Ilias S. Kotsireas
Eugene V. Zima *Editors*

Advances in Combinatorics

In Memory of Herbert S. Wilf

Springer

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Ilias S. Kotsireas • Eugene V. Zima
Editors

Advances in Combinatorics

Waterloo Workshop in Computer Algebra, W80, May 26-29, 2011

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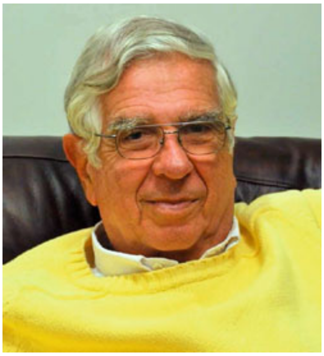
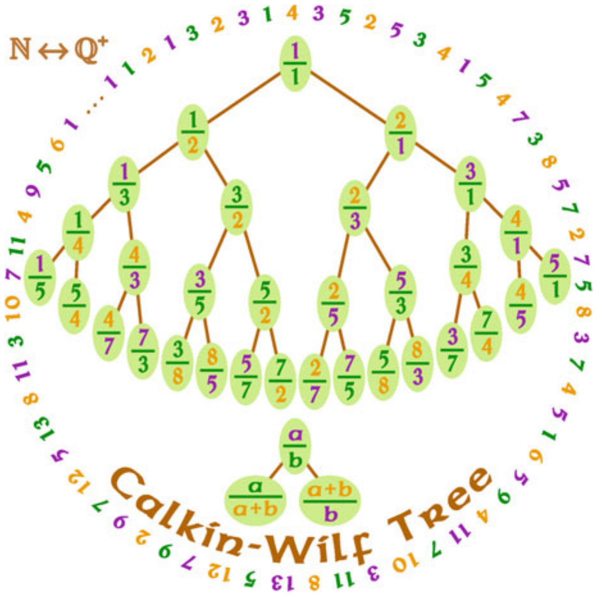


This book is dedicated to the life and scientific contributions of Herbert Saul Wilf.



$$F(n+1,k) - F(n,k) = G(n,k+1) - G(n,k)$$

Calkin-Wilf tree, courtesy of Douglas Zare

Foreword

This volume commemorates and celebrates the life and achievements of an extraordinary person, Herb Wilf. The planning of the book started while he was still alive. It was hoped to present it to him in person, but unfortunately he passed away before that could happen. While he was brought down by a neuromuscular degenerative disease, he had been active in research until shortly before his death, and this volume even contains a paper he coauthored.

Among the most prominent qualities that endeared Herb to his many students and colleagues was his warm personality. Deeply devoted to mathematics, he was an enthusiastic supporter of other researchers, especially of young students struggling to establish themselves. Always generous with suggestions and credit, he delighted when others improved on his own results. He was also very supportive of women mathematicians at a time when they faced high barriers and had an unusually large number of women among his PhD students.

Herb Wilf was a superb teacher and writer. His books have had extensive impact on a variety of fields. His many publications with their lucid explanations of abstruse mathematical results give a taste of his abilities as an expositor. He received a variety of teaching prizes, including the Deborah and Franklin Tepper Haimo Award of the Mathematical Association of America, which is given to "teachers of mathematics who have been widely recognized as extraordinarily successful." He devoted substantial effort to editorial activities, including a stint as the editor in chief of the *American Mathematical Monthly*, and was a cofounder of the *Journal of Algorithms* and of the *Electronic Journal of Combinatorics*.

However, Herb was foremost a researcher, driven by the desire to discover the inner workings of the mathematical world, as expressed by Hilbert's famous quote, "We must know. We will know." This volume consists of high-quality refereed research contributions by some of his colleagues, students, and collaborators. The origins of this book project were in the conference held on the occasion of Herb's 80th birthday in May 2011. But this is not a conference proceedings, in that many of the papers presented at that meeting are not included and some papers here were not part of the conference program. They are meant as a tribute to Herb

Wilf's contributions to mathematics and mathematical life. Some are very close to areas he worked in, and some are further apart. But they are all on topics he knew well and cared deeply about.

Although all the papers in this volume have some connection to Herb, they touch mostly on the last (although longest) phase of his career, that associated with combinatorics. It therefore seems appropriate to say a few words about his development as a mathematician. One of the many notable features of his life was the willingness to undertake new projects and change directions. Thus, in the 1990s, while he was already in his 60s and well established as an author and editor in the traditional print world, he saw the promise of electronic communication and moved to set up the free and completely scholar-operated *Electronic Journal of Combinatorics.* In the spirit of practicing what he preached, he also arranged for as many of his books as possible to be available for free downloads. In a rare case of a good deed being properly rewarded, he found, contrary to predictions, that sales of print copies of those freely downloadable books increased! This flexibility and willingness to experiment extended to research directions. Even close to the end of his life, he was always open to new ideas and wrote some papers in mathematical biology. But this was just a continuation of a lifelong pattern.

The repeated appearance of certain intellectual themes in Herb's work is illustrated nicely by one of his most famous contributions, namely, the work with Doron Zeilberger on automated proofs of identities. The computational aspect of this research offers a link to the start of Herb's professional career, which was closely linked to computers. He did direct hands-on programming of some of the first electronic digital computers, in order to implement early optimization algorithms. He then went on to write a PhD thesis on numerical analysis and carry out a substantial research program in that field, including producing books on mathematical models. Later yet he moved on to more theoretical work on complex analysis and inequalities. And then he was smitten by the charms of combinatorics, and this became the main passion for the rest of his life. Not that he forgot or abandoned his earlier interests completely. Computers, for example, continued to play a major role in his life. As just one example, in 1975, he and Albert Nijenhuis published *Combinatorial Algorithms*. It is not used as widely as it used to be, since the methods it contains are incorporated into standard software programs, such as Maple, Matlab, and Mathematica. But for that time, it was a tremendously useful collection that not only explained the methods but provided working code that could be used when needed. Another illustration of his later work drawing on earlier experience is provided by his work on complex analysis, which played a role in his extensive involvement with generating functions in combinatorics.

In conclusion, we can say that it is difficult to give a full picture of the many facets of Herb Wilf's life and work. There will be more formal obituary notices that will cover his contributions in detail. The brief sketch here serves only as an introduction to this collection of papers, original research contributions by some of Herb's many students, collaborators, and other admirers and beneficiaries, who dedicate their works to his memory. Herb heard presentations of some of these papers at his 80th birthday conference. What is certain is that he would have loved to read them all and appreciate the advances they represent in penetrating ever deeper into the mysteries of mathematics.

Minneapolis, USA
March 2013

Andrew M. Odlyzko

Preface

The Third Waterloo Workshop on Computer Algebra (WWCA 2011, W80) was held May 26–29, 2011 at Wilfrid Laurier University, Waterloo, Canada.

The conference was devoted to the 80th birthday of distinguished combinatorialist Professor Herbert S. Wilf (University of Pennsylvania, USA). Several of Professor Wilf's books are considered classical; we mention for instance Generatingfunctionology, Algorithms and Complexity, $A = B$.

Topics discussed at the workshop were closely related to several research areas in which Herbert Wilf has contributed and influenced.

WWCA 2011 was a real celebration of combinatorial mathematics, with some of the most famous combinatorial mathematicians of the world coming together to present their talks. We had more than a 100 participants at the conference. The list of scheduled invited lectures and presentations made at the conference includes:

- Herbert Wilf, University of Pennsylvania, USA, "Two exercises in combinatorial biology"
- Gert Almkvist, University of Lund, Sweden, "Ramanujan-like formulas for $\frac{1}{\pi^2}$ and String Theory"
- George E. Andrews, Pennsylvania State University, USA, "Partition Function Differences, and Anti-Telescoping"
- Miklos Bona, University of Florida, USA, "Permutations as Genome Rearrangements"
- Rod Canfield, University of Georgia, USA, "The Asymptotic Hadamard Conjecture"
- Sylvie Corteel, Univ. Paris 7, France, "Enumeration of staircase tableaux"
- Aviezri Fraenkel, Weizmann Institute of Science, Israel, "What's a question to Herb Wilf's answer?"
- Ira Gessel, Brandeis University, USA, "On the WZ method"
- Ian Goulden, University of Waterloo, Canada, "Combinatorics and the KP hierarchy"
- Ronald Graham, UCSD, USA, "Joint statistics for permutations in S_n and Eulerian numbers"

- Andrew Granville, Universite de Montreal, Canada, “More combinatorics and less analysis: A different approach to prime numbers”
- Curtis Greene, Haverford College, USA, “Some Posets Related to Muirhead’s, Maclaurin’s, and Newton’s Inequalities”
- Joan Hutchinson, Macalester College, USA, “Some challenges in list-coloring planar graphs”
- David Jackson, University of Waterloo, Canada, “Enumerative aspects of cactus graphs”
- Christian Krattenthaler, University of Vienna, Austria, “Cyclic sieving for generalised non-crossing partitions associated to complex reflection groups”
- Victor H. Moll, Tulane University, USA, “p-adic valuations of sequences: examples in search of a theory”
- Andrew Odlyzko, University of Minnesota, USA, “Primes, graphs, and generating functions”
- Peter Paule, RISC-Linz, Austria, “Proving strategies of WZ-type for modular forms”
- Robin Pemantle, University of Pennsylvania, USA, “Zeros of complex polynomials and their derivatives”
- Marko Petkovsek, University of Ljubljana, Slovenia, “On enumeration of structures with no forbidden substructures”
- Bruce Sagan, Michigan State University, USA, “Mahonian Pairs”
- Carla D. Savage, NCSU, USA, “Generalized Lecture Hall Partitions and Eulerian Polynomials”
- Jeffrey Shallit, University of Waterloo, Canada, “50 Years of Fine and Wilf”
- Richard Stanley, MIT, USA, “Products of Cycles”
- John Stembridge, University of Michigan, USA, “A finiteness theorem for W-graphs”
- Volker Strehl, Universitaet Erlangen, Germany, “Aspects of a combinatorial annihilation process”
- Michelle Wachs, University of Miami, USA, “Unimodality of q-Eulerian Numbers and p,q-Eulerian Numbers”
- Doron Zeilberger, Rutgers University, USA, “Automatic Generation of Theorems and Proofs on Enumerating Consecutive-Wilf classes”
- Eugene Zima, Wilfrid Laurier University, Canada, “Synthetic division in the context of indefinite summation”

The workshop was financially supported by the Fields Institute and various offices of Wilfrid Laurier University.

This book presents a collection of selected formally refereed papers submitted after the workshop. The topics discussed in this book are closely related to Herb’s influential works. Initially it was planned as a celebratory volume. Herb’s sudden death implied that this has now become a book commemorating his contributions to mathematics and computer science.

This book would not have been possible without the dedication and hard work of the anonymous referees, who supplied detailed referee reports and helped authors to

improve their papers significantly. Finally, we wish to thank the people at Springer-Verlag, in particular Ruth Allewelt and Martin Peters, for working closely with us and for their dedicated and unwavering support throughout the entire publication process.

We feel very fortunate that we were entrusted in the organization of this conference – “unforgettable conference of historical dimension” according to comments of one of the invitees.

Waterloo, Canada | Ilias S. Kotsireas
December 2012 | Eugene Zima

A Tribute to Herb Wilf

Doron Zeilberger

To Herbert Saul Wilf (June 13, 1931–Jan. 7, 2012), in memoriam

Herbert Wilf was one of the greatest combinatorialists of our time, but his influence far transcends the boundaries of any specific area. He was way ahead of his time when, as a fresh (28-year-old) PhD, he coedited (with Anthony Ralston) the pioneering book "Mathematical Methods for Digital Computers"; – 3 years later wrote the beautiful classic textbook "Mathematics for the Physical Sciences"; when algorithms just started to pop up everywhere, pioneered (with Don Knuth) the Journal of Algorithms; and when the Internet started, pioneered the Electronic Journal of Combinatorics. Herb also realized the great potential of the Internet for the sharing of knowledge and had several of his classic textbooks available for a free download!

Not to mention his great mathematical contributions!

Not to mention that he academically fathered 28 (a perfect number!) brilliant combinatorial children, including 8 females (way back when there were very few female PhDs).

Many of these brilliant academic children became distinguished academic mathematicians, for example, Fan Chung, Joan Hutchinson, the late Rodica Simion, Felix Lazebnik, and many others. But some of them had brilliant careers elsewhere. These include:

- Richard Garfield, of Magic the Gathering fame, one-time teenage idol, and still a household name among gamesters
- The Most Rev. Dr. Anthony Mikovsky, Prime Bishop of the Polish National Catholic Church

D. Zeilberger (✉)
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- Alkes Price, an ex-prodigy, who made a bundle in finance and wisely went back to academia and is now a rising star in statistical genetics
- Michael Wertheimer, CTO of the National Security Agency from 2005 to 2010

The first scientific contribution of Herb Wilf (b. June 13, 1931) was in astronomy. In the Oct. 1945 issue of Sky and Telescope, in an article that reported on readers' observations of a solar eclipse, one can find the following: "Herbert Wilf of NY City, sent in times of the first and last contacts agreeing closely with those predicted for his location. He used a stop watch of known rate set with radio time signals."

After that, Herb focused on mathematics, but his interests ranged far and wide and went through several phases. In a short (probably auto-) biographical footnote for a 1982 American Mathematical Monthly article, it says:

> His principal research interests have been in analysis: numerical, mathematical, and in the past several years, combinatorical.

Herb's "religious" conversion to combinatorics was already cited by Fan Chung and Joan Hutchinson's lovely tribute on the occasion of his 65th birthday: In 1965, Gian-Carlo Rota came to the University of Pennsylvania to give a colloquium talk on his then-recent work on Mobius functions and their role in combinatorics. Herb recalled, "That talk was so brilliant and so beautiful that it lifted me right out of my chair and made me a combinatorialist on the spot."

But Herb returned the debt and made me convert to the religion of combinatorics.

The bio attached to one of my own articles reads:

Doron Zeilberger was born, as a person, on July 2, 1950. He was born, as a mathematician, in 1976, when he got his PhD under the direction of Harry Dym (in analysis). He was born-again, as a combinatorialist, 2 years later, when he read a lovely proof of the so-called Hook-Length Formula (enumerating Standard Young Tableaux) by Curtis Greene, Albert Nijenhuis, and Herb Wilf. He lived happily ever after.

I still live happily, and all thanks to Herb (and Albert Nijenhuis and Curtis Greene, now Herb's beloved son-in-law).

Thanks Herb for the great inspiration that you bestowed on me and on so many other people whose lives – both mathematically and personally – you have touched.

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Glaisher's Formulas for $\frac{1}{\pi^2}$ and Some Generalizations

Gert Almkvist

In memory of Herb Wilf

Abstract Glaisher's formulas for $\dfrac{1}{\pi^2}$ are reviewed. Two generalized formulas are proved by using the WZ-method (named after Wilf and Zeilberger). Also an improvement of Fritz Carlson's theorem (proved in an Appendix by Arne Meurman) is used.

Keywords π • Glaisher

1 Introduction

Ramanujan-like formulas for $\dfrac{1}{\pi^2}$ are rare. Only a dozen genuine (not obtained by "squaring" formulas for $\dfrac{1}{\pi}$) formulas are known, most of them due to Guillera. Only five of them are proved, all by Guillera, using the WZ-method. Until I found Wenchang Chu's paper [2] I did not know of Glaisher's formulas for $\dfrac{1}{\pi^2}$ from 1905 (see [3]). His paper is not easy to read (also literary, the exponents in Quaterly Journal are very small) and I decided to write a self-contained survey.
After finding a slight generalization of Glaisher's formulas and inspired of Levrie's paper, I was lead to the following two new formulas for $\dfrac{1}{\pi}$.

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Theorem 1.

(i)

$$\sum_{n=0}^{\infty} \frac{(4n+1)}{(n+1)(n+2)\ldots(n+k)(2n-1)(2n-3)\ldots(2n-(2k-1))} \frac{\binom{2n}{n}^4}{256^n} = (-1)^k \frac{2^{5k+1} k!^4}{k \cdot (2k)!^3} \frac{1}{\pi^2}$$

(ii)

$$\sum_{n=0}^{\infty} \frac{(4n+1)}{(n+1)^3(n+2)^3\ldots(n+k)^3(2n-1)^3(2n-3)^3\ldots(2n-(2k-1))^3} \frac{\binom{2n}{n}^4}{256^n} = (-1)^k \frac{2}{3} \frac{2^{15k} k!^3 (3k)!}{k \cdot (4k)!^3} \frac{1}{\pi^2}$$

2 Glaisher's Formulas

We will make use of Legendre polynomials $P_n(x)$, defined by the generating function

$$\frac{1}{\sqrt{1-2xt+t^2}} = \sum_{n=0}^{\infty} P_n(x) t^n$$

They form an orthogonal system with inner product

$$\int_{-1}^{1} P_m(x) P_n(x) dx = \delta_{m,n} \frac{2}{2n+1}$$

Lemma 1.

$$P'_{n+1}(x) - x P'_n(x) = (n+1) P_n(x)$$

Proof. Differentiate the generating function with respect to x

$$\frac{d}{dx}\frac{1}{\sqrt{1-2xt+t^2}} = \frac{t}{(1-2xt+t^2)^{3/2}} = \sum_{n=0}^{\infty} P_n'(x)t^n$$

Hence

$$\sum_{n=0}^{\infty}(P_{n+1}'(x) - xP_n'(x))t^n = \frac{1-xt}{(1-2xt+t^2)^{3/2}}$$

$$= \frac{d}{dt}\frac{t}{\sqrt{1-2xt+t^2}} = \sum_{n=0}^{\infty}(n+1)P_n(x)t^n \qquad \square$$

Lemma 2.

$$xP_n'(x) - P_{n-1}'(x) = nP_n(x)$$

Proof. We have

$$\sum_{n=0}^{\infty}(xP_n'(x) - P_{n-1}'(x))t^n = \frac{xt-t^2}{(1-2xt+t^2)^{3/2}} = t\frac{d}{dt}\frac{1}{\sqrt{1-2xt+t^2}}$$

$$= \sum_{n=0}^{\infty} nP_n(x)t^n \qquad \square$$

Lemma 3.

$$P_{n+1}'(x) - P_{n-1}'(x) = (2n+1)P_n(x)$$

Proof. Add Lemmas 1 and 2. $\square$

Lemma 4.

$$\int_{-1}^{1}\frac{P_n(x)}{\sqrt{1-x^2}}dx = \pi\frac{\binom{2m}{m}^2}{16^m} \quad \textit{if } n = 2m \textit{ and } 0 \textit{ if } n \textit{ odd.}$$

Proof. We make the substitution $x = \cos(\varphi)$ and obtain

$$LHS = \int_0^{\pi} P_n(\cos(\varphi))d\varphi = \frac{1}{2}\int_{-\pi}^{\pi} P_n(\cos(\varphi))d\varphi$$

Then

$$\sum_{n=0}^{\infty} P_n(\cos(\varphi))t^n = \frac{1}{\sqrt{1-2t\cos(\varphi)+t^2}}$$
$$= \frac{1}{(1-t\exp(i\varphi))^{1/2}} \frac{1}{(1-t\exp(-i\varphi))^{1/2}}$$
$$= \sum_{j,k=0}^{\infty} \binom{2j}{j}\binom{2k}{k} \frac{t^{j+k}}{4^{j+k}} \exp(i(j-k)\varphi)$$

which gives

$$P_n(\cos(\varphi)) = \frac{1}{4^n} \sum_{j=0}^{n} \binom{2j}{j}\binom{2n-2j}{n-j} \exp(i(2j-n)\varphi)$$

Integrating, the only nonzero term is when $2j = n$ giving

$$\frac{1}{2}\int_{-\pi}^{\pi} P_{2j}(\cos(\varphi))d\varphi = \pi \frac{\binom{2j}{j}^2}{4^{2j}} \qquad \square$$

Lemma 5.

$$\int_{-1}^{1} \frac{xP_n(x)}{\sqrt{1-x^2}}dx = \pi \frac{2m+1}{2m+2} \frac{\binom{2m}{m}^2}{16^m} \quad \textit{if } n = 2m+1 \textit{ and } 0 \textit{ if } n \textit{ even.}$$

Proof. We have

$$\int_{-1}^{1} \frac{xP_n(x)}{\sqrt{1-x^2}}dx = \frac{1}{2}\int_{-\pi}^{\pi} \cos(\varphi)P_n(\cos(\varphi))d\varphi$$

and

$$\cos(\varphi)P_n(\cos(\varphi))$$
$$= \frac{1}{2\cdot 4^n} \sum_{j=0}^{n} \binom{2j}{j}\binom{2n-2j}{n-j} \{\exp(i(2j-n+1)\varphi) + \exp(i(2j-n-1)\varphi)\}$$

Integrating, we get a nonzero result only if $n = 2m+1$ and $j = m$ or $j = m+1$. The result is

$$\frac{1}{4^{2m+1}}\binom{2m}{m}\binom{2m+2}{m+1}$$ □

Proposition 1.

$$\frac{1}{\sqrt{1-x^2}} = \frac{\pi}{2}\sum_{n=0}^{\infty}(4n+1)\frac{\binom{2n}{n}^2}{16^n}P_{2n}(x)$$

Proof. Expanding

$$\frac{1}{\sqrt{1-x^2}} = \sum_{n=0}^{\infty} c_n P_n(x)$$

we get, using the orthogonality of the Legendre polynomials

$$c_n = \frac{2n+1}{2}\int_{-1}^{1}\frac{P_n(x)}{\sqrt{1-x^2}}dx = \frac{4m+1}{2}\pi\frac{\binom{2m}{m}^2}{16^m} \quad \text{if } n=2m \text{ and } 0 \text{ otherwise.}$$

□

Remark 1. Putting $x = 0$ in the generating function we obtain

$$\frac{1}{\sqrt{1+t^2}} = \sum_{m=0}^{\infty}(-1)^m\frac{\binom{2m}{m}}{4^m}t^{2m}$$

and hence

$$P_{2m}(0) = (-1)^m\frac{\binom{2m}{m}}{4^m} \quad \text{and} \quad P_{2m-1}(0) = 0$$

Then putting $x = 0$ in Proposition 1 implies

$$\sum_{n=0}^{\infty}(-1)^n(4n+1)\frac{\binom{2n}{n}^3}{64^n} = \frac{2}{\pi}$$

which was found by Bauer already in 1859 (see [1]). The convergence is very slow, as $\dfrac{1}{\sqrt{n}}$.

Proposition 2.

$$\arcsin(x) = \frac{\pi}{8}\sum_{n=0}^{\infty}\frac{4n+3}{(n+1)^2}\frac{\binom{2n}{n}^2}{16^n}P_{2n+1}(x)$$

Proof. We integrate the formula in Proposition 1. By Lemma 3 we have, assuming that $P_{-1}(x) = 0$

$$P_{2n}(x) = \frac{1}{4n+1}(P'_{2n+1}(x) - P'_{2n-1}(x))$$

and

$$\int_0^x P_{2n}(t)dt = \frac{1}{4n+1}(P_{2n+1}(x) - P_{2n-1}(x)) + C$$

where $C = 0$ since $P_{2n+1}(0) = P_{2n-1}(0) = 0$. We get

$$\arcsin(x) = \frac{\pi}{2}\sum_{n=0}^{\infty}\frac{\binom{2n}{n}^2}{16^n}(P_{2n+1}(x) - P_{2n-1}(x))$$

$$= \frac{\pi}{2}\sum_{n=0}^{\infty}\left\{\frac{\binom{2n}{n}^2}{16^n} - \frac{\binom{2n+2}{n+1}^2}{16^{n+1}}\right\}P_{2n+1}(x)$$

$$= \frac{\pi}{8}\sum_{n=0}^{\infty}\frac{4n+3}{(n+1)^2}\frac{\binom{2n}{n}^2}{16^n}P_{2n+1}(x)$$

□

Theorem 2.

$$\sum_{n=0}^{\infty}\frac{(2n+1)(4n+3)}{(n+1)^3}\frac{\binom{2n}{n}^4}{256^n} = \frac{32}{\pi^2}$$

Proof. We have

$$\int_{-1}^{1} \frac{x}{\sqrt{1-x^2}} \arcsin(x) dx = \frac{\pi}{8} \sum_{n=0}^{\infty} \frac{4n+3}{(n+1)^2} \frac{\binom{2n}{n}^2}{16^n} \int_{-1}^{1} \frac{x}{\sqrt{1-x^2}} P_{2n+1}(x) dx$$

Partial integration gives

$$\int_{-1}^{1} \frac{x}{\sqrt{1-x^2}} \arcsin(x) dx = [-\sqrt{1-x^2} \arcsin(x)]_{-1}^{1} + \int_{-1}^{1} \frac{\sqrt{1-x^2}}{\sqrt{1-x^2}} dx = 2$$

and we finish using Lemma 5. □

Proposition 3.

$$\sqrt{1-x^2} = \frac{\pi}{4} \left\{ 1 - \sum_{n=1}^{\infty} \frac{4n+1}{(n+1)(2n-1)} \frac{\binom{2n}{n}^2}{16^n} P_{2n}(x) \right\}$$

Proof. Assume

$$\sqrt{1-x^2} = \sum_{n=0}^{\infty} c_n P_n(x)$$

Then

$$c_n = \frac{2n+1}{2} \int_{-1}^{1} \sqrt{1-x^2} P_n(x) dx = \frac{2n+1}{4} \int_{-\pi}^{\pi} P_n(\cos(\varphi)) \sin^2(\varphi) d\varphi$$
$$= \frac{2n+1}{8} \int_{-\pi}^{\pi} P_n(\cos(\varphi))(1-\cos(2\varphi)) d\varphi$$

Clearly $c_n = 0$ if n is odd, so let $n = 2m$. Now we know from the proof of Lemma 4

$$P_{2m}(\cos(\varphi)) = \frac{1}{16^m} \sum_{j=0}^{2m} \binom{2j}{j} \binom{4m-2j}{2m-j} \exp(2i(j-m))$$

When integrating we get nonzero terms for $j = m$, $j = m + 1$ and $j = m - 1$. We have $c_0 = \frac{\pi}{4}$ and for $m \geq 1$

$$c_m = \frac{\pi}{4} \frac{4m+1}{16^m} \left\{ \binom{2m}{m}^2 - \binom{2m+2}{m+1}\binom{2m-2}{m-1} \right\}$$

$$= -\frac{\pi}{4} \frac{4m+1}{(m+1)(2m-1)} \frac{\binom{2m}{m}^2}{16^m}$$

□

Theorem 3.

$$\sum_{n=0}^{\infty} \frac{4n+1}{(n+1)(2n-1)} \frac{\binom{2n}{n}^4}{256^n} = -\frac{8}{\pi^2}$$

Proof. Divide the formula in Proposition 3 by $\sqrt{1-x^2}$

$$1 = \frac{\pi}{4} \left\{ \frac{1}{\sqrt{1-x^2}} - \sum_{n=1}^{\infty} \frac{4n+1}{(n+1)(2n-1)} \frac{\binom{2n}{n}^2}{16^n} \frac{P_{2n}(x)}{\sqrt{1-x^2}} \right\}$$

Integrating from -1 to 1 and using Lemma 4 we are done. □

Remark 2. The series converges as $\frac{1}{n^3}$.

Now

$$\frac{4n+1}{(2n+2)(2n-1)} = \frac{1}{2n-1} + \frac{1}{2n+2}$$

and

$$\frac{1}{2n}\frac{\binom{2n-2}{n-1}^4}{256^{n-1}}+\frac{1}{2n-1}\frac{\binom{2n}{n}^4}{256^n}$$
$$=\frac{\binom{2n}{n}^4}{256^n}\left\{\frac{1}{2n-1}+\frac{1}{2n}\frac{256n^4}{16(2n-1)^4}\right\}$$
$$=\frac{(2n-1)^3+(2n)^3}{(2n-1)^4}\frac{\binom{2n}{n}^4}{256^n}$$

and we get

$$1-\sum_{n=1}^{\infty}\frac{(2n-1)^3+(2n)^3}{(2n-1)^4}\frac{\binom{2n}{n}^4}{256^n}=\frac{4}{\pi^2}$$

Similarly we can rewrite Theorem 2 as

$$\sum_{n=1}^{\infty}\frac{2n(4n-1)}{(2n-1)^3}\frac{\binom{2n}{n}^4}{256^n}=\frac{4}{\pi^2}$$

Adding we obtain

Theorem 4.

$$\sum_{n=0}^{\infty}\frac{1-4n}{(2n-1)^4}\frac{\binom{2n}{n}^4}{256^n}=\frac{8}{\pi^2}$$

Remark 3. Using the Pochhammer symbol this can be written as

$$\sum_{n=0}^{\infty}(1-4n)\frac{(-1/2)_n^4}{n!^4}=\frac{8}{\pi^2}$$

which converges as $\dfrac{1}{n^5}$ (not as $\dfrac{1}{n^6}$ as Glaisher claims).

Another formula with the same convergence is the following (not in Glaisher):

Theorem 5.

$$\sum_{n=0}^{\infty} \frac{4n+1}{(n+1)(n+2)(2n-1)(2n-3)} \frac{\binom{2n}{n}^4}{256^n} = \frac{32}{27\pi^2}$$

Proof. Assume

$$(1-x^2)^{3/2} = \sum_{n=0}^{\infty} c_{2m} P_{2m}(x)$$

Doing as in the proof of Proposition 3 we obtain

$$c_{2m} = \frac{9\pi}{8} \frac{4m+1}{(m+1)(m+2)(2m-1)(2m-3)} \frac{\binom{2m}{m}^2}{16^m}$$

Dividing by $\sqrt{1-x^2}$ and integrating from -1 to 1 we find the formula. □

Remark 4. By expanding $(1-x^2)^{(2k-1)/2}$, the above result can be generalized to the first formula below. Coming so far I received the paper [4] by Levrie from Zudilin. Using the hints on p. 229 and experimenting a little one finds formula (ii):

Theorem 6.

(i)

$$\sum_{n=0}^{\infty} \frac{(4n+1)}{(n+1)(n+2)\ldots(n+k)(2n-1)(2n-3)\ldots(2n-(2k-1))} \frac{\binom{2n}{n}^4}{256^n}$$
$$= (-1)^k \frac{2^{5k+1} k!^4}{k \cdot (2k)!^3} \frac{1}{\pi^2}$$

(ii)

$$\sum_{n=0}^{\infty} \frac{(4n+1)}{(n+1)^3(n+2)^3\ldots(n+k)^3(2n-1)^3(2n-3)^3\ldots(2n-(2k-1))^3} \frac{\binom{2n}{n}^4}{256^n}$$
$$= (-1)^k \frac{2}{3} \frac{2^{15k} k!^3 (3k)!}{k \cdot (4k)!^3} \frac{1}{\pi^2}$$

Proof.
Proof of (i):
The first formula can be written as

$$\sum_{n=0}^{\infty} G(n,k) = \frac{2}{\pi^2}$$

where

$$G(n,k) = \frac{(-1)^k k(4n+1)\binom{2k}{k}^2 \binom{2n}{n+k}\binom{2n}{n}^3}{16^{2n+k}\binom{2n}{2k}}$$

Zeilberger's imaginary friend EKHAD (i.e using "WZMethod" in Maple) gives us

$$F(n,k) = \frac{4(-1)^k n^3(n-k)\binom{2k}{k}^2 \binom{2n}{n+k}\binom{2n}{n}^3}{16^{2n+k}(k+1)(2k+1)\binom{2n}{2k+2}}$$

such that

$$F(n+1,k) - F(n,k) = G(n,k+1) - G(n,k)$$

Write this as

$$\begin{aligned} \frac{F(n+1,k)}{F(n,k)} - 1 &= \frac{G(n,k+1)}{F(n,k)} - \frac{G(n,k)}{F(n,k)} \\ &= -\frac{(4n+1)(8n^2k+4nk+2k+1)}{16n^3(n+k+1)} \end{aligned}$$

an algebraic identity which is valid for any complex number k. The usual telescoping gives for $H(z) = \sum_{n=0}^{\infty} G(n,z)$

$$\begin{aligned} H(z+1) - H(z) &= \sum_{n=0}^{\infty} G(n,z+1) - \sum_{n=0}^{\infty} G(n,z) \\ &= \lim(F(n+1,z) - F(0,z)) = 0 \end{aligned}$$

so $H(z)$ is periodic with period one. We want to use Meurman's version of Fritz Carlson's theorem (see the Appendix). We write

$$G(n,z)=\frac{z\cos(\pi z)(4n+1)\binom{2z}{z}^2\binom{2n}{n+z}\binom{2n}{n}^3}{16^{2n+z}\binom{2n}{2z}}$$

First we notice that

$$\cos(\pi z)=\sin(\pi(\frac{1}{2}-z))=\frac{\pi}{\Gamma(\frac{1}{2}-z)\Gamma(\frac{1}{2}+z)}$$

and

$$\frac{(2z)!}{z!}=\frac{2\Gamma(2z)}{\Gamma(z)}=\frac{4^z}{\sqrt{\pi}}\Gamma(z+\frac{1}{2})$$

Consider

$$\frac{z\cos(\pi z)\binom{2z}{z}^2\binom{2n}{n+z}}{16^z\binom{2n}{2z}}$$

$$=\frac{8\pi z}{z!16^z\Gamma(\frac{1}{2}-z)\Gamma(\frac{1}{2}+z)(z+n)!}\left\{\frac{\Gamma(2z)}{\Gamma(z)}\right\}^3\frac{\Gamma(2n-2z)}{\Gamma(n-z)}$$

$$=\frac{4^n\Gamma(z+\frac{1}{2})^2\Gamma(\frac{1}{2}-z+n)}{\pi\Gamma(z)\Gamma(\frac{1}{2}-z)\Gamma(1+z+n)}$$

Since $H(z)$ has period one, we can assume that $1\le\Re(z)\le 2$. Let $z=x+iy$. Then we have

$$|\Gamma(x+iy)|\approx\sqrt{2\pi}\,|y|^{x-1/2}\exp(-\frac{\pi}{2}\,|y|)$$

and

$$\left|\frac{\Gamma(\frac{1}{2}-z+n)}{\Gamma(1+z+n)}\right| \approx \frac{1}{n^{1/2+2x}} \leq \frac{1}{n^{5/2}} \text{ for large } n$$

Furthermore

$$\left|\frac{\Gamma(z+\frac{1}{2})^2}{\Gamma(z)\Gamma(\frac{1}{2}-z)}\right| \approx |y|^{2x+1/2} \leq |y|^{9/2}$$

We have for large n

$$\frac{(4n+1)\binom{2n}{n}^3}{16^{2n}} \approx \frac{4n}{4^n(\pi n)^{3/2}}$$

Collecting the evidence we obtain

$$|G(n,z)| \leq \frac{4^n}{\pi}\frac{1}{n^{5/2}}\frac{4}{4^n(\pi)^{3/2}n^{1/2}}|y|^{9/2} \leq \frac{2|y|^{9/2}}{\pi^{5/2}}\frac{1}{n^3}$$

and

$$|H(z)| \leq \frac{2|y|^{9/2}}{\pi^{5/2}}\varsigma(3) = O(\exp(c|y|))$$

for any positive $c < 2\pi$, so $H(z) = A$, a constant by Meurman's Theorem. To determine the constant A we put $z = \frac{1}{2}$. We find $G(0,z) \to \frac{2}{\pi^2}$ when $z \to \frac{1}{2}$, while $G(n,\frac{1}{2}) = 0$ for $n > 0$.

Proof of (ii):

Here we have

$$G(n,k) = \frac{(-1)^k k(4n+1)\binom{2k}{k}^2\binom{4k}{2k}^3\binom{2n}{n+k}^3\binom{2n}{n}}{16^{2n+3k}\binom{3k}{k}\binom{2n}{2k}^3}$$

and

$$F(n,k) = \frac{1}{8}\frac{(-1)^k n(n-k)^3 \binom{2k}{k}^2 \binom{4k}{2k}^3 \binom{2n}{n+k}^3 \binom{2n}{n} P(n,k)}{16^{2n+3k}(k+1)^4(2k+1)^4 \binom{3k+3}{k+1}\binom{2n}{2k+2}^3}$$

where

$$P(n,k) = 64n^3(n-1)(3k+1)(3k+2) - 8n^2(3k+2)(80k^3+72k^2+12k-1)$$
$$+4n(2k+1)(3k+2)(40k^2+16k+1) + (2k+1)^2(592k^4+752k^3+300k^2+48k+3)$$

As before we check

$$F(n+1,k) - F(n,k) = G(n,k+1) - G(n,k)$$

To use Meurman's theorem we write

$$G(n,z) = \frac{z\cos^3(\pi z)(4n+1)\binom{2z}{z}^2\binom{4z}{2z}^3\binom{2n}{n+z}^3\binom{2n}{n}}{16^{2n+3z}\binom{3z}{z}\binom{2n}{2z}^3}$$

We consider

$$\frac{z\cos^3(\pi z)\binom{2z}{z}^2\binom{4z}{2z}^3\binom{2n}{n+z}^3}{16^{3z}\binom{3z}{z}\binom{2n}{2z}^3}$$

$$= \frac{4^{3n}}{3\pi^2}\frac{\Gamma(z+\frac{1}{2})\Gamma(2z+\frac{1}{2})^3}{z\Gamma(z)\Gamma(3z)\Gamma(\frac{1}{2}-z)^3}\left\{\frac{\Gamma(n+\frac{1}{2}-z)}{\Gamma(n+1+z)}\right\}^3$$

Now for $1 \le \Re(z) \le 2$ we have

$$\left|\frac{\Gamma(z+\frac{1}{2})\Gamma(2z+\frac{1}{2})^3}{z\Gamma(z)\Gamma(3z)\Gamma(\frac{1}{2}-z)^3}\right| \le |y|^{6x+1} \le |y|^{13}$$

Furthermore

$$\left|\frac{\Gamma(\frac{1}{2}-z+n)^3}{\Gamma(1+z+n)^3}\right| \approx \frac{1}{n^{3/2+6x}} \le \frac{1}{n^{15/2}} \text{ for large } n$$

We have

$$\frac{(4n+1)\binom{2n}{n}}{16^{2n}} \approx \frac{4n}{4^{3n}(\pi n)^{1/2}}$$

We obtain

$$|G(n,z)| \le \frac{4^{3n}}{3\pi^2}\frac{1}{n^{15/2}}\frac{4n}{4^{3n}(\pi)^{1/2}n^{1/2}}|y|^{13} \le \frac{4|y|^{13}}{3\pi^{5/2}}\frac{1}{n^7}$$

and

$$|H(z)| \le \frac{4|y|^{13}}{3\pi^{5/2}}\varsigma(7) = O(\exp(c|y|))$$

for any positive $c < 2\pi$. Hence $H(z)$ is constant. As above we find $G(0,z) \to \frac{2}{3\pi^2}$ when $z \to \frac{1}{2}$, while $G(n, \frac{1}{2}) = 0$ for $n > 0$. □

Remark 5. For $n < k$ we must replace $\frac{\binom{2n}{n+k}}{\binom{2n}{2k}}$ with $(-1)^{k-n}\frac{\binom{2k}{n+k}}{\binom{2k-2n}{k-n}}$ and we obtain the formulas

(i)

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

(ii)

$$\frac{(-1)^k k\binom{2k}{k}^2\binom{4k}{2k}^3}{16^{3k}\binom{3k}{k}}$$

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

Remark 6. By using "WZMethod" in Maple on $F(n,k+n)$ in the proof of Conjecture (i) we get an enormous expression, which after putting $k = 0$ simplifies to

$$\sum_{n=0}^{\infty}(-1)^n\binom{2n}{n}^5(20n^2+8n+1)\frac{1}{2^{12n}}=\frac{8}{\pi^2}$$

which is Guillera's first formula for $\frac{1}{\pi^2}$. Similarly for $F(n,k+2n)$ we obtain

$$\sum_{n=0}^{\infty}(-1)^n\frac{\binom{2n}{n}^3\binom{4n}{2n}^3}{\binom{3n}{n}}\frac{1376n^4+1808n^3+784n^2+138n+9}{(3n+1)(3n+2)}\frac{1}{2^{16n}}=\frac{32}{\pi^2}$$

In Maple's answer occur expressions like $\binom{2n}{4n}$ which need interpretation. Hereby one needs the following expansions to turn the binomial coefficients "upside down"

$$\binom{2(n+\varepsilon)}{4(n+\varepsilon)}=\frac{1}{n\binom{4n}{2n}}\varepsilon+O(\varepsilon^2)$$

$$\binom{2(n+\varepsilon)}{3(n+\varepsilon)}=\frac{(-1)^n}{n\binom{3n}{2n}}\varepsilon+O(\varepsilon^2)$$

$$\binom{2(n+\varepsilon)}{4(n+\varepsilon)+2} = \frac{1}{(n+1)\binom{4n+2}{2n}}\varepsilon + O(\varepsilon^2)$$

$$\binom{2(n+\varepsilon)+2}{4(n+\varepsilon)+6} = \frac{1}{(n+2)\binom{4n+6}{2n+2}}\varepsilon + O(\varepsilon^2)$$

Finally for $F(n, k+3n)$ we get

$$\sum_{n=0}^{\infty}(-1)^n \frac{\binom{2n}{n}^3\binom{6n}{3n}^2\binom{6n}{2n}}{\binom{4n}{2n}} \frac{P(n)}{(3n+1)(3n+2)(4n+1)^2(4n+3)^2} \frac{1}{2^{20n}} = \frac{256}{\pi^2}$$

where

$$\begin{aligned}P(n) = 4038912n^8 + 13296384n^7 + 18184448n^6 + 13423232n^5\\ +5828864n^4 + 1523184n^3 + 234144n^2 + 19440n + 675\end{aligned}$$

Conjecture.

(a) If $p > k$ is a prime then

$$\frac{(-1)^k k\binom{2k}{k}^2}{16^k} \times \left\{\sum_{n=0}^{k-1} \frac{(-1)^{k-n}(4n+1)\binom{2k}{n+k}\binom{2n}{n}^3}{16^{2n}\binom{2k-2n}{k-n}} + \sum_{n=k}^{p-1} \frac{(4n+1)\binom{2n}{n+k}\binom{2n}{n}^3}{16^{2n}\binom{2n}{2k}}\right\} \equiv 0 \mod p^3$$

(b) If $p > 7$ is prime then

$$\sum_{n=0}^{p-1}(-1)^n \binom{2n}{n}^5 \frac{(2n+1)^2}{(n+1)^2}(40n^3+84n^2+54n+9)\frac{1}{2^{12n}} \equiv 8p^2 \mod p^3$$

3 Consequences of Levrie's Work

Levrie's Theorem 7 in [4] can be proved by using the WZ-pair

$$G(n,k) = \frac{(4n+1)k\binom{2k}{k}^2\binom{4k}{2k}\binom{2n}{n}^2\binom{2n}{n+k}^2}{16^{2n+2k}\binom{2n}{2k}^2}$$

$$F(n,k) = -\frac{n^2(-8n^2+4n+16k^2+10k+1)\binom{2k}{k}^2\binom{4k}{2k}\binom{2n}{n}^2\binom{2n}{n+k}^2}{2\cdot 16^{2n+2k}(2n-2k-1)^2\binom{2n}{2k}^2}$$

Using the "WZMethod" on $F(n,k+n)$ and putting $k=0$ we have a new proof of Guillera's formula

$$\sum_{n=0}^{\infty}\binom{2n}{n}^4\binom{4n}{2n}\frac{120n^2+34n+3}{2^{16n}} = \frac{32}{\pi^2}$$

Similarly for $F(n,k+2n)$ we get

$$\sum_{n=0}^{\infty}\frac{\binom{2n}{n}^2\binom{4n}{2n}^4\binom{8n}{4n}}{\binom{3n}{n}^2}\frac{P(n)}{(2n+1)(3n+1)^2(3n+2)^2}\frac{1}{2^{24n}} = \frac{1{,}024}{\pi^2}$$

where

$$P(n) = 968704n^7+2683904n^6+3013376n^5+1758208n^4$$
$$+568224n^3+100200n^2+8844n+315.$$

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Appendix

A Periodic Version of Fritz Carlson's Theorem

Arne Meurman[1]

When using the WZ-method one often needs Fritz Carlson's theorem (see e.g. [1]) to find the value of a constant. Usually the function $H(z)$ which one wants to prove constant is periodic, $H(z+1) = H(z)$. The following theorem uses the full strength of the periodicity and also improves the size of the constant in the growth condition to $c < 2\pi$.

Theorem. Let $H(z)$ be an entire function such that $H(z+1) = H(z)$ and there is $c \in \mathbf{R}$ such that $c < 2\pi$ and

$$H(z) = O(\exp(c\,|Im(z)|))$$

for $z \in \mathbf{C}$. Then $H(z)$ is constant.

Proof. Replacing $H(z)$ by $H(z) - H(0)$ we may assume that $H(k) = 0$ for all $k \in \mathbf{Z}$. Then $H(z)$ is divisible by $e^{2\pi iz} - 1$ in the sense that

$$H(z) = (e^{2\pi iz} - 1)H_1(z)$$

with H_1 entire. As H_1 is also periodic with period 1 we can express $H_1(z) = h(e^{2\pi iz})$ with h analytic in the punctured plane $\mathbf{C} \setminus \{0\}$. Expanding h in a Laurent series we obtain

$$H(z) = (e^{2\pi iz} - 1) \sum_{n=-\infty}^{\infty} a_n e^{2\pi inz}.$$

The coefficients satisfy

$$a_n = \int_{a+yi}^{a+1+yi} \frac{H(z)}{(e^{2\pi iz} - 1)e^{2\pi inz}}\, dz$$

for any $a, y \in \mathbf{R}$. For $n < 0$ we let $y \to +\infty$ and the assumed estimate on $|H(z)|$ gives

$$a_n = \lim_{y\to+\infty} \int_{a+yi}^{a+1+yi} \frac{H(z)}{(e^{2\pi iz} - 1)e^{2\pi inz}}\, dz = 0.$$

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For $n \geq 0$ we let $y \to -\infty$ and obtain

$$a_n = \lim_{y \to -\infty} \int_{a+yi}^{a+1+yi} \frac{H(z)}{(e^{2\pi iz} - 1)e^{2\pi inz}}\, dz = 0.$$

Hence $H(z) \equiv 0$. □

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Complementary Bell Numbers: Arithmetical Properties and Wilf's Conjecture

Tewodros Amdeberhan, Valerio De Angelis, and Victor H. Moll

To Herb Wilf, with admiration and gratitude

Abstract The 2-adic valuations of Bell and complementary Bell numbers are determined. The complementary Bell numbers are known to be zero at $n = 2$ and H. S. Wilf conjectured that this is the only case where vanishing occurs. N. C. Alexander and J. An proved (independently) that there are at most two indices where this happens. This paper presents yet an alternative proof of the latter.

Keywords Valuations • Bell numbers • Complementary Bell numbers • Closed-form summation • Wilf's conjecture

1 Introduction

The Stirling numbers of the second kind $S(n,k)$, defined for $n \in \mathbb{N}$ and $0 \leq k \leq n$, count the number of ways to partition a set of n elements into exactly k nonempty subsets (blocks). The *Bell numbers*

$$B(n) = \sum_{k=0}^{n} S(n,k) \tag{1}$$

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count all such partitions independent of size and the *complementary Bell numbers*

$$\tilde{B}(n) = \sum_{k=0}^{n} (-1)^k S(n,k) \tag{2}$$

takes the parity of the number of blocks into account. The exponential generating functions are given by

$$\sum_{n=0}^{\infty} B_n \frac{x^n}{n!} = \exp(\exp(x) - 1) \text{ and } \sum_{n=0}^{\infty} \tilde{B}(n) \frac{x^n}{n!} = \exp(1 - \exp(x)). \tag{3}$$

In this paper we consider arithmetical properties of the Bell and complementary Bell numbers. The results described here are part of a general program to describe properties of p-adic valuations of classical sequences. The example of Stirling numbers is described in [3], the ASM numbers that count the number of alternating sign matrices appear in [15] and a not-so-classical sequence appearing in the evaluation of a rational integral is described in [2, 10]. On the other hand, much of our interest in the valuations of the complementary Bell numbers is motivated by

$$\textit{Wilf's conjecture}: \tilde{B}(n) = 0 \text{ only for } n = 2.$$

The guiding strategy for us is this: if we manage to prove that $\nu_2(\tilde{B}(n))$ is finite for $n > 2$, the non-vanishing result will follow. The authors [4] have succeeded in employing this method to prove that the sequence

$$x_n = \frac{n + x_{n-1}}{1 - n x_{n-1}}, \text{ starting at } x_1 = 1 \tag{4}$$

only vanishes at $n = 3$. The more natural question that $x_n \notin \mathbb{Z}$ for $n > 5$ remains open.

The following notation is adopted throughout this paper: for $n \in \mathbb{N}$ and a prime p, the *p-adic valuation of n*, denoted by $\nu_p(n)$, is the largest power of p that divides n. The value $\nu_p(0) = +\infty$ is consistent with the fact that any power of p divides 0. As an example, the complementary Bell number $\tilde{B}(14) = 110{,}176$ factors as $2^5 \cdot 11 \cdot 313$; therefore $\nu_2(\tilde{B}(14)) = 5$ and $\nu_3(\tilde{B}(14)) = 0$. Legendre [9] established the formula

$$\nu_p(n!) = \frac{n - s_p(n)}{p - 1} \tag{5}$$

where $s_p(n)$ is the sum of the digits of n in base p.

The exponential generating function (3) and the series representation

$$\tilde{B}(n) = e \sum_{r=0}^{\infty} (-1)^r \frac{r^n}{r!}, \tag{6}$$

as well as elementary properties of the complementary Bell numbers are presented in [16]. The numbers $\tilde{B}(n)$ also appear in the literature as the Uppuluri-Carpenter numbers. Subbarao and Verma [14] established the asymptotic growth of $\tilde{B}(n)$, showing that

$$\limsup_{n\to\infty} \frac{\log|\tilde{B}(n)|}{n \log n} = 1. \tag{7}$$

The non-vanishing of $\tilde{B}(n)$ has been considered by M. Klazar [7, 8] in the context of partitions and by M. R. Murty [11] in reference to p-adic irrationality. Y. Yang [17] established the result $|\{n \leq x : \tilde{B}(n) = 0\}| = O(x^{2/3})$ and De Wannemacker [13] proved that if $n \not\equiv 2, 2{,}944{,}838 \pmod{3 \cdot 2^{20}}$, then $\tilde{B}(n) \neq 0$. The main result of [13] is that $\tilde{B}(n) = 0$ has at most two solutions. This has been achieved by different techniques by N. C. Alexander [1] and Junkyu An [5]. Our interest in the non-vanishing questions comes from the theory of summation in finite terms.

The methods developed by R. Gosper show that the finite sum

$$\sum_{k=1}^{n} k! \tag{8}$$

does not admit a closed-form expression as a hypergeometric function of n. The identity

$$\sum_{k=1}^{n-1} k^a k! = \sum_{\ell=1}^{a} (-1)^{\ell+a} r_\ell(a) + (-1)^{a+1} \tilde{B}(a+1) \sum_{k=0}^{n-1} k! \tag{9}$$

where

$$r_\ell(a) = S(a+1, \ell+1) \sum_{i=0}^{\ell-1} \left((n+i)! - i!\right), \tag{10}$$

shows that a positive verification of Wilf's conjecture implies that the elementary identity

$$\sum_{k=1}^{n} k k! = (n+1)! - 1 \tag{11}$$

is unique in this category. M. Petkovsek, H. S. Wilf and D. Zeilberger [12] is the standard reference for issues involving closed-form summation. The details for (9) are provided in [6].

Section 2 presents a family of polynomials that play a crucial role in the study of the 2-adic valuations of Bell numbers given in Sect. 3. The main arguments presented here are based on the representation of the polynomials introduced in Sect. 2 in terms of rising and falling factorials. This is discussed in Sect. 4. An alternative proof of the analytic expressions for the valuations of regular Bell numbers is presented in Sect. 5. This serves as a motivating example for the more difficult case of the 2-adic valuations of complementary Bell numbers. Experimental data on these valuations are presented in Sect. 6. The data suggests that only those indices congruent to 2 modulo 3 need to be considered. The study of this case begins in Sect. 7, where these valuations are determined for all but two classes modulo 24. The two remaining classes require the introduction of an infinite matrix. This is done in Sect. 8. The two remaining classes are analyzed in Sects. 9 and 10, respectively. The final section presents the exponential generating functions of the two classes of polynomials employed in this work, and some open problems.

2 An Auxiliary Family of Polynomials

The recurrence for the Stirling numbers of second kind

$$S(n+1,k) = S(n,k-1) + kS(n,k) \tag{12}$$

is summed over $0 \leq k \leq n+1$ to produce

$$\sum_{k=0}^{n+1} S(n+1,k) = \sum_{k=0}^{n} (k+1) S(n,k) \tag{13}$$

using the vanishing of $S(n,k)$ for $k<0$ or $k>n$. Iteration of this procedure leads to the next result.

Lemma 1. *The family of polynomials $\mu_j(k)$, defined by*

$$\mu_{j+1}(k) = k\mu_j(k) + \mu_j(k+1), \tag{14}$$

$$\mu_0(k) = 1, \tag{15}$$

satisfy

$$B(n+j) = \sum_{k=0}^{n+j} S(n+j,k) = \sum_{k=0}^{n} \mu_j(k) S(n,k), \tag{16}$$

for all $n,\ j \geq 0$.

Proof. The proof is by induction on j. The inductive step gives

$$\sum_{k=0}^{(n+1)+j} S((n+1)+j,k) = \sum_{k=0}^{n+1} \mu_j(k) S(n+1,k). \tag{17}$$

The recurrence (12) and (14) yield the result. □

Note. The polynomials $\mu_j(k)$ have positive integer coefficients and the first few are given by

$$\begin{aligned}
\mu_0(k) &= 1\\
\mu_1(k) &= k+1\\
\mu_2(k) &= k^2+2k+2\\
\mu_3(k) &= k^3+3k^2+6k+5.
\end{aligned}$$

The degree of μ_j is j, so the family $Z_m := \{\mu_j : 0 \leq j \leq m\}$ forms a basis for the space of polynomials of degree at most m.

The special polynomial

$$\begin{aligned}
\mu_{12}(k) = k^{12} &+ 12k^{11} + 132k^{10} + 1100k^9 + 7425k^8 + 41184k^7 \\
&+ 187572k^6 + 694584k^5 + 2049300k^4 + 4652340k^3 \\
&+ 7654350k^2 + 8142840k + 4{,}213{,}597
\end{aligned} \tag{18}$$

plays a crucial role in the study of 2-adic valuation of Bell numbers discussed in Sect. 3.

3 The 2-adic Valuation of Bell Numbers

In this section we determine the 2-adic valuation of the Bell numbers. The data presented in Fig. 1 suggests examining this valuation according to the equivalence classes modulo 12.

Theorem 1. *The* 2*-adic valuation of the Bell numbers satisfy*

$$\nu_2(B(n)) = 0 \quad \textit{if}\ n \equiv 0,\ 1 \pmod 3. \tag{19}$$

In the missing case, $n \equiv 2 \pmod 3$*, the sequence* $\nu_2(B(3n+2))$ *is a periodic function of period* 4*. The repeating values are* $\{1, 2, 2, 1\}$*. In particular, the* 2*-adic valuation of the Bell numbers is completely determined modulo* 12*. In detail,*

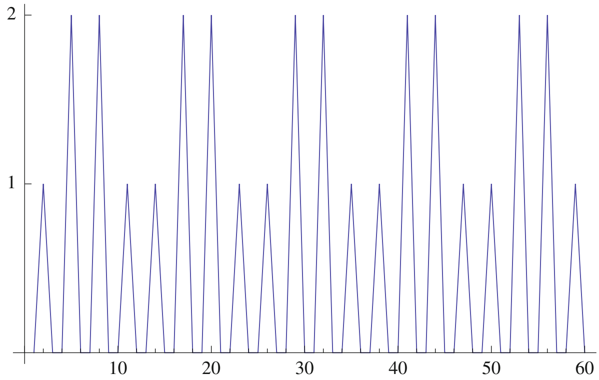

Fig. 1 The 2-adic valuation of Bell numbers

$$\nu_2(B(12n+j)) = \begin{cases} 0 & \textit{if } j \equiv 0,\ 1\ 3,\ 4,\ 6,\ 7,\ 9,\ 10 \pmod{12}; \\ 1 & \textit{if } j \equiv 2,\ 11 \pmod{12}; \\ 2 & \textit{if } j \equiv 5,\ 8 \pmod{12}. \end{cases} \tag{20}$$

The proof of the theorem starts with a congruence for the Bell numbers.

Lemma 2. *The Bell numbers satisfy*

$$B(n+24) \equiv B(n) \pmod{8}. \tag{21}$$

Proof. The identity (16) gives

$$\sum_{k=0}^{n+12} S(n+12,k) = \sum_{k=0}^{n} \mu_{12}(k) S(n,k). \tag{22}$$

The polynomial $\mu_{12}(k)$ given in (18) is now expressed in terms of the basis of rising factorials

$$(k)^{[m]} := k(k+1)(k+2)\cdots(k+m-1),\ m \in \mathbb{N},\ \text{with } (k)^{[0]} = 1. \tag{23}$$

A direct calculation shows that

$$\mu_{12}(k) \equiv \sum_{m=0}^{12} a_m (k)^{[m]} \tag{24}$$

with $a_0 = 421{,}359 \equiv 5$, $a_1 = 3{,}633{,}280 \equiv 0$, $a_2 = 1{,}563{,}508 \equiv 4$, and $a_3 = 414{,}920 \equiv 0 \pmod{8}$. Also, for $m \geq 4$, we have $(k)^m \equiv 0 \pmod{8}$. Thus

$$\mu_{12}(k) \equiv 5 + 4k(k+1) \equiv 5 \pmod{8}. \tag{25}$$

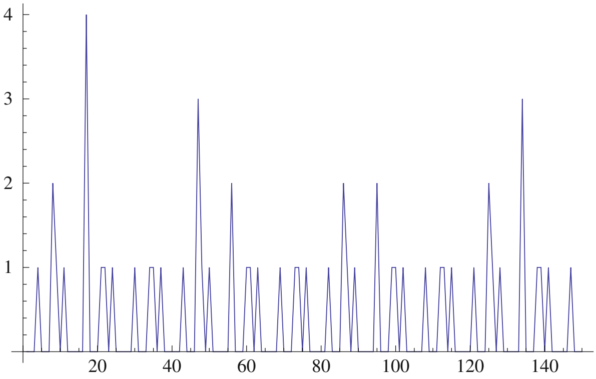

Fig. 2 The 3-adic valuation of Bell numbers

Now (22) produces

$$\sum_{k=0}^{n+12} S(n+12,k) \equiv 5\sum_{k=0}^{n} S(n,k) \pmod 8, \tag{26}$$

that is, $B(n+12) \equiv 5B(n) \pmod 8$. Repeating this yields $B(n+24) \equiv 5B(n+12) \equiv 25B(n) \equiv B(n) \pmod 8$. □

The result of the theorem now follows from computing of the first 24 Bell numbers modulo 8 to obtain the pattern asserted in the theorem.

Remark 1. The p-adic valuation of Bell numbers for primes $p \neq 2$ exhibit some patterns. Figure 2 shows the case $p = 3$.

Experimental observations show that, if $j \not\equiv 2 \pmod 3$, then

$$\nu_3(B_{12n+13j}) = \nu_3(B_{12n}), \text{ for } n \geq 0. \tag{27}$$

In other words, up to a shift, the valuations $\nu_3(B_{12n+j})$ are independent of j.

4 A Representation in Two Bases

The set

$$Z_m = \{\mu_j(k) : 0 \leq j \leq m\} \tag{28}$$

is a basis of the vector space of polynomials of degree at most m. This section explores the representation of this basis in terms of the usual *rising factorials*, defined by

$$(k)^{[r]} := k(k+1)(k+2)\cdots(k+r-1) \quad \text{for } r > 0, \tag{29}$$
$$(k)^{[0]} := 1,$$

and the *falling factorials*, given by

$$(k)_r := k(k-1)(k-2)\cdots(k-r+1) \quad \text{for } r > 0, \tag{30}$$
$$(k)_0 := 1,$$

Definition 1. The coefficients of $\mu_n(r)$ with respect to these bases are denoted

$$\mu_j(k) = \sum_{r=0}^{j} a_j(r)(k)^{[r]} \quad \text{and } \mu_j(k) = \sum_{r=0}^{j} d_j(r)(k)_r. \tag{31}$$

These coefficients are stored in the vectors

$$\mathbf{a_j} := \left[a_j(0),\, a_j(1),\, \cdots\right] \quad \text{and} \quad \mathbf{d_j} := \left[d_j(0),\, d_j(1),\, \cdots\right] \tag{32}$$

where $a_j(r) = d_j(r) = 0$ for $r > j$.

Certain properties of $(k)_r$ and $(k)^{[r]}$ required in the analysis of the 2-adic valuations are stated below.

Lemma 3. *The rising factorial symbol satisfies*

$$\begin{aligned}(k-1)^{[r]} &= (k)^{[r]} - r(k)^{[r-1]}\\ k(k)^{[r]} &= (k)^{[r+1]} - r(k)^{[r]}.\end{aligned}$$

The corresponding relations for the falling factorials are

$$\begin{aligned}(k+1)_r &= (k)_r + r(k)_{r-1}\\ k(k)_r &= (k)_{r+1} + r(k)_r.\end{aligned}$$

The next step is to transform the recurrence for μ_j in (14) into recurrences for the coefficients $a_j(r)$ and $d_j(r)$.

Proposition 1. *The coefficients $a_j(r)$ in Definition 1 satisfy*

$$a_{j+1}(r)-(r+1)a_{j+1}(r+1) = a_j(r-1)-2ra_j(r)+(r+1)^2a_j(r+1), \tag{33}$$

with the assumptions that $a_j(r) = 0$ if $r < 0$ or $r > j$.

Proof. This follows directly from the recurrence for μ_j and the properties described in Lemma 3. □

Note. The recurrences for the coefficients $\mathbf{a_j}$ can be written using the (infinite) matrices

$$\mathbf{M} = (m_{ij})_{i,j\geq 0} \quad \text{and } \mathbf{N} = (n_{ij})_{i,j\geq 0} \tag{34}$$

with

$$m_{ij} = \begin{cases} 1 & \text{if } i = j; \\ -(i+1) & \text{if } i = j-1; \\ 0 & \text{otherwise;} \end{cases} \quad \text{and} \quad n_{ij} = \begin{cases} 1 & \text{if } i = j+1; \\ -2(i-1) & \text{if } i = j; \\ i^2 & \text{if } i = j-1; \\ 0 & \text{otherwise;} \end{cases}$$

in the form

$$\mathbf{Ma_{j+1}} = \mathbf{Na_j}. \tag{35}$$

The analogue of Proposition 1 for falling factorials is stated next.

Proposition 2. *The coefficients $d_j(r)$ in (1) satisfy*

$$d_{j+1}(r) = d_j(r-1) + (r+1)d_j(r) + (r+1)d_j(r+1), \tag{36}$$

with the assumptions that $d_j(r) = 0$ if $r < 0$ or $r > j$.

Note. The recurrence for $\mathbf{d_j}$ is now written using $\mathbf{T} = (t_{ij})_{i,j\geq 0}$, where

$$t_{ij} = \begin{cases} i+1 & \text{if } i = j; \\ i & \text{if } i = j-1; \\ 1 & \text{if } i = j+1; \\ 0 & \text{otherwise;} \end{cases}$$

in the form

$$\mathbf{d_{j+1}} = \mathbf{Td_j}. \tag{37}$$

5 An Alternative Approach to Valuation of Bell Numbers

This section presents an alternative proof of the congruence (2) based on the results of Sect. 4. Recall that this congruence provides complete structure of the 2-adic valuation of the Bell numbers. The ideas introduced here provide a partial description of the 2-adic valuations of complementary Bell numbers.

The first step is to identify the Bell numbers as the first entry of the vectors $\mathbf{a}_j$ and $\mathbf{d}_j$.

Lemma 4. *The Bell numbers are given by*

$$B(j) = \mu_j(0) = a_j(0) = d_j(0). \tag{38}$$

Proof. Let $n = 0$ in the identity (16) to obtain $B(j) = \mu_j(0)$. The other two expressions for the Bell numbers $B(j)$ are obtained by letting $k = 0$ in (31). □

The congruence for the Bell numbers now arises from the analysis of the relations (35) and (37) modulo 8. The key statement is provided next.

Lemma 5. *If* $k \in \mathbb{N}$ *and* $r \geq 4$, *then*

$$(k)^{[r]} \equiv (k)_r \equiv 0 \pmod 8. \tag{39}$$

Proof. Among any set of four consecutive integers there is one that is a multiple of 2 and a different one that is a multiple of 4. □

The system (35) now reduces to

$$\begin{bmatrix} 1 & -1 & 0 & 0 \\ 0 & 1 & -2 & 0 \\ 0 & 0 & 1 & -3 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} a_{j+1}(0) \\ a_{j+1}(1) \\ a_{j+1}(2) \\ a_{j+1}(3) \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & -2 & 4 & 0 \\ 0 & 1 & -4 & 9 \\ 0 & 0 & 1 & -6 \end{bmatrix} \begin{bmatrix} a_j(0) \\ a_j(1) \\ a_j(2) \\ a_j(3) \end{bmatrix}.$$

Inverting the matrix on the left and taking entries modulo 8 leads to

$$\mathbf{a}_{\mathbf{j+1}}^{\mathbf{(4)}} \equiv X_4 \mathbf{a}_{\mathbf{j}}^{\mathbf{(4)}} \pmod 8 \tag{40}$$

where $\mathbf{a}_{\mathbf{j}}^{\mathbf{(4)}}$ represents the first four entries of the coefficient vector $\mathbf{a}_{\mathbf{j}}$ and

$$X_4 = \begin{bmatrix} 1 & 1 & 2 & 6 \\ 1 & 0 & 2 & 6 \\ 0 & 1 & 7 & 7 \\ 0 & 0 & 1 & 2 \end{bmatrix}.$$

Now observe that

$$\mathbf{a}_{\mathbf{j+2}}^{\mathbf{(4)}} \equiv X_4 \mathbf{a}_{\mathbf{j+1}}^{\mathbf{(4)}} \equiv X_4^2 \mathbf{a}_{\mathbf{j}}^{\mathbf{(4)}} \pmod 8 \tag{41}$$

and this extends to

$$\mathbf{a}_{\mathbf{j+s}}^{\mathbf{(4)}} \equiv X_4^s \mathbf{a}_{\mathbf{j}}^{\mathbf{(4)}} \pmod 8 \tag{42}$$

for any $s \in \mathbb{N}$.

Lemma 6. *The matrix X satisfies $X^{24} \equiv I \pmod 8$.*

Proof. Direct (symbolic) calculation. □

The Bell number $B(j)$ is the first entry of the vector $\mathbf{a}_{\mathbf{j}}^{\mathbf{(4)}}$. Then considering the first entry in the relation

$$\mathbf{a}_{\mathbf{j+24}}^{\mathbf{(4)}} \equiv X_4^{24} \mathbf{a}_{\mathbf{j}}^{\mathbf{(4)}} \pmod 8 \tag{43}$$

gives the congruence $B(j+24) \equiv B(j) \pmod 8$.

Note. The corresponding relation for the coefficient vector $\mathbf{d_j}$ is simpler: the system (37) reduces to

$$\begin{bmatrix} d_{j+1}(0) \\ d_{j+1}(1) \\ d_{j+1}(2) \\ d_{j+1}(3) \end{bmatrix} \equiv T_4 \times \begin{bmatrix} d_j(0) \\ d_j(1) \\ d_j(2) \\ d_j(3) \end{bmatrix} \pmod 8 \tag{44}$$

where

$$T_4 = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 2 & 2 & 0 \\ 0 & 1 & 3 & 3 \\ 0 & 0 & 1 & 4 \end{bmatrix}. \tag{45}$$

The matrix T_4 also satisfies $T_4^{24} \equiv I \pmod 8$ and the argument proceeds as before.

6 Some Experimental Data on $\nu_2(\tilde{B}(n))$

This section discusses the 2-adic valuations of the complementary Bell numbers $\tilde{B}(n)$. The data is depicted in Fig. 3 in the range $3 \leq n \leq 1{,}000$.
This discussion begins with some empirical data from the sequence $\nu_2(\tilde{B}(n))$. For $3 \leq n \leq 30$, the list is

$$\{0, 0, 1, 0, 0, 1, 0, 0, 2, 0, 0, 5, 0, 0, 1, 0, 0, 1, 0, 0, 2, 0, 0, 5, 0, 0, 1, 0\}. \tag{46}$$

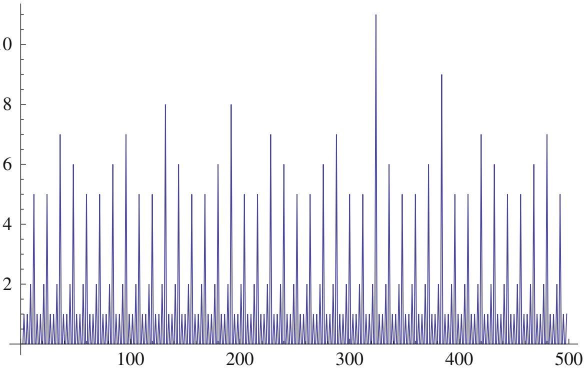

Fig. 3 The 2-adic valuation of the complementary Bell numbers

This suggests that $\nu_2(\tilde{B}(n)) = 0$ if $n \not\equiv 2 \pmod 3$. The list of values of $\nu_2(\tilde{B}(3n+2))$ is

$$\{1,\ 1,\ 2,\ 5,\ 1,\ 1,\ 2,\ 5,\ 1,\ 1,\ 2,\ 7,\ 1,\ 1,\ 2,\ 6,\ 1,\ 1,\ 2,\ 5,\ 1,\ 1,\ 2,\ 5,\ 1,\ 1,\ 2,\ 6,\ 1,\ 1\}$$

and the patterns $\{1,\ 1,\ 2,\ *\}$ suggests considering the sequence $\nu_2(\tilde{B}(n))$ for n modulo 12. The values $n \equiv 2 \pmod 3$ split into classes 2, 5, 8 and 11 modulo 12. The data suggests

$$\nu_2(\tilde{B}(12n+5)) = 1,\ \nu_2(\tilde{B}(12n+8)) = 1,\ \nu_2(\tilde{B}(12n+11)) = 2,$$

while the class $n \equiv 2 \pmod 1$2 does not exhibit such a pattern.

The first step in the analysis of 2-adic valuations of $\tilde{B}(n)$ is to present some elementary congruences to establish that both $\tilde{B}(3n)$ and $\tilde{B}(3n+1)$ are always odd integers. The proof relies on the recurrence

$$\tilde{B}(n) = -\sum_{k=0}^{n-1} \binom{n-1}{k} \tilde{B}(k), \qquad \text{for } n \geq 1 \text{ and } \tilde{B}(0) = 1. \tag{47}$$

Proposition 3. *The complementary Bell numbers $\tilde{B}(n)$ satisfy*

$$\tilde{B}(3n) \equiv \tilde{B}(3n+1) \equiv 1, \textit{ and } \tilde{B}(3n+2) \equiv 0 \pmod 2. \tag{48}$$

Proof. Proceed by induction. The recurrence (47) yields

$$-\tilde{B}(3n) = \sum_{k=0}^{3n-1} \binom{3n-1}{k} \tilde{B}(k). \tag{49}$$

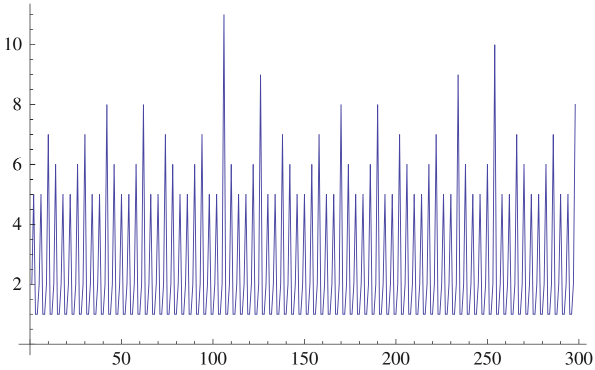

Fig. 4 The 2-adic valuation of $\tilde{B}(3n+2)$

Splitting the sum as

$$-\tilde{B}(3n) = \sum_{k=0}^{n-1} \binom{3n-1}{3k} \tilde{B}(3k) + \sum_{k=0}^{n-1} \binom{3n-1}{3k+1} \tilde{B}(3k+1) + \sum_{k=0}^{n-1} \binom{3n-1}{3k+2} \tilde{B}(3k+2)$$

and using the inductive hypothesis gives

$$-\tilde{B}(3n) \equiv \sum_{k=0}^{n-1} \binom{3n-1}{3k} + \sum_{k=0}^{n-1} \binom{3n-1}{3k+1} \pmod 2. \tag{50}$$

The two sums appearing in the previous line add up to

$$2^{3n-1} - \sum_{k=0}^{n-1} \binom{3n-1}{3k+2}. \tag{51}$$

The result now follows from the identity

$$\sum_{k=0}^{n-1} \binom{3n-1}{3k+2} = \frac{2^{3n-1} + (-1)^n}{3}. \tag{52}$$

Both sides satisfies the recurrence $x_{n+2} - 7x_{n+1} - 8x_n = 0$ and have the same initial conditions $x_1 = 1$ and $x_2 = 11$. □

Proposition 3 shows that

$$\nu_2(\tilde{B}(3n)) = \nu_2(\tilde{B}(3n+1)) = 0, \tag{53}$$

leaving the case $\nu_2(\tilde{B}(3n+2))$ for discussion. This is presented in Sect. 7. Figure 4 shows the data for this sequence and its erratic behavior can be seen from the graph.

7 The 2-Adic Valuation of $\tilde{B}(3n+2)$

The results from the previous section show that $\tilde{B}(3n)$ and $\tilde{B}(3n+1)$ are odd integers and $\tilde{B}(3n+2)$ is an even integer. This section explores the value of the sequence $\nu_2(\tilde{B}(3n+2))$. The family of polynomials $\{\lambda_j(k) : j \geq 0\}$ play the same role as $\mu_j(k)$ did for the regular Bell numbers $B(n)$.

Lemma 7. *The family of polynomials $\lambda_j(k)$, defined by*

$$\begin{aligned} \lambda_{j+1}(k) &= k\lambda_j(k) - \lambda_j(k+1), \\ \lambda_0(k) &= 1, \end{aligned} \tag{54}$$

satisfy

$$\tilde{B}(n+j) = \sum_{k=0}^{n+j} (-1)^k S(n+j,k) = \sum_{k=0}^{n} (-1)^k \lambda_j(k) S(n,k), \tag{55}$$

for all $n, j \geq 0$.

Proof. Use the recurrence (54) and proceed as in the proof of Lemma 1. □

Corollary 1. *The evaluation $\tilde{B}(j) = \lambda_j(0)$ is valid for $j \in \mathbb{N}$.*

The recursions for the falling factorials, given in Proposition 3, yields an evaluation of $\tilde{B}(n)$ in terms of the powers of an infinite matrix.

Note. The (i,j)-entry of a matrix A is denoted by $A(i,j)$. This notation is used to prevent confusion with the presence of a variety of subindices.

Theorem 2. *Let $P = P(r,s),\ r,s \geq 0$ be the infinite matrix defined by*

$$P(r+1,r) = 1, P(r,r) = r-1, P(r,r+1) = -r-1, \quad P(r,s) = 0 \text{ for } |r-s| > 1 \tag{56}$$

or

$$P = \begin{pmatrix} -1 & -1 & 0 & 0 & 0 & 0 & \cdots \\ 1 & 0 & -2 & 0 & 0 & 0 & \cdots \\ 0 & 1 & 1 & -3 & 0 & 0 & \cdots \\ 0 & 0 & 1 & 2 & -4 & 0 & \cdots \\ 0 & 0 & 0 & 1 & 3 & -5 & \cdots \\ 0 & 0 & 0 & 0 & 1 & 4 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \tag{57}$$

Then

$$\tilde{B}(n) = P^n(0,0). \tag{58}$$

Proof. The first step is to express the polynomials $\lambda_n(x)$ in terms of the falling factorial:

$$\lambda_n(k) = \sum_{r=0}^{n} c_n(r)(k)_r. \tag{59}$$

The recurrence relation in Lemma 7 shows that $c_n(r)$ are integers with $c_0(0) = 1$, $c_0(r) = 0$ for $r > 0$ and $c_n(r) = 0$ if $r > n$. Moreover, this recurrence may be expressed as

$$\mathbf{c_{n+1}} = P\mathbf{c_n}, \tag{60}$$

with P defined in (57) and $\mathbf{c_n}$ is the vector $(c_n(r) : r \geq 0)$.

Note that powers of P can be computed with a finite number of operations: each row or column has only finitely many non-zero entries. Iterating (60) gives

$$c_n(r) = P^n(r,0), r \geq 0. \tag{61}$$

The result now follows from Corollary 1 and $c_n(0) = \lambda_n(0)$. □

The next lemma contains a precise description of the fact that the falling factorial $(k)_r$ is divisible by a large power of 2. This is a fundamental tool in the analysis of the 2-adic valuation of $\tilde{B}(n)$.

Lemma 8. *For each $m \geq 0$ and $k \geq 1$, the congruence*

$$(k)_r \equiv 0 \pmod{2^{2^m-1}} \text{ holds for all } r \geq 2^m. \tag{62}$$

Proof. Since $(k)_r$ divides $(k)_j$ for $j \geq r$, it may be assumed that $r = 2^m$. Now observe that $(k)_r/r! = \binom{k}{r}$, thus $\nu_2((k)_r) \geq \nu_2(r!)$. For $r = 2^m$, Legendre's formula (5) gives the value $\nu_2(r!) = 2^m - s_2(2^m) = 2^m - 1$. □

Now we exploit the previous lemma to derive congruences for $\tilde{B}(n)$ modulo a large power of 2. The first step is to show a result analogous to Theorem 2, with P replaced by a $2^m \times 2^m$ matrix, provided the computations are conducted modulo 2^{2^m-1}. Proposition 4 is not necessary for the results that follow it, but it is of interest because it allows us to express $\tilde{B}(n)$ as the top left entry of the power of a finite matrix (with size depending on n).

Proposition 4. *Let $P[n]$ be the $n \times n$ matrix defined by*

$$P[n](r,s) = P(r,s), \quad 0 \leq r,s \leq n-1. \tag{63}$$

For each $n \geq 1$ and $i \geq 1$,

$$(P[n])^i\,(r,s) = P^i(r,s) \ \textit{for}\ 0 \leq r,s \leq n-1, \quad r+s+i \leq 2n-1.$$

Proof. Fix $n \geq 1$ and proceed by induction on i. The statement is clearly true for $i = 1$. Assume that $r+s+i+1 \leq 2n-1$, then the claim follows by computing

$$(P[n])^{i+1}\,(r,s) = \sum_{t=0}^{n-1} (P[n])^i\,(r,t)P[n](t,s). \tag{64}$$

□

Corollary 2. *For $i \leq 2n-1$, the complementary Bell number is given by*

$$\tilde{B}(i) = (P[n])^i\,. \tag{65}$$

For $m \geq 1$ fixed, denote $P[2^m]$ by P_m. This is a matrix of size $2^m \times 2^m$, indexed by $\{0, 1, \ldots, 2^m - 1\}$. Lemma 8 gives

$$\lambda_n(k) \equiv \sum_{r=0}^{2^m-1} c_n(r)(k)_r \pmod{2^{2^m-1}}, \quad n \geq 1, k \geq 0, \tag{66}$$

and then the same argument as before gives

$$c_n(r) \equiv P_m^n(r,0) \qquad \pmod{2^{2^m-1}}, \ \text{ for } 0 \leq r \leq 2^m-1, n \geq 1. \tag{67}$$

The next proposition summarizes the discussion.

Proposition 5. *For $n \in \mathbb{N}$,*

$$\tilde{B}(n) \equiv P_m^n(0,0) \qquad \pmod{2^{2^m-1}}. \tag{68}$$

Corollary 3. *The complementary Bell numbers satisfy*

$$\tilde{B}(n+j) \equiv \sum_{r=0}^{2^m-1} P_m^j(0,r)P_m^n(r,0) \qquad \pmod{2^{2^m-1}}, n \geq 1, j \geq 0. \tag{69}$$

Proof. This is simply the identity $P_m^{n+j} = P_m^n \times P_m^j$. □

Proposition 6. *The following table gives the values of $\tilde{B}(24n+j)$ modulo 8 for $0 \leq j \leq 23$:*

j	$\tilde{B}(24n+j) \mod 8$
0	1
1	7
2	0
3	1
4	1
5	6
6	7
7	7
8	2
9	3
10	5
11	4

j	$\tilde{B}(24n+j) \mod 8$
12	5
13	3
14	0
15	5
16	5
17	6
18	3
19	3
20	2
21	7
22	1
23	4

Proof. Choose $m = 2$, and check that $P_2^{24} \equiv I \pmod 8$. Corollary 3 gives

$$\tilde{B}(24n+j) \equiv \sum_{r=0}^{3} P_2^j(0,r) P_2^{24n}(r,0) \equiv P_2^j(0,0) \equiv \tilde{B}(j) \pmod 8. \quad (70)$$

Therefore the value of $\tilde{B}(j)$ modulo 8 is a periodic function with period 24. The result follows by computing the values $\tilde{B}(j)$ for $0 \le j \le 23$. □

Corollary 4. *Assume* $j \not\equiv 2,\ 14 \pmod{24}$. *Then*

$$\nu_2(\tilde{B}(j)) = \begin{cases} 1 & \text{if } j \equiv 5,\ 8,\ 17,\ 20 \pmod{24}; \\ 2 & \text{if } j \equiv 11,\ 23 \pmod{24}; \\ 0 & \text{otherwise}. \end{cases} \quad (71)$$

Corollary 5. *Assume* $j \not\equiv 2,\ 14 \pmod{24}$. *Then* $\tilde{B}(j) \neq 0$.

The remaining sections discuss the more difficult cases $n \equiv 2$ and $n \equiv 14 \pmod{24}$.

8 The Top-Left Block of Powers of the Matrix P_m

The analysis of the 2-adic valuation of $\tilde{B}(n)$ employs the sequence of matrices appearing in the top-left block of powers of the matrix P_m. This section describes properties of this sequence.

A convention on their block structure is presented next:
let $n \in \mathbb{N}$ and $i,\ j$ integers with $1 \le i,\ j \le n-1$. For an $n \times n$ matrix Q and an $i \times j$ matrix A, the block structure is

$$Q = \begin{pmatrix} A & B \\ C & D \end{pmatrix}. \tag{72}$$

Since the size of the top left corner determines the rest, the notation

$$Q = \begin{pmatrix} \overbrace{A}^{i\times j} & B \\ C & D \end{pmatrix}$$

will be used to specify the size of all blocks when necessary. The default convention is that whenever a $2^m \times 2^m$ matrix is written in block form $\begin{pmatrix} A & B \\ C & D \end{pmatrix}$, it will be understood that the blocks are of size $2^{m-1} \times 2^{m-1}$.

The next lemma is the essential part of the argument for the 2-adic analysis of $\tilde{B}(n)$. The proof is a simple check with the definitions.

Definition 2. For each $m \geq 0$, define $2^m \times 2^m$ matrices B_m, D_m, V_m inductively as follows: $B_0 = -1$, $D_0 = 1$, $V_0 = 1$,

$$B_{m+1} = \begin{pmatrix} 0 & 0 \\ B_m & 0 \end{pmatrix}, \; D_{m+1} = \begin{pmatrix} D_m & B_m \\ 0 & D_m \end{pmatrix}, \; V_{m+1} = \begin{pmatrix} 0 & V_m \\ 0 & 0 \end{pmatrix},$$

where all blocks are $2^m \times 2^m$ matrices.

Recall the P_m is the $2^m \times 2^m$ matrix obtained from the top left corner of the infinite matrix P defined in (57).

Lemma 9. *The matrices P_m satisfy the recurrence*

$$P_{m+1} = \begin{pmatrix} P_m & 0 \\ V_m & P_m \end{pmatrix} + 2^m \begin{pmatrix} 0 & B_m \\ 0 & D_m \end{pmatrix}.$$

The first point in the analysis is to show that, for every power of P_m, the top half of the last column is zero modulo a large power of 2.

Lemma 10. *For all $m \geq 1$, $n \geq 1$, and $0 \leq i \leq 2^m - 1$, the inequality*

$$\nu_2 \left(P_m^n(i, 2^m - 1) \right) \geq 2^m - m - 1 - \nu_2(i!). \tag{73}$$

holds.

Proof. The right-hand side vanishes for $m = 1$. Fix $m \geq 2$. If $n = 1$, the last column of P_m has $2^m - 2$ zeros at the beginning and its last two entries are $-(2^m - 1)$ and $2^m - 2$. Therefore, $\nu_2 \left(P_m(i, 2^m - 1)\right) = \infty$ for $0 \leq i \leq 2^m - 3$, and

$$\nu_2 \left(P_m(2^m - 2, 2^m - 1)\right) = \nu_2(-(2^m - 1)) = 0,$$
$$\nu_2 \left(P_m(2^m - 1, 2^m - 1)\right) = \nu_2(2^m - 2) = 1.$$

Legendre's formula (5) shows that the right-hand side of (73) is $2^m - m - 1 - i + s_2(i)$, so it vanishes for $i = 2^m - 2$ and $i = 2^m - 1$. This proves the case for $n = 1$.

The inductive step is presented next:

$$\begin{aligned} P_m^{n+1}(i, 2^m - 1) &= \sum_{j=0}^{2^m-1} P_m(i, j) P_m^n(j, 2^m - 1) \\ &= P_m(i, i-1) P_m^n(i-1, 2^m - 1) + P_m(i, i) P_m^n(i, 2^m - 1) \\ &\quad + P_m(i, i+1) P_m^n(i+1, 2^m - 1) \\ &= P_m^n(i-1, 2^m - 1) + (i-1) P_m^n(i, 2^m - 1) - (i+1) P_m^n(i+1, 2^m - 1). \end{aligned}$$

Observe that the three terms on the last line are elements of the last column of the matrix P_m^n. The inductive argument provides a lower bound on the power of 2 that divides these integers. Therefore, there are integers q_1, q_2, q_3 such that

$$P_m^{n+1}(i, 2^m - 1) = 2^{2^m - m - 1} \left(2^{-\nu_2((i-1)!)} q_1 + 2^{\nu_2(i-1) - \nu_2(i!)} q_2 - 2^{\nu_2(i+1) - \nu_2((i+1)!)} q_3 \right).$$

It follows that

$$\nu_2\left(P_m^{n+1}(i, 2^m - 1)\right) \geq \\ 2^m - m - 1 + \min\{-\nu_2((i-1)!), \nu_2(i-1) - \nu_2(i!), \nu_2(i+1) - \nu_2((i+1)!)\}. \tag{74}$$

Now use $\nu_2(i+1) - \nu_2((i+1)!) = -\nu_2(i!)$ and $-\nu_2((i-1)!) \geq -\nu_2(i!)$, to verify that the minimum on the right is $-\nu_2(i!)$. This completes the argument. □

The next step is to describe the relation of the matrix P_m (of size $2^m \times 2^m$) to P_{m+1} (of size $2^{m+1} \times 2^{m+1}$). The additional block matrices appearing in this transition are defined recursively:

Fix $m \geq 0$, define $2^m \times 2^m$ matrices $V_{m,n}, A_{m,n}, B_{m,n}, C_{m,n}, D_{m,n}$ inductively by

$$V_{m,1} = V_m, \quad V_{m,n+1} = V_{m,n} P_m + P_m^m V_{m,n}$$

$$B_{m,1} = B_m, \quad B_{m,n+1} = P_m^n B_m + B_{m,n} P_m$$

$$A_{m,1} = 0, \quad A_{m,n+1} = A_{m,n} P_m + B_{m,n} V_m$$

$$D_{m,1} = D_m, \quad D_{m,n+1} = V_{m,n} B_m + P_m^n D_m + D_{m,n} P_m$$

$$C_{m,1} = 0, \quad C_{m,n+1} = C_{m,n} P_m + D_{m,n} V_m$$

The relation between P_m and P_{m+1} is stated next.

Lemma 11. *For each $n \geq 1$, the congruence*

$$P_{m+1}^{n} \equiv \begin{pmatrix} P_m^n & 0 \\ V_{m,n} & P_m^n \end{pmatrix} + 2^m \begin{pmatrix} A_{m,n} & B_{m,n} \\ C_{m,n} & D_{m,n} \end{pmatrix} \pmod{2^{2m}} \tag{75}$$

holds.

Proof. The result is clear for $n = 1$. Computing $P_{m+1}^{n+1} = P_{m+1}^{n} P_{m+1}$, it follows that

$$\begin{aligned} P_{m+1}^{n+1} &\equiv \begin{pmatrix} P_m^n + 2^m A_{m,n} & 2^m B_{m,n} \\ V_{m,n} + 2^m C_{m,n} & P_m^n + 2^m D_{m,n} \end{pmatrix} \begin{pmatrix} P_m^n & 2^m B_m \\ V_{m,n} & P_m^n + 2^m D_m \end{pmatrix} \\ &\equiv \begin{pmatrix} P_m^{n+1} & 0 \\ V_{m,n} P_m + P_m^n V_m & P_m^{n+1} \end{pmatrix} \\ &+ 2^m \begin{pmatrix} A_{m,n} P_m + B_{m,n} V_m & P_m^n B_m + B_{m,n} P_m \\ C_{m,n} P_m + D_{m,n} V_m & V_{m,n} B_m + P_m^n D_m + D_{m,n} P_m \end{pmatrix} \pmod{2^{2m}}. \end{aligned}$$

The recurrence for the matrices A, B, C, D and V are designed to complete the inductive step. □

Corollary 6.

$$V_{m,2n} \equiv V_{m,n} P_m^n + P_m^n V_{m,n} \pmod{2^{2m}} \tag{76}$$

Proof. This follows from Lemma 11 by computing $P_{m+1}^{2n} = P_{m+1}^{n} P_{m+1}^{n}$. □

The next lemma shows some operational rules for the matrices A, B introduced above. The symbol $*$ indicates an unspecified integer or matrix.

Lemma 12. *(a) For any $2^m \times 2^m$ matrix $M(i,j)$ and arbitrary $i \in \mathbb{N}$, we have*

$$(MB_m)(i,0) = -M(i, 2^m - 1).$$

(b) For $m \geq 2$ and $n \geq 1$, both $B_{m,n}$ and $A_{m,n}$ have the form

$$\begin{pmatrix} 0 & 0 \\ * & * \end{pmatrix} \pmod{2^{2^{m-1}-1}}$$

Proof. Part (a) follows directly from the definition of B_m. Part (b) is established by induction. The statement holds for $B_{m,1}$. Now observe that

$$(P_m^n B_m)(i,0) = -P_m^n(i, 2^m - 1) \equiv 0 \pmod{2^{2^{m-1}-1}} \text{ for } 0 \leq i \leq 2^{m-1} - 1,$$

by part (a) and Lemma 10. The induction hypothesis implies that

$$B_{m,n} \equiv \begin{pmatrix} 0 & 0 \\ * & * \end{pmatrix} \qquad (\text{mod } 2^{2^{m-1}-1}),$$

and this leads to

$$B_{m,n+1} = P_m^n B_m + B_{m,n} P_m \equiv \begin{pmatrix} 0 & 0 \\ * & * \end{pmatrix} \qquad (\text{mod } 2^{2^{m-1}-1}).$$

A similar argument shows that

$$A_{m,n+1} = A_{m,n} P_m + B_{m,n} V_m \equiv \begin{pmatrix} 0 & 0 \\ * & * \end{pmatrix} \qquad (\text{mod } 2^{2^{m-1}-1}). \qquad \square$$

The next results describe the powers of P_m considered modulo 2^i. This leads to explicit formula for the 2-adic valuation of $\tilde{B}(n)$.

Notation: $d_m = 3 \times 2^m$.

Proposition 7. *For all* $m \geq 1$,

$$P_m^{d_m} \equiv I \qquad (\text{mod } 4), \quad \textit{and} \quad V_{m,d_m} \equiv 0 \qquad (\text{mod } 2).$$

Proof. For $m = 1$, a direct calculation shows that $P_1^3 = I$ and so $P_1^{d_1} = P_1^6 = I$. Also,

$$V_{1,2} \equiv V_1 P_1 + P_1 V_1 \equiv \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} \qquad (\text{mod } 2),$$

$$V_{1,3} \equiv V_{1,2} P_1 + P_1^2 V_1 \equiv \begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix} \qquad (\text{mod } 2),$$

and this produces

$$V_{1,d_1} = V_{1,6} \equiv V_{1,3} P_1^3 + P_1^3 V_{1,3} \equiv \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \qquad (\text{mod } 2).$$

Assume now $P_m^{d_m} \equiv I \pmod 4$ and $V_{m,d_m} \equiv 0 \pmod 2$. For simplicity, drop the subscripts in the matrices. Lemma 11 gives

$$P_{m+1}^{d_m} \equiv \begin{pmatrix} P & 0 \\ V & P \end{pmatrix} \equiv \begin{pmatrix} I & 0 \\ V & I \end{pmatrix} \quad (\text{mod } 4)$$

and

$$P_{m+1}^{d_{m+1}} = \left(P_{m+1}^{d_m}\right)^2 \equiv \begin{pmatrix} I & 0 \\ V & I \end{pmatrix} \begin{pmatrix} I & 0 \\ V & I \end{pmatrix} \equiv \begin{pmatrix} I & 0 \\ 2V & I \end{pmatrix} \equiv \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix} \pmod 4.$$

Using the notation

$$V_{m+1,d_m} = \begin{pmatrix} X & Y \\ Z & W \end{pmatrix}$$

it follows that

$$\begin{aligned}
V_{m+1,d_{m+1}} &= V_{m+1,2d_m} \equiv V_{m+1,d_m} P_{m+1}^{d_m} + P_{m+1}^{d_m} V_{m+1,d_m} \\
&\equiv \begin{pmatrix} X & Y \\ Z & W \end{pmatrix} \begin{pmatrix} P & 0 \\ V & P \end{pmatrix} + \begin{pmatrix} P & 0 \\ V & P \end{pmatrix} \begin{pmatrix} X & Y \\ Z & W \end{pmatrix} \\
&\equiv \begin{pmatrix} X & Y \\ Z & W \end{pmatrix} \begin{pmatrix} I & 0 \\ V & I \end{pmatrix} + \begin{pmatrix} I & 0 \\ V & I \end{pmatrix} \begin{pmatrix} X & Y \\ Z & W \end{pmatrix} \\
&\equiv \begin{pmatrix} X + YV & Y \\ Z + WV & W \end{pmatrix} + \begin{pmatrix} X & Y \\ VX + Z & VY + W \end{pmatrix} \\
&\equiv \begin{pmatrix} 2X + YV & 2Y \\ 2Z + WV + VX & VY + 2W \end{pmatrix} \equiv \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \pmod 2. \qquad \square
\end{aligned}$$

The next proposition provides the structure of $P_m^{d_m}$ modulo 2^{m+3}, for $m \geq 4$. Introduce the notation

$$Q = \begin{pmatrix} 1 & 2 & 6 & 0 \\ 6 & 1 & 0 & 6 \\ 3 & 4 & 5 & 4 \\ 0 & 1 & 4 & 3 \end{pmatrix}$$

and define recursively for $m \geq 4$ the $4 \times (2^m - 4)$ matrices R_m by

$$R_4 = \begin{pmatrix} 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

$$R_{m+1} = \begin{pmatrix} R_m & 0 \end{pmatrix}.$$

Notation: $q(*)$ indicates a matrix or number that is a multiple of q.

Proposition 8. *Let $m \geq 4$. Then*

$$P_m^{d_m} \equiv I + \overbrace{\begin{pmatrix} 2^m Q & 2^{m+2} R_m \\ 4(*) & 4(*) \end{pmatrix}}^{4\times 4} \pmod{2^{m+3}}.$$

Proof. The claim holds for $m = 4$ by *simple task*: evaluate P_4^{48} modulo 2^7. Keep in mind that P_4 is a 16×16 matrix.

Assume the claim holds for m. Observe that $2m \geq m+4$ for $m \geq 4$, therefore the congruence modulo 2^{2m} of Lemma 11 can be replaced with a congruence modulo 2^{m+4}. Write $V = \begin{pmatrix} X & Y \\ Z & W \end{pmatrix}$ to obtain

$$\begin{aligned} P_{m+1}^{d_m} &\equiv \begin{pmatrix} P & 0 \\ V & P \end{pmatrix} + 2^m \begin{pmatrix} A & B \\ C & D \end{pmatrix} \\ &\equiv \begin{pmatrix} I + 2^m Q & 2^{m+2} R & 0 & 0 \\ 4(*) & I + 4(*) & 2^m(*) & 2^m(*) \\ X + 2^m(*) & Y + 2^m(*) & I + 2^m(*) & 2^m(*) \\ Z + 2^m(*) & W + 2^m(*) & 4(*) & I + 4(*) \end{pmatrix} \pmod{2^{m+4}}. \end{aligned}$$

Squaring this matrix gives

$$P_{m+1}^{d_{m+1}} \equiv \begin{pmatrix} I + 2^{m+1} Q & 2^{m+3} R & 0 & 0 \\ 4(*) & I + 4(*) & 4(*) & 4(*) \\ 2X + 4(*) & 2Y + 4(*) & I + 4(*) & 4(*) \\ 2Z + 4(*) & 2W + 4(*) & 4(*) & I + 4(*) \end{pmatrix} \pmod{2^{m+4}}.$$

The previous proposition shows that $V = \begin{pmatrix} X & Y \\ Z & W \end{pmatrix} \equiv 0 \pmod 2$, therefore

$$P_{m+1}^{d_{m+1}} \equiv I + \begin{pmatrix} 2^{m+1} Q & 2^{m+3} R_{m+1} \\ 4(*) & 4(*) \end{pmatrix} \pmod{2^{m+4}}.$$

This completes the induction argument. □

The next corollary is employed in the next section to establish the 2-adic valuation of complementary Bell numbers.

Corollary 7. *For each $n \geq 1$,*

$$P_m^{nd_m} \equiv I + n \overbrace{\begin{pmatrix} 2^m Q & 2^{m+2} R_m \\ 4(*) & 4(*) \end{pmatrix}}^{4\times 4} \pmod{2^{m+3}}.$$

Proof. The result follows immediately from Proposition 8 and the binomial theorem. □

9 The Case $n \equiv 2 \pmod{24}$

The 2-adic valuations for the complementary Bell numbers $\tilde{B}(n)$ are given in Corollary 4 for $j \not\equiv 2, 14 \pmod{24}$. This section determines the case $j \equiv 2$.

The main result is:

Theorem 3. *For $n \in \mathbb{N}$,*

$$\nu_2\left(\tilde{B}(24n+2)\right) = 5 + \nu_2(n).$$

Proof. Write $n = 2^m q$ with q odd. Corollary 3 and Proposition 8 give

$$\begin{aligned} \tilde{B}(24n+2) = \tilde{B}(3 \cdot 2^{m+3} q + 2) &\equiv \sum_{r=0}^{2^{m+3}-1} P_{m+3}^{qd_{m+3}}(0,r) P_{m+3}^2(r,0) \\ &\equiv P_{m+3}^{qd_{m+3}}(0,0) P_{m+3}^2(0,0) + P_{m+3}^{qd_{m+3}}(0,1) P_{m+3}^2(1,0) \\ &\quad + P_{m+3}^{qd_{m+3}}(0,2) P_{m+3}^2(2,0) \\ &\equiv (1 + 2^{m+3} q)(0) - q 2^{m+4} + 6q 2^{m+3} \\ &\equiv q 2^{m+5} \equiv 2^{m+5} \pmod{2^{m+6}}. \end{aligned}$$

The expression for the valuation $\nu_2\left(\tilde{B}(24n+2)\right)$ follows immediately. □

The tree shown in Fig. 5 summarizes the information derived so far on the 2-adic valuation of $\tilde{B}(n)$. The top three edges of the tree correspond to the residue class of $n \pmod 3$. The number by the side of the edge (if present) gives the (constant) 2-adic valuation of $\tilde{B}(n)$ for that residue class. For example $\nu_2(\tilde{B}(3n+1)) = 0$. If there is no number next to the edge, the 2-adic valuation is not constant for that residue class, so n needs to be split further. The split at each stage is conducted by replacing the index n of the sequence by $2n$ and $2n+1$. For example, the sequence $\nu_2(\tilde{B}(12n+2))$ is not constant so it generates the two new sequences $\nu_2(\tilde{B}(24n+2))$ and $\nu_2(\tilde{B}(24n+14))$. Constant sequences include

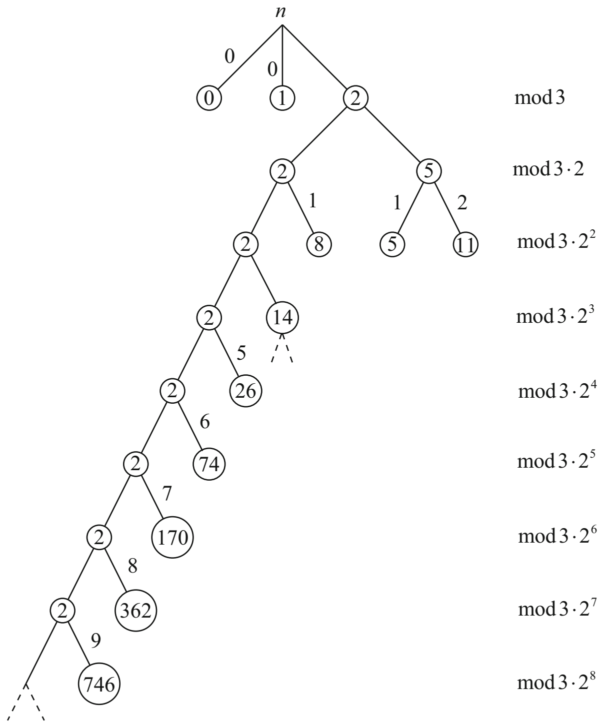

Fig. 5 The 2-adic valuation of $\tilde{B}(24n + 2)$

$\nu_2(\tilde{B}(12n + 8)) = \nu_2(\tilde{B}(12n + 5)) = 1$ and $\nu_2(\tilde{B}(12n + 11)) = 2$. The main theorem of this section shows that the infinite branch on the left, coming from the splitting of $24n + 2$, has a well-determined structure. The other infinite branch, corresponding to $24n + 14$, does not exhibit such a regular pattern. This is the topic of the next section.

10 The Case $n \equiv 14 \pmod{24}$

This section discusses the last missing case in the 2-adic valuations of $\tilde{B}(n)$. The main result of this section is:

Theorem 4. *There is at most one integer $n > 2$ such that $\tilde{B}(n) = 0$.*

Outline of the proof. The proof consists of a sequence of steps. □

Step 1. Define two sequences $\{x_m,\ y_m\}$ recursively via

$$y_{m+1} = \begin{cases} y_m & \text{if } \nu_2(\tilde{B}(x_m)) > m+5; \\ \\ y_m + 2^m & \text{if } \nu_2(\tilde{B}(x_m)) \leq m+5; \end{cases}$$

$$x_{m+1} = 24y_{m+1} + 14.$$

Step 2. Let $y_m = \sum_{i=0}^{m} s_{m,i} 2^i$ and let $s_i = \lim_{m\to\infty} s_{m,i}$ and define $s = (s_0,\ s_1,\ s_2, \cdots)$.

Step 3. For $n \in \mathbb{N}$ let $n = \sum_k b_k(n) 2^k$ be its binary expansion. Let

$$\omega(n) = \begin{cases} \text{first index } k \text{ such that } b_k(n) \neq s_k; \\ \infty \qquad \text{otherwise.} \end{cases} \tag{77}$$

Then $\omega(n) < \infty$ unless s has ony finitely many ones and s is the binary expansion of n. If such n exists, it is called *exceptional*.

Step 4. The 2-adic valuation of $\tilde{B}(24n+14)$ is given by

$$\nu_2(\tilde{B}(24n+14)) = \omega(n) + 5. \tag{78}$$

In particular $\tilde{B}(n) = 0$ only if n is exceptional. This concludes the proof of the theorem.

Proof of Theorem 4. The r-th entry of the top row of P_m^j needs to be expressed as a linear combination of $\tilde{B}(j+i) \pmod{2^{2^m-1}}$, $0 \leq i \leq r$. This is the content of the next lemma. □

Lemma 13. *Define $b_r(i)$ recursively by*

$$\begin{aligned} b_0(0) &= 1, \\ b_{r+1}(i) &= b_r(i-1) + (1-r)b_r(i) + rb_{r-1}(i), \quad 0 \leq i \leq r \\ b_r(i) &= 0 \ \textit{for } i < 0 \textit{ or } i > r. \end{aligned}$$

Then for each $m \geq 1$, $j \geq 1$, and $0 \leq r \leq 2^m - 1$, we have

$$P_m^j(0,r) \equiv \sum_{i=0}^{r} b_r(i)\tilde{B}(j+i) \pmod{2^{2^m-1}}.$$

Proof. The proof is by induction on r. If $r = 0$, the statement is Proposition 5. Assuming the statement for r, it follows that

$$P_m^{j+1}(0,r) \equiv \sum_{i=0}^{r} b_r(i)\tilde{B}(j+1+i) \pmod{2^{2^m-1}}$$

and also

$$\begin{aligned} P_m^{j+1}(0,r) &= P_m^j(0,r-1)P_m(r-1,r) + P_m^j(0,r)P_m(r,r) \\ &\quad + P_m^j(0,r+1)P_m(r+1,r) \\ &= -rP_m^j(0,r-1) + (r-1)P_m^j(0,r) + P_m^j(0,r+1). \end{aligned}$$

Comparing the two expressions and using induction, $P_m^j(0,r+1)$ is expressed as a linear combination of $\tilde{B}(j+i)$, $0 \le i \le r$, with coefficients as in the right side of the equation defining $b_{r+1}(i)$. □

Extensive calculations suggest that $\nu_2(\tilde{B}(24n+14))$ is always at least 5, and it is rather irregular. After examining the experimental data, we were led to define the following sequences.

Define x_m, y_m inductively by:

$$y_0 = 0, \quad x_0 = 24y_0 + 14,$$

and if x_m, y_m have been defined, set

$$y_{m+1} = \begin{cases} y_m & \text{if } \nu_2\left(\tilde{B}(x_m)\right) > m+5 \\ 2^m + y_m & \text{if } \nu_2\left(\tilde{B}(x_m)\right) \le m+5 \end{cases}, \quad x_{m+1} = 24y_{m+1} + 14.$$

This is the statement of Step 1.

The next table gives the first few values of y_m and x_m.

m	0	1	2	3	4	5	6	7	8	9	10
y_m	0	1	1	5	13	13	13	77	77	333	845
x_m	14	38	38	134	326	326	326	1,862	1,862	8,006	20,294

The next lemma provides a lower bound for the 2-adic valuation of the subsequence of complementary Bell numbers indexed by x_m.

Lemma 14. *For $m \in \mathbb{N}$, $\nu_2(\tilde{B}(x_m)) \ge m+5$.*

Proof. The proof employs the values of $b_r(i)$ for $0 \leq r \leq 2$. These are given in Lemma 13 for $r = 0, 1, 2$. It turns out that $b_1(0) = b_1(1) = b_2(0) = b_2(1) = b_2(2) = 1$. (In case one wonders here if all non-zero terms of $b_r(i)$ are 1, this is not true for $r \geq 3$).

Direct calculation shows that $\nu_2(\tilde{B}(x_0)) = \nu_2(\tilde{B}(14)) = 5$, and $\nu_2(\tilde{B}(x_1)) = \nu_2(\tilde{B}(38)) = 7$. Therefore the statement holds for $m = 0,\ 1$. Assume the result for $m \geq 1$. Therefore $\nu_2(\tilde{B}(x_m)) \geq m + 5$. If $\nu_2(\tilde{B}(x_m)) > m + 5$, then by definition $x_{m+1} = x_m$, and it follows that $\nu_2(\tilde{B}(x_{m+1})) \geq m + 6$. On the other hand, if $\nu_2(\tilde{B}(x_m)) = m+5$, write $\tilde{B}(x_m) = 2^{m+5}q$, with q is odd. Then $y_{m+1} = 2^m + y_m$, and $x_{m+1} = 24(2^m + y_m) + 14 = 3 \cdot 2^{m+3} + x_m$. Corollary 3 (with $n = 3 \cdot 2^{m+3}$, $j = x_m$, and m replaced by $m+3$) and Proposition 8 (with m replaced by $m+3$), produce

$$\begin{aligned}
\tilde{B}(x_{m+1}) = \tilde{B}(3 \cdot 2^{m+3} + x_m) &\equiv \sum_{r=0}^{2^{m+3}-1} P_{m+3}^{x_m}(0,r) P_{m+3}^{d_{m+3}}(r,0) \pmod{2^{2^{m+3}-1}} \\
&\equiv (1 + 2^{m+3}) P_{m+3}^{x_m}(0,0) + 6 \cdot 2^{m+3} P_{m+3}^{x_m}(0,1) + 3 \cdot 2^{m+3} P_{m+3}^{x_m}(0,2) \\
&\quad + \sum_{r=4}^{2^{m+3}-1} P_{m+3}^{x_m}(0,r) P_{m+3}^{d_{m+3}}(r,0) \pmod{2^{m+6}}.
\end{aligned}$$

Proposition 8 shows that the first term in the last sum is divisible by 2^{m+5} and the second term is divisible by 4. Then, Lemma 13 yields

$$\begin{aligned}
\tilde{B}\,(x_{m+1}) &\equiv (1 + 2^{m+3})\tilde{B}\,(x_m) + 3 \cdot 2^{m+4} \left(\tilde{B}\,(x_m) + \tilde{B}\,(x_m + 1)\right) \\
&\quad + 3 \cdot 2^{m+3} \left(\tilde{B}\,(x_m) + \tilde{B}\,(x_m + 1) + \tilde{B}\,(x_m + 2)\right) \pmod{2^{m+6}}.
\end{aligned}$$

Since $x_m + 1 \equiv 15$ and $x_m + 2 \equiv 16 \pmod{24}$, Proposition 6 shows that $\tilde{B}\,(x_m + 1) \equiv \tilde{B}\,(x_m + 2) \equiv 5 \pmod 8$. So we find

$$\begin{aligned}
\tilde{B}\,(x_{m+1}) &\equiv (1 + 2^{m+3})2^{m+5}q + 3 \cdot 2^{m+4} \left(2^{m+5}q + 5 + 8(*)\right) \\
&\quad + 3 \cdot 2^{m+3} \left(2^{m+5}q + 5 + 8(*) + 5 + 8(*)\right) \\
&\equiv 2^{m+5}q + 15 \cdot 2^{m+4} + 15 \cdot 2^{m+3} + 15 \cdot 2^{m+3} \\
&\equiv 2^{m+5}q + 15 \cdot 2^{m+5} \equiv (q + 15)2^{m+5} \equiv 0 \pmod{2^{m+6}}.
\end{aligned}$$

This completes the inductive step. □

Lemma 15. *The binary expansion of* y_m *has the form*

$$y_m = \sum_{i=0}^{m} s_{m,i} 2^i \tag{79}$$

and $s_i = \lim_{m \to \infty} s_{m,i}$ *exists.*

Proof. By construction $y_m \leq 2^m - 1$, showing that the binary expansion of y_m ends at 2^{m-1}. Moreover, the binary expansion of y_{m+1} is the same as that of y_m with possibly and extra leading 1. This confirms the existence of the limit s_i. □

Note. Step 2 concludes by defining $s = (s_0, s_1, \ldots) = (1, 0, 1, 1, 0, 0, 1, 0, 1, 1, \ldots)$.

Theorem 5. *Let n be a positive integer with binary expansion $n = \sum_k b_k 2^k$, and let $\omega(n)$ be the first index for which $b_k \neq s_k$. If no such index exists, let $\omega(n) = \infty$. Then*

$$\nu_2(\tilde{B}(24n + 14)) = \omega(n) + 5.$$

Note. As discussed in Step 3, there is at most one index $n > 2$ for which $\omega(n) = \infty$. This happens when s, defined above, has finitely many ones. In this situation, s is the binary expansion of this exceptional index. The conjecture of Wilf states that this situation *does not happen*.

Proof. The notation $m = \omega(n)$ is employed in the proof. If $m = \infty$, then $\tilde{B}(24n + 14) = 0$ and the formula holds. Suppose now that $m \neq \infty$. Then there is $p \in \mathbb{N}$ such that $24n + 14 = 3 \cdot 2^{m+3} p + x_m$.

Write $\tilde{B}(x_m) = 2^{m+5+i} q$, with q odd and $i \geq 0$. Then, as in the previous proof (and also using Lemma 7), it follows that

$$\begin{aligned}
\tilde{B}(24n + 14) &= \tilde{B}\left(3 \cdot 2^{m+3} p + x_m\right) \\
&\equiv (1 + 2^{m+3} p) 2^{m+5+i} q + 3p \cdot 2^{m+4} \left(2^{m+5+i} q + 5 + 8(*)\right) \\
&+ 3p \cdot 2^{m+3} \left(2^{m+5+i} q + 5 + 8(*) + 5 + 8(*)\right) \\
&\equiv 2^{m+5+i} q + 15p \cdot 2^{m+4} + 15p \cdot 2^{m+3} + 15p \cdot 2^{m+3} \\
&\equiv 2^{m+5+i} q + 15p \cdot 2^{m+5} \equiv 2^{m+5}(2^i q + 15p) \qquad (\text{mod } 2^{m+6}).
\end{aligned}$$

If $i = 0$, then $s_m = 1$, and p must be even (because this is where n and s disagree). Thus the quantity in parentheses on the last line is odd, and $\nu_2(\tilde{B}(24n + 14)) = m + 5$. If $i > 0$, then $s_m = 0$, and p must be odd and, as in the previous case, the quantity in parentheses is odd. The result follows from here. □

Note. The tree shown in Fig. 6 updates Fig. 5 by including the 2-adic valuation of $\tilde{B}(24n + 14)$. It is a curious fact that $\nu_2(\tilde{B}(n))$ takes on all non-negative values except 3 and 4.

Final comment. It remains to decide if the exceptional case exists. If it does not, then $\tilde{B}(n) \neq 0$ for $n > 2$, Wilf's conjecture is true and the sequence $\nu_2(\tilde{B}(24n + 14))$ is unbounded. If this exceptional index exists, then it is unique. Observe that the exceptional case exists if and only if the sequence x_m is eventually constant.

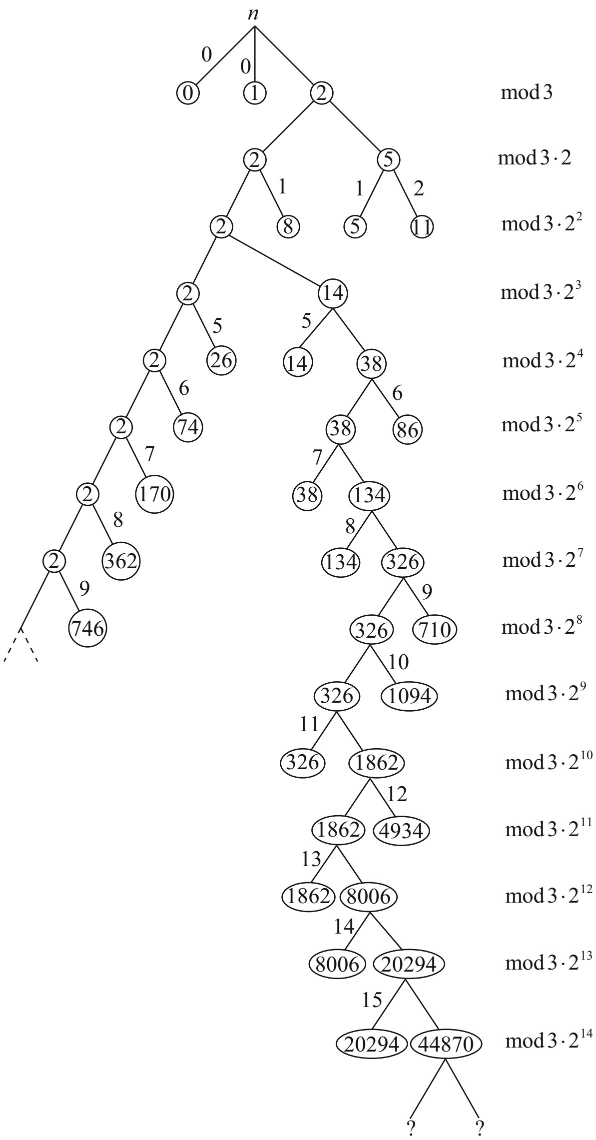

Fig. 6 The 2-adic valuation of $\tilde{B}(24n + 14)$

11 Two Classes of Polynomials

Two families of polynomials have been considered in Lemmas 1 and 7: $\mu_0(x) \equiv 1, \lambda_0(x) \equiv 1$, and

$$\mu_{j+1}(x) = x\mu_j(x) + \mu_j(x+1); \quad \text{for } n \geq 0; \tag{80}$$

$$\lambda_{j+1}(x) = x\lambda_j(x) - \lambda_j(x+1); \quad \text{for } n \geq 0. \tag{81}$$

The corresponding exponential generating functions are provided below.

Lemma 16. *The polynomials μ_j and λ_j have generating functions given by*

$$\sum_{j=0}^{\infty} \frac{z^j}{j!}\mu_j(x) = e^{xz-1+e^z} \quad \textit{and} \sum_{j=0}^{\infty} \frac{z^j}{j!}\lambda_j(x) = e^{xz+1-e^z}. \tag{82}$$

Proof. Let $F(x,z) = \sum_{j\geq 0} \frac{z^j}{j!}\mu_j(x)$ and $G(x,z) = e^{xz-1+e^z}$. Multiplying the polynomial recurrence through by $z^j/j!$ yields

$$\mu_{j+1}(x)\frac{z^j}{j!} = x\mu_j(x)\frac{z^j}{j!} + \mu_j(x+1)\frac{z^n}{j!}.$$

Now sum over all non-negative integers j to find

$$\frac{\partial}{\partial z}F(x,z) = xF(x,z) + F(x+1,z). \tag{83}$$

Since $G(x+1,z) = e^z G(x,z)$, it follows

$$\frac{\partial}{\partial z}G(x,z) = G(x,z)(x+e^z) = xG(x,z) + G(x+1,z). \tag{84}$$

On the other hand, $F(x,0) = \mu_0(x) = 1 = G(x,0)$. Therefore, $F(x,z) = G(x,z)$. The same argument verifies the second assertion of the lemma. The proof is complete. □

Corollary 8. *The polynomials μ_j and λ_j satisfy*

$$\mu_j(0) = B(j) \textit{ and } \lambda_j(0) = \tilde{B}(j). \tag{85}$$

Corollary 9. *There are double-indexed exponential generating functions for $\mu_j(n)$, $\lambda_j(n)$:*

$$\sum_{j,n\geq 0} \mu_j(n)\frac{z^j y^n}{j!n!} = e^{-1+(y+1)e^z}, \quad \sum_{j,n\geq 0} \lambda_j(n)\frac{z^j y^n}{j!n!} = e^{-1+(y-1)e^z}.$$

Proof. Direct computation shows

$$\sum_{j,n} \mu_j(n) \frac{z^j y^n}{j!n!} = \sum_n e^{nz-1+e^z} \frac{y^n}{n!} = e^{-1+e^z} \sum_n \frac{(ye^z)^n}{n!} \tag{86}$$

with a similar argument for λ_j. □

Corollary 10. *The polynomials $\mu_j(x), \lambda_j(x)$ are binomial convolutions of Bell numbers,*

$$\mu_j(x) = \sum_r \binom{j}{r} B(r) x^{j-r}, \quad \lambda_j(x) = \sum_r \binom{j}{r} \tilde{B}(r) x^{j-r}.$$

Proof. This follows directly from

$$\sum_{j\geq 0} \mu_j(x) \frac{z^j}{j!} = e^{e^z-1} e^{xz} = \sum_{k\geq 0} B(k) \frac{z^k}{k!} \times \sum_{n\geq 0} x^n \frac{z^n}{n!} \tag{87}$$

and a similar argument for λ_j. □

Corollary 11. *The family of polynomials $\lambda_j(x)$ have a missing strip of coefficients, i.e.*

$$[x^{j-2}]\lambda_j(x) = 0.$$

Proof. Follows from Corollary 10 and $\tilde{B}(2) = 0$. □

Define the functions $e^{(k)}(x)$ inductively, as follows:

$$e(x) = e^{(1)}(x) = 1 - e^x$$
$$e^{(k+1)}(x) = e(e^{(k)}(x)).$$

These are called *super-exponentials*. For example,

$$e^{(2)}(x) = 1 - e^{1-e^x} \quad \text{and} \quad e^{(3)}(x) = 1 - e^{1-e^{1-e^x}}.$$

Introduce the *super-complementary Bell numbers*, $\tilde{B}^{(k)}(n)$, according to

$$\sum_{n\geq 0} \tilde{B}^{(k)}(n) \frac{x^n}{n!} = 1 - e^{(k+1)}(x). \tag{88}$$

The usual complementary Bell numbers $\tilde{B}(n)$ become $\tilde{B}^{(1)}(n)$ due to the relation

$$\sum_n \tilde{B}(n) \frac{x^n}{n!} = e^{1-e^x} = 1 - e^{(2)}(x). \tag{89}$$

The next conjecture is a natural extension of Wilf's original question.

Conjecture 1. Let $k \in \mathbb{N}$ be odd. Then $\tilde{B}^{(k)}(n) = 0$ if and only if $n = 2$. For $k \in \mathbb{N}$ even and $k \neq 2$, it is conjectured that $\tilde{B}^{(k)}(n) \neq 0$. The case $k = 2$ is peculiar: the corresponding conjecture is that $\tilde{B}^{(2)}(n) = 0$ if and only if $n = 3$.

Combinatorial meanings: $B_1^{(1)}(n)$ = number of set partitions of $\{1, \ldots, n\}$ with an even number of parts, minus the number of such partitions with an odd number of parts; $B_1^{(2)}(n)$ = number of set partitions of $\{1, \ldots, n\}$ with an even number of parts, minus the number of such partitions with an odd number of parts, and then repeating this process for each block. Similar number of chain reactions yield $B_1^{(k)}(n)$. For instance,

$$\tilde{B}^{(2)}(n) = \sum_{j=0}^{n} (-1)^j S(n, j) \tilde{B}(j). \tag{90}$$

Illustrative example. Take $n = 3$, and partition the set $\{1, 2, 3\}$. For $k = 1$: $\{1, 2, 3\}$; for $k = 2$: $\{1, \{2, 3\}\}$, $\{2, \{1, 3\}\}$, $\{3, \{1, 2\}\}$; for $k = 3$: $\{\{1\}, \{2\}, \{3\}\}$. In the next step, partition blocks as follows. When $k = 1$: $\{1, 2, 3\}$ is its own partition as a 1-element set; when $k = 2$, partition each of $\{1, \{2, 3\}\}$, $\{2, \{1, 3\}\}$, $\{3, \{1, 2\}\}$ as 2-element sets; when $k = 3$, partition $\{\{1\},\{2\},\{3\}\}$ as a 3-element set. The resulting collection looks like this:

$$\begin{aligned}
&\{1, 2, 3\},\\
&\{1, \{2, 3\}\},\\
&\{\{1\}, \{\{2, 3\}\}\},\\
&\{2, \{1, 3\}\},\\
&\{\{2\}, \{\{1, 3\}\}\},\\
&\{3, \{1, 2\}\},\\
&\{\{3\}, \{\{1, 2\}\}\},\\
&\{\{1\}, \{2\}, \{3\}\},\\
&\{\{1\}, \{\{2\}, \{3\}\}\},\\
&\{\{2\}, \{\{1\}, \{3\}\}\},\\
&\{\{3\}, \{\{1\}, \{2\}\}\},\\
&\{\{1\}, \{\{2\}\}, \{\{3\}\}\}.
\end{aligned}$$

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Partitions with Early Conditions

George E. Andrews*

In honor of my friend, Herb Wilf, on the occasion of his 80th birthday.

Abstract In an earlier paper, partitions in which the smaller parts were required to appear at least k-times were considered. Some of those results were tied up with Rogers-Ramanujan type identities and mock theta functions. By considering more general conditions on initial parts we are led to natural explanations of many more identities contained in Slater's compendium of 130 Rogers-Ramanujan identities.

1 Introduction

In 1886, J. J. Sylvester [17] posed a couple of problems in the Educational Times that are precursors to the study undertaken here. We reproduce the problems in their entirety:

> Definition. If, in any arrangement of integers, each of the numbers $1, 2, 3, \ldots$ up to any odd number (unity inclusive), say $2i - 1$, occurs once or any odd number of times, but the even number following, say $2i$, does not occur any odd number of times, the arrangement is said to be flushed; if such kind of sequence does not occur, it is said to be unflushed.
>
> 1. Required to prove, that if any number be partitioned in every possible way, the number of unflushed partitions containing an odd number of parts is equal to the number of unflushed partitions containing an even number of parts.

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Ex.gr.: The total partitions of 7 are
7; 6, 1; 5,2; 5, 1, 1; 4, 3; 4, 2, 1; 4, 1, 1, 1; 3, 3, 1; 3, 2, 2; 3, 2, 1, 1; 2, 2, 2, 1; 3, 1, 1, 1, 1; 2, 2, 1, 1, 1; 2, 1, 1, 1, 1, 1; 1, 1, 1, 1, 1, 1, 1.
Of these, 6, 1; 4, 1, 1, 1; 3, 3, 1; 2, 2, 1, 1, 1; 1, 1, 1, 1, 1, 1, 1 alone are flushed. Of the remaining unflushed partitions, five contain an odd number of parts, and five an even number.
Again, the total partitions of 6 are
6; 5, 1; 4, 2; 4, 1, 1; 3, 3; 3, 2, 1; 2, 2, 2; 3, 1, 1, 1; 2, 2, 1, 1; 2, 1, 1, 1, 1; 1, 1, 1, 1, 1, 1; of which 5, 1; 3, 2, 1; 3, 1, 1, 1 alone are flushed. Of the remainder, four contain an odd and four an even number of parts.
N.B.—This transcendental theorem compares singularly with the well-known algebraical one, that the total number of the permuted partitions of a number with an odd number of parts is equal to the same of the same with an even number.

2. Required to prove that the same proposition holds when any odd number is partitioned without repetitions in every possible way.

Sylvester did not publish solutions to these problems. In 1970, solutions to both problems were published [1] and the generating function for flushed partitions (corrected) was revealed as

$$\frac{\sum_{n=1}^{\infty} q^{n(3n-1)/2}(1-q^n)}{(q;q)_\infty},$$

where

$$(A;q)_n = (1-A)(1-Aq)\cdots(1-Aq^{n-1}).$$

The solutions of Sylvester's problems involved generating functions. It is completely unknown whether this was Sylvester's approach and how he came upon flushed partitions in the first place.

Sylvester's flushed partitions suggest a more extensive study of partitions subject to variations on the following three constraints which we shall call the *Sylvester constraints*:

1. Some of the smaller parts are required to appear a specified number of times (e.g. in the case of flushed partitions, an odd number of times).
2. Immediately following the parts considered in (1) there may be one or two special parts (e.g. in the case of flushed partitions, the first integer appearing an even number of times is even).
3. The larger parts are constrained differently if at all (e.g. in the case of flushed partitions there are no constraints).

In the subsequent decades of the twentieth century, N. J. Fine appears to have been the only one to consider questions of this type. In lectures at Penn State, he observed that the conjugates of partitions into distinct parts are "partitions without gaps," i.e. partitions in which every integer smaller than the largest part is also a part. For example, here are the partitions of 6 into distinct parts paired with their conjugates:

6	1 + 1 + 1 + 1 + 1 + 1
5 + 1	2 + 1 + 1 + 1 + 1
4 + 2	2 + 2 + 1 + 1
3 + 2 + 1	3 + 2 + 1

Fine also noted in his book [7, p. 57] (see also [18]) that in one of Ramanujan's third order mock theta functions

$$\psi(q) := \sum_{n=0}^{\infty} \frac{q^{n^2}}{(q;q^2)_n} = \sum_{n=0}^{\infty} \beta(n) q^n,$$

the coefficient $\beta(n)$ is the number of partitions of n into *odd* parts where each odd integer smaller than the largest part must also be a part.

In 2009, the theme initiated by Sylvester was further developed in a paper titled "Partitions with initial repetitions" [5].

Definition 1. A partition with initial k-repetitions is a partition in which if any j appears at least k times as a part, then each positive integer less than j appears k times as a part.

As noted in [5, Theorem 1], partitions with initial k-repetitions fit naturally into an expanded version of the Glaisher/Euler theorem [2, Corollary 1.3, p. 6].

Theorem 1. *The number of partitions of n with initial k-repetitions equals the number of partitions of n into parts not divisible by $2k$ and also equals the number of partitions of n in which no part is repeated more than $2k-1$ times.*

This idea was further developed in [5] and sets the stage for the results in this paper.

Definition 2. Let $F_e(n)$ (resp. $F_o(n)$) denote the number of partitions of n in which no odd (resp. no even) parts are repeated and no odd part (resp. even part) is smaller than a repeated even part (resp. odd part), and if an even (resp. odd) part is repeated then each smaller even (resp. odd) positive integer is also a repeated part.

Theorem 2. *$F_e(n)$ equals the number of partitions of n into parts $\not\equiv 0, \pm 2 \pmod 7$.*

This result follows immediately from the second Rogers-Selberg identity [16, p. 155, Eq. (32)]

$$\sum_{n=0}^{\infty} \frac{q^{2n^2+2n}(-q^{2n+1};q)_\infty}{(q^2;q^2)_n} = \prod_{\substack{n=1 \\ n\not\equiv 0\pm 2 \ (\mathrm{mod}\ 7)}}^{\infty} \frac{1}{1-q^n}.$$

Theorem 3. $\sum_{n=0}^{\infty} F_o(n)q^n = (-q;q)_\infty f(q^2)$, *where* $f(q)$ *is one of Ramanujan's seventh order mock theta functions [14, p. 355]*

$$f(q) = \sum_{n=1}^{\infty} \frac{q^{n^2}}{(q^n;q)_n}.$$

Our object in this paper is to apply the Sylvester constraints to various other Rogers-Ramanujan type identities found by Slater [16], (cf. [14, Appendix A]). In each instance odds and evens will be subject to different restrictions. Interchanging the roles of odds and evens (as was done in passing from Theorems 2 to 3) has an interesting outcome. Sometimes mock theta functions (cf. [18]) arise (cf. (7), (8) and Sect. 4), and sometimes other Rogers-Ramanujan type identities arise (cf. Sect. 3).

In Sect. 2, we analyze two theorems that were originally found by F. H. Jackson and are listed as identities (38) and (39) in Slater [16]. In this case the exchange of the roles of odds and evens yields two of the mock theta functions listed in [6].

In Sect. 3, we begin with Slater's identity (119) [16, p. 165]. In this case, the reversed roles of odds and evens leads to a result equivalent to Slater's (81) [16, p. 160].

In Sect. 4, events take a surprising turn. We begin with Slater's (44) and (46) [16, p. 156]. Each of these makes condition (2) of the Sylvester constraints rather cumbersome. So the terms of the series in (44) and (46) are slightly altered to streamline condition (2). The result is new Hecke-type series, and the odd even reversal yields a further instance.

Finally in Sect. 5, we start with Slater's (53). This requires us to move from odd-even (or modulus 2) conditions to modulus 4 conditions. In this case, the role reversal takes us from Slater's (53) to Slater's (55).

Section 6 is the conclusion where we discuss a variety of potential projects foreshadowed by this paper.

2 Identities of Modulus 8

Of course, there are two famous modulus 8, Rogers-Ramanujan identities. They are due to Lucy Slater [14, Eqs. (36) and (34)]:

$$\sum_{n=0}^{\infty} \frac{(-q;q^2)_n q^{n^2}}{(q^2;q^2)_n} = \prod_{\substack{n=1 \\ n\equiv 1,4,7 \pmod 8}}^{\infty} \frac{1}{1-q^n}, \tag{1}$$

and

$$\sum_{n=0}^{\infty} \frac{(-q;q^2)_n q^{n^2+2n}}{(q^2;q^2)_n} = \prod_{\substack{n=1 \\ n\equiv 3,4,5 \pmod 8}}^{\infty} \frac{1}{1-q^n}. \tag{2}$$

Although Slater first obtained these results in her Ph.D. thesis in the late 1940s, they have become known as the Göllnitz-Gordon identities because in the early 1960s both H. Göllnitz [9] and B. Gordon [10] discovered their partition theoretic interpretation.

As A. Sills notes in [15, p. 103], F. H. Jackson [11] found, and Slater [16, Eqs. (39) and (38)] re-found closely related results which we now consider in slightly altered form:

$$\sum_{n=0}^{\infty} \frac{q^{2n^2}(-q^{2n+1};q^2)_\infty}{(q^2;q^2)_n} = \prod_{\substack{n=1 \\ n\equiv 1,4,7 \pmod 8}}^{\infty} \frac{1}{1-q^n}, \tag{3}$$

and

$$\sum_{n=0}^{\infty} \frac{q^{2n^2+2n}(-q^{2n+3};q^2)_\infty}{(q^2;q^2)_n} = \prod_{\substack{n=1 \\ n\equiv 3,4,5 \pmod 8}}^{\infty} \frac{1}{1-q^n}. \tag{4}$$

Let us rewrite these series in a form where the partition theoretic interpretation is obvious.

$$\sum_{n=0}^{\infty} \frac{q^{2+2+4+4+\cdots+(2n-2)+(2n-2)+2n}(1+q^{2n+1})(1+q^{2n+3})(1+q^{2n+5})\cdots}{(1-q^2)(1-q^4)\cdots(1-q^{2n})} = \prod_{\substack{n=1 \\ n\equiv 1,4,7 \pmod 8}}^{\infty} \frac{1}{1-q^n}, \tag{5}$$

$$\sum_{n=0}^{\infty} \frac{q^{2+2+4+4+\cdots+2n+2n}(1+q^{2n+3})(1+q^{2n+5})(1+q^{2n+7})\cdots}{(1-q^2)(1-q^4)\cdots(1-q^{2n})} = \prod_{\substack{n=1 \\ n\equiv 3,4,5 \pmod 8}}^{\infty} \frac{1}{1-q^n}. \tag{6}$$

The standard methods for generating partitions from q-series and products [2, Chap. 1] allows us to interpret (5) and (6) as follows.

Theorem 4. *Let $G_1(n)$ denote the number of partitions of n into parts* $\equiv 1, 4$ *or* 7 (mod 8)*. Let $R_1(n)$ denote the number of partitions of n in which, (i) odd parts are distinct and each is larger than any even part, and (ii) all even integers less than the largest even part appears at least twice. Then for each $n \geq 0$,*

$$G_1(n) = R_1(n).$$

For example, the 12 partitions enumerated by $G_1(15)$ are 15, $12+1+1+1$, $9+4+1+1$, $9+1+1+\cdots+1$, $7+7+1$, $7+4+4$, $7+4+1+1+1+1$, $7+1+1+\cdots+1$, $4+4+4+1+1+1$, $4+4+1+1+\cdots+1$, $4+1+1+\cdots+1$, $1+1+\cdots+1$, and the 12 partitions enumerated by $R_1(15)$ are 15, $11+3+1$, $9+5+1$, $7+5+3$, $13+2$, $11+2+2$, $9+2+2+2$, $7+2+2+2+2$, $5+2+2+2+2+2$, $3+2+2+\cdots+2$, $7+4+2+2$, $5+4+2+2+2$.

Theorem 5. *Let $G_2(n)$ denote the number of partitions of n into parts* $\equiv$ 3, 4*, or* 5 (mod 8)*. Let $R_2(n)$ denote the number of partitions of n in which, (i) odd parts are distinct, greater than 1, and each is larger than the largest even+2, and (ii) all even integers up to and including the largest even part appear at least twice. Then for each $n \geq 0$*

$$G_2(n) = R_2(n).$$

For example, the 7 partitions enumerate by $G_2(16)$ are $13+3$, $12+4$, $11+5$, $5+5+3+3$, $5+4+4+3$, $4+4+4+4$, $4+3+3+3$, and the 7 partitions enumerated by $R_2(16)$ are $13+3$, $11+5$, $9+7$, $7+5+2+2$, $4+4+2+2+2+2$, $4+4+4+2+2$, $2+2+\cdots+2$.

Now let us reverse the roles played by the evens and odds. The resulting counterpart of (5) is

$$\begin{aligned}\sum_{n\geq 1}\frac{q^{1+1+3+3+\cdots+(2n-3)+(2n-3)+(2n-1)}(-q^{2n};q^2)_\infty}{(q;q^2)_n} &= q\sum_{n\geq 0}\frac{q^{2n^2+2n}(-q^{2n+2};q^2)_\infty}{(q;q^2)_{n+1}}\\ &= q(-q^2;q^2)_\infty\sum_{n=0}^{\infty}\frac{q^{2n^2+2n}}{(q;-q)_{2n+1}}\\ &:= q(-q^2;q^2)_\infty \mathcal{G}_1(q), \qquad (7)\end{aligned}$$

where [6]

$$\begin{aligned}\mathcal{G}_1(-q) &= \sum_{n=0}^{\infty}\frac{q^{2n^2+2n}}{(-q;q)_{2n+1}}\\ &= \frac{1}{(q^2;q^2)_\infty}\sum_{n=0}^{\infty} q^{4n^2-3n}(q^{14n+7}-1)\sum_{j=-n}^{n}(-1)^j q^{-j^2}.\end{aligned}$$

The latter is the now familiar form of a Hecke-type series involving an indefinite quadratic form (see also [6, Eq. (1.15)]).

The resulting counterpart of (6) is

$$\begin{aligned}\sum_{n\geq 1}\frac{q^{1+1+3+3+\cdots+(2n-1)+(2n-1)}(-q^{2n+2};q^2)_\infty}{(q;q^2)_n} &= \sum_{n\geq 0}\frac{q^{2n^2}(-q^{2n+2};q^2)_\infty}{(q;q^2)_n}\\ &= (-q^2;q^2)_\infty\sum_{n=0}^{\infty}\frac{q^{2n^2}}{(q;-q)_{2n}}\\ &= (-q^2;q^2)_\infty \mathcal{G}_2(q), \qquad (8)\end{aligned}$$

where [6, Eq. (1.14)]

$$\begin{aligned}\mathcal{G}_2(-q) &= \sum_{n=0}^{\infty}\frac{q^{2n^2}}{(-q;q)_{2n}}\\ &= \frac{1}{(q^2;q^2)_\infty}\sum_{n=0}^{\infty}q^{4n^2+n}(1-q^{6n+3})\sum_{j=-n}^{n}(-1)^j q^{-j^2}.\end{aligned}$$

Thus, as was mentioned in the Introduction, the even-odd reversal transformed the related generating functions from classical theta functions into mock theta functions.

3 Identities of Modulus 28

Suppose now we allow some mixing of odds and evens in our Sylvester constraints. Let us turn to identity (119) in Slater's [16, p. 165] which we write as follows:

$$\sum_{n=0}^{\infty}\frac{q^{1+3+\cdots+(2n+1)}(-q^{2n+2};q^2)_\infty}{(q;q)_{2n+1}} = q\prod_{\substack{n=1\\ n\not\equiv 0,\pm 4,\pm 5,\pm 9,14 \pmod{28}}}^{\infty}\frac{1}{1-q^n}. \qquad (9)$$

We directly deduce from this the following partition identity.

Theorem 6. *Let* $H_1(n)$ *denote the number of partitions of n into parts* $\not\equiv 0,\pm 4,\pm 5,$ $\pm 9, 14 \pmod{28}$. *Let* $S_1(n)$ *denote the number of partitions of n in which odd parts do appear and without gaps while the evens larger than the largest odd part are distinct. Then for* $n\geq 1$

$$H_1(n-1) = S_1(n).$$

For example, the 18 partitions enumerated by $H_1(9)$ are $8+1$, $7+2$, $7+1+1$, $6+3$, $6+2+1$, $6+1+1+1$, $3+3+3$, $3+3+2+1$, $3+3+1+1+1$, $3+2+2+2$,

$3+2+2+1+1$, $3+2+1+1+1+1$, $3+1+\cdots+1$, $2+2+2+2+1$, $2+2+1+1+1$, $2+2+1+1+1+1+1$, $2+1+1+\cdots+1$, $1+1+\cdots+1$, and the 18 partitions enumerated by $S_1(10)$ are $8+1+1$, $6+3+1$, $6+2+1+1$, $6+1+1+1+1$, $5+3+1+1$, $4+3+2+1$, $4+3+1+1+1$, $4+2+1+1+1+1$, $3+3+3+1$, $4+1+1+\cdots+1$, $3+3+2+1+1$, $3+3+1+1+1+1$, $3+2+2+2+1$, $3+2+2+1+1+1$, $3+2+1+1+\cdots+1$, $3+1+1+\cdots+1$, $2+1+1+\cdots+1$, $1+1+\cdots+1$.

When we now reverse the roles of evens and odds, we find that, instead of a mock theta function arising, we obtain another identity of Slater's [16]. Thus

$$\begin{aligned}\sum_{n=0}^{\infty} \frac{q^{2+4+\cdots+2n}(-q^{2n+1};q^2)_\infty}{(q;q)_{2n}} &= (-q;q^2)_\infty \sum_{n=0}^{\infty} \frac{q^{n^2+n}}{(q;q)_{2n}(-q;q^2)_n} \\ &= (-q;q^2)_\infty \sum_{n=0}^{\infty} \frac{q^{n^2+n}}{(q^2;q^2)_n(q^2;q^4)_n} \\ &= \prod_{\substack{n=1 \\ n\not\equiv 0,\pm 2,\pm 10,\pm 12,14 \pmod{28}}}^{\infty} \frac{1}{1-q^n},\end{aligned}$$

by Slater [16, p. 160, Eq. (81)].

This result is then directly interpretable in the following theorem.

Theorem 7. *Let $H_2(n)$ denote the number of partitions of n into parts $\not\equiv 0, \pm 2, \pm 10, \pm 12, 14 \pmod{28}$. Let $S_2(n)$ denote the number of partitions of n in which even parts appear without gaps and the odd parts larger than the largest even part are distinct. Then*

$$H_2(n) = S_2(n).$$

For example, the 15 partitions enumerated by $H_2(9)$ are 9, $8+1$, $7+1+1$, $6+3$, $6+1+1+1$, $5+4$, $5+3+1$, $5+1+1+1+1$, $4+4+1$, $4+3+1+1$, $4+1+1+\cdots+1$, $3+3+3$, $3+3+1+1+1$, $3+1+1+\cdots+1$, $1+1+\cdots+1$, and the 15 partitions enumerated by $S_2(9)$ are 9, $7+2$, $5+3+1$, $5+2+2$, $5+2+1+1$, $4+3+2$, $4+2+1+1+1$, $4+2+2+1$, $3+2+2+2$, $3+2+2+1+1$, $3+2+1+1+1+1$, $2+2+2+2+1$, $2+2+2+1+1+1$, $2+2+1+1+\cdots+1$, $2+1+1+\cdots+1$.

4 Identities Stemming from Modulus 20

As is apparent by now, each section of this paper is devoted to some different outcome when extending Sylvester's three conditions to the interpretation of Slater's identities. In this section we begin with two of Slater's formulas that, upon inspection, suggest rather cumbersome partition identities. The modifications necessary to reduce the awkwardness again lead us to mock theta functions.

The identities in question are Slater's (44) and (46) [16, p. 156] slightly rewritten:

$$\sum_{n\geq 0} \frac{q^{1+1+2+3+3+\cdots+(2n-1)+(2n-1)+2n+(2n+1)}(-q^{2n+3};q^2)_\infty}{(q)_{2n+1}} = q \prod_{\substack{n=1\\ n\not\equiv 0,\pm 2,\pm 4,\pm 6,10 \pmod{20}}}^{\infty} \frac{1}{1-q^n}. \tag{10}$$

and

$$\sum_{n\geq 0} \frac{q^{1+1+2+3+3+\cdots+(2n-3)+(2n-3)+(2n-2)+(2n-1)+2n}(-q^{2n+1};q^2)_\infty}{(q)_{2n}} = q \prod_{\substack{n=1\\ n\not\equiv 0,\pm 2,\pm 6,\pm 8,10 \pmod{20}}}^{\infty} \frac{1}{1-q^n}. \tag{11}$$

One can interpret (10) and (11) in the Sylvester manner, but, in doing so, condition (2) in the Sylvester constraints becomes quite complicated.

So instead we consider closely related series where the interpretations are more natural. Let

$$\sum_{n\geq 0} J_1(n)q^n := \sum_{n\geq 0} \frac{q^{1+1+2+3+3+4+\cdots+(2n-1)+(2n-1)+2n}(-q^{2n+1};q^2)_\infty}{(q)_{2n}} = \sum_{n\geq 0} \frac{q^{3n^2+n}(-q^{2n+1};q^2)_\infty}{(q)_{2n}}. \tag{12}$$

and

$$\sum_{n\geq 0} J_2(n)q^n := \sum_{n\geq 0} \frac{q^{1+1+2+3+3+4+\cdots+2n+(2n+1)+(2n+1)}(-q^{2n+3};q^2)_\infty}{(q)_{2n+1}} = \sum_{n\geq 0} \frac{q^{3n^2+5n+2}(-q^{2n+3};q^2)_\infty}{(q)_{2n+1}}. \tag{13}$$

Now $J_1(n)$ and $J_2(n)$ may be viewed as enumerating partitions that mix "partitions with initial 2-repetitions" with "partitions without gaps."

Namely, $J_1(n)$ is the number of partitions of n in which (1) all odd integers smaller than the largest even part appear at least twice, (2) even parts appear without gaps, and (3) odd parts larger than the largest even part are distinct.

The formulation of $J_2(n)$ is even more straightforward. $J_2(n)$ is the number of partitions of n in which (1) each odd integer smaller than a repeated odd part is a repeated odd part and (2) every even integer smaller than the largest repreated odd part is a part, and (3) there are no other even parts.

Theorem 8.

$$\sum_{n\geq 0} J_1(n)q^n = \frac{1}{\psi(-q)}\sum_{n=0}^{\infty} q^{4n^2+2n}(1-q^{4n+2}) \sum_{j=-\lfloor \frac{n}{2}\rfloor}^{\lfloor \frac{n}{2}\rfloor} (-1)^j q^{-6j^2+2j} \tag{14}$$

and

$$\sum_{n\geq 0} J_2(n)q^n = \frac{q^2}{\psi(-q)}\sum_{n=0}^{\infty} q^{4n^2+6n}(1-q^{4n+4}) \sum_{j=-\lfloor \frac{n}{2}\rfloor}^{\lfloor \frac{n+1}{2}\rfloor} (-1)^j q^{-6j^2+2j} \tag{15}$$

where

$$\psi(q) := \sum_{n=0}^{\infty} q^{n(n+1)/2}. \tag{16}$$

Proof. Using representations (12) and (13) we see that (14) and (15) are equivalent to the following assertions:

$$\sum_{n=0}^{\infty} \frac{q^{3n^2+n}}{(q^2;q^2)_n(q^2;q^4)_n} = \frac{1}{(q^2;q^2)_\infty}\sum_{n=0}^{\infty} q^{4n^2+2n}(1-q^{4n+2}) \sum_{|2j|\leq n} (-1)^j q^{-6j^2+2j} \tag{17}$$

and

$$\sum_{n=0}^{\infty} \frac{q^{3n^2+5n}}{(q^2;q^2)_n(q^2;q^4)_{n+1}} = \frac{1}{(q^2;q^2)_\infty}\sum_{n=0}^{\infty} q^{4n^2+6n}(1-q^{4n+4}) \sum_{-n\leq 2j\leq n+1} (-1)^j q^{-6j^2+2j}. \tag{18}$$

Identities (17) and (18) may be reduced to Bailey pair identities following the use of the strong form of Bailey's Lemma [3, p. 270]. In the case of (17) we replace q by q^2 in Bailey's Lemma and set $a = q^2$. In the case of (18) we replace q by q^2 in Bailey's Lemma and set $a = 1$. If we then invoke the weak form of Bailey's Lemma [4, p. 27, Eq. (3.33)] we see that (17) and (18) are equivalent to the assertions (27) and (28) below.

Let

$$a_1(n,q) = \sum_{j=0}^{n} \frac{(q^{-n};q)_j(q^{n+1};q)_j q^{\binom{j+1}{2}}}{(q;q)_j(q;q^2)_j}, \tag{19}$$

$$a_2(n,q) = \sum_{j=1}^{n} \frac{(q^{-n};q)_j(q^{n};q)_j q^{\binom{j+1}{2}}}{(q;q)_{j-1}(q;q^2)_j}, \tag{20}$$

$$a_3(n,q) = \sum_{j=0}^{n} \frac{(q^{-n};q)_j(q^{n};q)_j q^{\binom{j+1}{2}}}{(q;q)_j(q;q^2)_j}. \tag{21}$$

Our proof relies on proving the following three identities. This in the spirit of the method developed at length in [6].

$$a_1(n,q) + q^n a_1(n-1,q) = (1+q^n)a_3(n,q), \tag{22}$$

$$q^n a_2(n,q) - (1-q^n)a_1(n,q) = -(1-q^n)a_3(n,q), \tag{23}$$

$$a_3(n,q) = \begin{cases} 0 & \text{if } n \text{ is odd} \\ (-1)^\nu q^{-\nu^2} & \text{if } n = 2\nu. \end{cases} \tag{24}$$

First we prove (22).

$$\begin{aligned} a_1(n,q) + q^n a_1(n-1,q) &= \sum_{j=0}^{n} \frac{(q^{-n+1};q)_{j-1}(q^{n+1};q)_{j-1} q^{\binom{j+1}{2}}}{(q;q)_j (q;q^2)_j} \\ &\quad \times \left\{(1-q^{-n})(1-q^{n+j}) + q^n(1-q^{-n+j})(1-q^n)\right\} \\ &= (1+q^n)\sum_{j=0}^{n} \frac{(q^{-n};q)_j (q^n;q)_j q^{\binom{j+1}{2}}}{(q;q)_j (q;q^2)_j} \\ &= (1+q^n)a_3(n,q). \end{aligned}$$

Next we treat (23).

$$\begin{aligned} a_2(n,q) - (1-q^n)a_1(n,q) &= \sum_{j\ge 0} \frac{(q^{-n};q)_j (q^n;q)_j q^{\binom{j+1}{2}}}{(q;q)_j (q;q^2)_j} \Big((1-q^j) - (1-q^{n+j})\Big) \\ &= -(1-q^n)\sum_{j\ge 0} \frac{(q^{-n};q)_j (q^n;q)_j q^{\binom{j+1}{2}+j}}{(q;q)_j (q;q^2)_j} \\ &= -(1-q^n)\sum_{j\ge 0} \frac{(q^{-n};q)_j (q^n;q)_j q^{\binom{j+1}{2}} \big(1-(1-q^j)\big)}{(q;q)_j (q;q^2)_j} \\ &= -(1-q^n)a_3(n,q) + (1-q^n)a_2(n,q), \end{aligned}$$

which is equivalent to (23).

Finally we move to (24) using the notation of [8, p. 4] and invoking [8, p. 242, Eq. III.13].

$$\begin{aligned} a_3(n,q) &= \lim_{\tau\to 0} {}_3\phi_2\left(\begin{matrix} q^{-n}, q^n, -\frac{q}{\tau}; q, \tau \\ q^{\frac12}, -q^{\frac12} \end{matrix}\right) \\ &= \frac{1}{(-q^{\frac12};q)_n} \lim_{\tau\to 0} {}_3\phi_2\left(\begin{matrix} q^{-n}, -\frac{q}{\tau}, q^{\frac12-n}; q, q \\ q^{\frac12}, \frac{q^{\frac32-n}}{\tau} \end{matrix}\right) \end{aligned}$$

$$= \frac{1}{(-q^{\frac{1}{2}};q)_n} {}_2\phi_1\left(\begin{matrix} q^{-n}, q^{\frac{1}{2}-n}; q, -q^{\frac{1}{2}+n} \\ q^{\frac{1}{2}} \end{matrix}\right)$$

$$= \begin{cases} 0 & \text{if } n \text{ is odd} \\ (-1)^\nu q^{-\nu^2} & \text{if } n = 2\nu, \end{cases}$$

where the final line follows from the q-analog of Kummer's theorem [8, p. 236, Eq. (II.9)].

From (22) to (24) it is clear that each of $a_1(n,q)$, $a_2(n,q)$ and $a_3(n,q)$ is recursively defined as a Laurent polynomial in q. It is then a straightforward matter to show via mathematical induction that

$$a_1(n,q) = \begin{cases} -q^n a_1(n-1,q) & \text{if } n \text{ odd} \\ q^{\binom{n+1}{2}} \sum_{j=-\nu}^{\nu} (-1)^j q^{-j(3j+1)} & \text{if } n = 2\nu. \end{cases} \tag{25}$$

$$a_2(n,q) = (1-q^n)(-1)^n q^{\binom{n}{2}} \sum_{j=-\lfloor \frac{n}{2} \rfloor}^{\lfloor \frac{n-1}{2} \rfloor} (-1)^j q^{-j(3j+1)}. \tag{26}$$

Equating (19) and (25) are equivalent to the assertion that

$$\begin{cases} \alpha_n = \frac{(-1)^n q^{n^2-n}(1-q^{4n+2})}{(1-q^2)} a_1(n,q^2) \\ \beta_n = \frac{q^{n^2-n}}{(q^2;q^2)_n (q^2;q^4)_n} \end{cases} \tag{27}$$

are a Bailey pair (where $q \to q^2$ and $a = q^2$) (see [3] especially Bailey's Lemma on page 270 and Eq. (4.1) on page 278). We note that this Bailey pair can also be deduced from the more general Bailey pair given by Lovejoy [12, p. 1510, Eqs. (2.4) and (2.5)]. We may now insert this Bailey pair into the weak form of Bailey's Lemma [4, p. 27, Eq. (3.33)] with $q \to q^2$, $a = q^2$], and then (25) and simplification yields (17).

Equations (20) and (26) are equivalent to the assertion that

$$\begin{cases} \overline{\alpha}_n = (-1)^n q^{n^2-n}(1+q^{2n}) a_2(n,q) \\ \overline{\beta}_n = \frac{q^{n^2-n}(1-q^{2n})}{(q^2;q^2)_n (q^2;q^4)_n} \end{cases} \tag{28}$$

are a Bailey pair (with $q \to q^2$, $a = 1$) [3, pp. 270 and 278]. We may now insert this Bailey pair into the weak form of Bailey's Lemma [4, p. 27, Eq. (3.33) with $q \to q^2$, $a = 1$]; then (26) and simplification yields (18). □

Notice that our starting position in this section, namely (12) and (13) (inspired by (10) and (11)) landed us in the world of Hecke-type series immediately. So what will happen when we reverse the roles of evens and odds? We define

$$\sum_{n\geq 0} K_1(n)q^n := \sum_{n\geq 0} \frac{q^{1+2+2+3+4+4+\cdots+2n+2n+(2n+1)}(-q^{2n+2};q^2)_\infty}{(q)_{2n+1}}$$
$$= \sum_{n\geq 0} \frac{q^{3n^2+4n+1}(-q^{2n+2};q^2)_\infty}{(q)_{2n+1}}, \qquad (29)$$

and

$$\sum_{n\geq 0} K_2(n)q^n := \sum_{n\geq 0} \frac{q^{1+2+2+3+\cdots+2n+2n}(-q^{2n+2};q^2)_\infty}{(q)_{2n}}$$
$$= \sum_{n\geq 0} \frac{q^{3n^2+2n}(-q^{2n+2};q^2)_\infty}{(q)_{2n}}. \qquad (30)$$

We shall not formally provide the partition-theoretic interpretations of $K_1(n)$ and $K_2(n)$ because they are identical with those of $J_1(n)$ and $J_2(n)$ respectively where the roles of odds and evens have been exchanged.

Theorem 9.

$$\sum_{n\geq 0} K_1(n)(-q)^n = \frac{1}{(-q;q^2)_\infty(q^2;q^5)_\infty(q^3;q^5)_\infty} - \sum_{n=0}^{\infty} K_2(n)(-q)^n, \qquad (31)$$

and

$$\sum_{n\geq 0} K_2(n)q^n = \frac{1}{\phi(-q^2)} \sum_{n\geq 0} q^{4n^2+2n}(1-q^{4n+2}) \sum_{j=-n}^{n} (-1)^j(-q)^{-j(3j-1)/2}, \qquad (32)$$

with $\phi(q) = \sum_{n=-\infty}^{\infty} q^{n^2}$.

Proof. Using representations (29) and (30) we see that (31) and (32) are equivalent to the following assertions.

$$\sum_{n\geq 0} \frac{q^{3n^2+4n+1}}{(q;q)_{2n+1}(-q^2;q^2)_n}$$
$$= \frac{1}{(q^2;q^2)_\infty}\left(\sum_{n=-\infty}^{\infty} (-1)^n(-q)^{n(5n+3)/2}\right) - \sum_{n=0}^{\infty} \frac{q^{3n^2+2n}}{(q;q)_{2n}(-q^2;q^2)_n}. \qquad (33)$$

$$\sum_{n\geq 0} \frac{q^{3n^2+2n}}{(q;q)_{2n}(-q^2;q^2)_n}$$
$$= \frac{1}{(q^2;q^2)_\infty} \sum_{n=0}^{\infty} q^{4n^2+2n}(1-q^{4n+2}) \sum_{j=-n}^{n} (-1)^j(-q)^{-j(3j-1)/2}. \qquad (34)$$

Identities (33) and (34) may be reduced to Bailey pair identities following the use of the strong form of Bailey's Lemma [3, p. 270]. For both (33) and (34) we replace q by q^2 in Bailey's Lemma and set $a = q^2$. If we then invoke the weak form of Bailey's Lemma [4, p. 27, Eq. (3.33)] we see (33) and (34) are equivalent to the assertions (45) and (46) below.

Let

$$A_1(n,q) = \sum_{j=0}^{n} \frac{(q^{-2n};q^2)_j (q^{2n+2};q^2)_j q^{j^2+4j+1}}{(q;q)_{2j+1}(-q^2;q^2)_j}, \tag{35}$$

$$A_2(n,q) = \sum_{j=0}^{n} \frac{(q^{-2n};q^2)_j (q^{2n+2};q^2)_j q^{j^2+2j}}{(q;q)_{2j}(-q^2;q^2)_j}, \tag{36}$$

$$A_3(n,q) = \sum_{j=0}^{n} \frac{(q^{-2n};q^2)_j (q^{2n+2};q^2)_j q^{j^2+2j}}{(q;q)_{2j+1}(-q^2;q^2)_j}, \tag{37}$$

$$A_4(n,q) = \sum_{j=0}^{n} \frac{(q^{-2n};q^2)_j (q^{2n};q^2)_j q^{j^2+2j}}{(q;q)_{2j}(-q^2;q^2)_j}. \tag{38}$$

Our proof requires the following identities.

$$A_3(n,q) - A_1(n,q) = A_2(n,q), \tag{39}$$

$$A_2(n,q) + q^{2n} A_2(n-1,q) = (1+q^{2n}) A_4(n,q), \tag{40}$$

$$A_3(n,q) = \frac{(-q)^{-\binom{n}{2}}}{1-q^{2n+1}}, \tag{41}$$

$$A_4(n,q) = \frac{(-q)^{-\binom{n}{2}}(1+(-q)^n)}{1+q^{2n}}. \tag{42}$$

First we prove (39).

$$\begin{aligned} A_3(n,q) - A_1(n,q) &= \sum_{j=0}^{n} \frac{(q^{-2n};q^2)_j (q^{2n+2};q^2)_j q^{j^2+2j}(1-q^{2j+1})}{(q;q)_{2j+1}(-q^2;q^2)_j} \\ &= \sum_{j=0}^{n} \frac{(q^{-2n};q^2)_j (q^{2n+2};q^2)_j q^{j^2+2j}}{(q;q)_{2j}(-q^2;q^2)_j} = A_2(n,q). \end{aligned}$$

Next comes (40).

$$\begin{aligned} &A_2(n,q) + q^{2n} A_2(n-1,q) \\ &\qquad = \sum_{j\geq 0} \frac{(q^{-2n+2};q^2)_{j-1} (q^{2n+2};q^2)_{j-1} q^{j^2+2j}}{(q;q)_{2j}(-q^2;q^2)_j} \end{aligned}$$

$$\times \left\{(1-q^{2n})(1-q^{2n+2j}) + q^{2n}(1-q^{-2n+2j})(1-q^{2n})\right\}$$

$$= (1+q^{2n}) \sum_{j\geq 0} \frac{(q^{-2n};q^2)_j (q^{2n};q^2)_j q^{j^2+2j}}{(q;q)_{2j}(-q^2;q^2)_j}$$

Now we treat (41) using the notation of [8, p. 4].

$$A_3(n,q) = \frac{1}{1-q} \lim_{\tau\to 0} {}_3\phi_2\left(\begin{matrix} q^{-2n}, q^{2n+2}, -\frac{q}{\tau}; q^2, q^2\tau \\ q^3, -q^2 \end{matrix}\right)$$

$$= \frac{1}{(q;q^2)_{n+1}} \lim_{\tau\to 0} {}_3\phi_2\left(\begin{matrix} q^{-2n}, -\frac{q}{\tau}, -q^{-2n}; q^2, q^2 \\ -q^2, -\frac{q^{2n}}{\tau} \end{matrix}\right)$$

by Gasper and Rahman [8, p. 242, Eq. (III.13)]

$$= \frac{1}{(q;q^2)_{n+1}} {}_2\phi_1\left(\begin{matrix} q^{-2n}, -q^{2n}; q^2, q^{2n+3} \\ -q^2 \end{matrix}\right)$$

$$= \frac{1}{(q;q^2)_{n+1}} \sum_{j=0}^{n} \frac{(q^{-4n};q^4)_j q^{(2n+3)j}}{(q^4;q^4)_j}$$

$$= \frac{(q^{3-2n};q^4)_n}{(q;q^2)_{n+1}} = \frac{(-q)^{-\binom{n}{2}}}{1-q^{2n+1}},$$

where the penultimate assertion follows from [8, p. 236, Eq. (II.7)].

Finally we treat the fourth identity (42).

$$A_4(n,q) = \lim_{\tau\to 0} {}_3\phi_2\left(\begin{matrix} q^{-2n}, q^{2n}, -\frac{q}{\tau}; q^2, q^2\tau \\ -q^2, q \end{matrix}\right)$$

$$= \frac{1}{(q;q^2)_n} {}_2\phi_1\left(\begin{matrix} q^{-2n}, -q^{2-2n}; q^2, q^{1+2n} \\ -q^2 \end{matrix}\right)$$

by Gasper and Rahman [8, p. 241, Eq. (III.9)]

$$= \frac{1}{(q;q^2)_n} \sum_{j=0}^{n} \frac{(q^{4-4n};q^4)_{j-1}(1-q^{-2n})(1+q^{-2n+2j})q^{j(1+2n)}}{(q^4;q^4)_j}$$

$$= \frac{1}{(q;q^2)_n(1+q^{-2n})} \sum_{j=0}^{n} \frac{(q^{-4n};q^4)_j}{(q^4;q^4)_j} \left(q^{j(1+2n)} + q^{-2n+j(3+2n)}\right)$$

$$= \frac{q^{2n}}{(q;q^2)_n(1+q^{2n})} \left((q^{1-2n};q^4)_n + (q^{3-2n};q^4)_n\right)$$

$$= \frac{(-q)^{-\binom{n}{2}}(-q)^n}{1+q^{2n}} + \frac{(-q)^{-\binom{n}{2}}}{1+q^{2n}}$$

$$= (-q)^{-\binom{n}{2}} \frac{(1+(-q)^n)}{1+q^{2n}},$$

as desired.

From (39) to (42), it follows by mathematical induction that

$$A_1(n,q) = -q^{n^2+n}(-1)^n \sum_{j=-n}^{n} (-1)^j (-q)^{-j(3j-1)/2} + \frac{(-q)^{-\frac{n(n-1)}{2}}}{1-q^{2n+1}}, \tag{43}$$

$$A_2(n,q) = (-1)^n q^{n^2+n} \sum_{j=-n}^{n} (-1)^j (-q)^{-j(3j-1)/2}. \tag{44}$$

Let us treat (32) or rather its equivalent formulation (34) first. Identity (44) is equivalent to the assertion that

$$\begin{cases} \alpha'_n = \frac{q^{2n^2}(1-q^{4n+2})}{(1-q^2)} \sum_{j=-n}^{n} (-1)^j (-q)^{-j(3j-1)/2} \\ \beta'_n = \frac{q^{n^2}}{(q;q)_{2n}(-q^2;q^2)_n} \end{cases} \tag{45}$$

are a Bailey pair (where $q \to q^2$ and $a = q^2$). It should be noted that this Bailey pair was found earlier by A. Patkowski in [13]. Inserting this Bailey pair into the weak form of Bailey's Lemma, we obtain (34) by invoking (44) and simplifying.

As for (31), or rather its equivalent formulation (33), we see from (43) and (44) that

$$\begin{cases} \alpha''_n = -\alpha'_n + \frac{(-1)^n(-q)^{\binom{n}{2}}(1+q^{2n+1})}{(1-q^2)} \\ \beta''_n = \frac{q^{n^2+2n+1}}{(q;q)_{2n+1}(-q^2;q^2)_n} \end{cases} \tag{46}$$

form a Bailey pair. Furthermore

$$\begin{aligned} \sum_{n\geq 0} K_1(n)q^n &= \sum_{n=0}^{\infty} q^{2n^2+2n}\beta''_n \\ &= \frac{1}{(q^4;q^2)_\infty} \sum_{n=0}^{\infty} q^{2n^2+2n}\alpha''_n \\ &= \frac{1}{(q^4;q^2)_\infty} \sum_{n=0}^{\infty} q^{2n^2+2n} \left(-\alpha'_n + \frac{(-1)^n(-q)^{\binom{n}{2}}(1+q^{2n+1})}{1-q^2} \right) \\ &= -\sum_{n\geq 0} K_2(n)q^n + \frac{1}{(q^2;q^2)_\infty} \sum_{n=-\infty}^{\infty} (-1)^n(-q)^{\frac{5n^2}{2}+\frac{3n}{2}}, \end{aligned}$$

and invoking Jacobi's triple product identity [2, Theorem 2.8, p. 21], we see that (33) is established. □

5 Identities of Modulus 12

As is obvious by now, we are choosing a variety of examples from Slater's compendium to illustrate the variety that arises when we mix parity with the Sylvester constraints. We close our presentation with a move beyond parity to conditions modulo 4.

Recall that *evenly even* numbers are numbers divisible by 4 while *oddly even* numbers are numbers congruent to 2 modulo 4.

We shall examine Slater's (53) and (55) [16, p. 157].

$$\prod_{\substack{n=1 \\ n\equiv \pm 1,\pm 3,\pm 4 \pmod{12}}} \frac{1}{1-q^n} = \sum_{n\geq 0} \frac{q^{4n^2}}{(q^4;q^4)_{2n}(q^{4n+1};q^2)_\infty} \tag{47}$$

$$= \frac{1}{(q;q^2)_\infty} + \frac{q^{2+2}}{(1-q^{2+2})(1-q^{4+4})(q^5;q^2)_\infty} + \frac{q^{2+2+6+6}}{(1-q^{2+2})(1-q^{4+4})(1-q^{6+6})(1-q^{8+8})(q^9;q^2)_\infty} + \cdots$$

and

$$\prod_{\substack{n=1 \\ n\equiv \pm 3,\pm 4,\pm 5 \pmod{12}}} \frac{1}{1-q^n} \tag{48}$$

$$= \sum_{n\geq 0} \frac{q^{4n^2+4n}}{(q^4;q^4)_{2n+1}(q^{4n+3};q^2)_\infty}$$

$$= \frac{1}{(1-q^{2+2})(q^3;q^2)_\infty} + \frac{q^{4+4}}{(1-q^{2+2})(1-q^{4+4})(1-q^{6+6})(q^7;q^2)_\infty} + \frac{q^{4+4+8+8}}{(1-q^{2+2})(1-q^{4+4})(1-q^{6+6})(1-q^{8+8})(1-q^{10+10})(q^{11};q^2)_\infty} + \cdots .$$

In both (47) and (48), the extended final forms are given so that the following theorems are immediately interpreted from these forms.

Theorem 10. *Let* $L_1(n)$ *denote the number of partitions of* n *into parts that are* $\equiv \pm 1, \pm 3, \pm 4 \pmod{12}$. *Let* $T_1(n)$ *denote the number of partitions of* n *in which (1) all* *even parts must appear an even number of times, (2) each oddly even integer not exceeding the largest even part must appear, (3) each odd part is at least 3 greater than each oddly even part. Then for* $n \geq 0$,

$$L_1(n) = T_1(n).$$

For example, the 20 partitions enumerated by $T_1(13)$ are 13, $11+1+1$, $9+3+1$, $9+2+2$, $9+1+1+1+1$, $7+5+1$, $7+3+3$, $7+3+1+1+1$, $7+1+1+\cdots+1$, $5+5+3$, $5+5+1+1+1$, $5+3+3+1+1$, $5+3+1+\cdots+1$, $5+2+2+\cdots+2$, $5+1+1+\cdots+1$, $3+3+3+3+1$, $3+3+3+1+1+1+1$, $3+3+1+1+\cdots+1$, $3+1+1+\cdots+1$, $1+1+\cdots+1$, and the 20 partitions enumerated by $L_1(13)$ are 13, $11+1+1$, $9+4$, $9+3+1$, $9+1+1+1+1$, $8+4+1$, $8+3+1+1$, $8+1+1+\cdots+1$, $4+4+4+1$, $4+4+3+1+1$, $4+4+1+1+\cdots+1$, $4+3+3+3$, $4+3+3+1+1+1$, $4+3+1+1+\cdots+1$, $4+1+1+\cdots+1$, $3+3+3+3+1$, $3+3+3+1+1+1+1$, $3+3+1+1+\cdots+1$, $3+1+1+\cdots+1$, $1+1+\cdots+1$,

Theorem 11. *Let* $L_2(n)$ *denote the number of partitions of* n *into parts that are* $\equiv \pm 3, \pm 4, \pm 5 \pmod{12}$. *Let* $T_2(n)$ *denote the number of partitions of* n *in which (1) all even parts must appear an even number of times, (2) each evenly even integer not exceeding the largest even part must appear as a part, (3) each odd part is larger than 1 and at least 3 larger than the largest evenly even part. Then for* $n \geq 0$,

$$L_2(n) = T_2(n).$$

For example the 10 partitions enumerated by $L_2(15)$ are 15, $9+3+3$, $8+7$, $8+4+3$, $7+5+3$, $7+4+4$, $5+5+5$, $5+4+3+3$, $4+4+4+3$, $3+3+3+3+3$, and the 10 partitions enumerated by $T_2(15)$ are 15, $11+2+2$, $9+3+3$, $7+5+3$, $7+4+4$, $7+2+2+2+2$, $5+5+5$, $5+3+3+2+2$, $3+3+3+3+3$, $3+2+2+\cdots+2$.

6 Conclusion

This paper is in no way meant to be exhaustive. Indeed we have chosen a handful of Slater's identities for consideration. The examples were chosen to illustrate the variety of possible outcomes.

There are many further formulas in Slater's paper [16] that can be interpreted using the approach we have developed. Indeed this can be done for the original Rogers-Ramanujan identities [14, pp. 133–134 (14)–(18)] and also for variants on the Rogers-Ramanujan identities (cf. Slater's (15), (16), (19), (20) and (25)). Others like the modulus 6 results (Slater's (22)–(30)) are either quite classical (e.g. (23) is effectively due to Euler) or seem to require some alternative analysis. The identities with modulus 27 (Slater's (88)–(93)) seem quite distant from these developments as do those identities like (97), or (101)–(112), or (125)–(130) that apparently are not reducible to a single product.

It would certainly be interesting to determine if there is an alternative to Sylvester's constraints that leads to explanations of further Slater identities that could not be treated here.

It is interesting to note that in each case where a Slater identity was modified to fit the Sylvester paradigm, the resulting infinite product was always of the nicest form imaginable, namely

$$\prod_{n=1}^{\infty}{}' \frac{1}{1-q^n}$$

where the $'$ indicates only that the n are restricted to a specified set of arithmetic progressions.

Finally the relation of (33) to the original Rogers-Ramanujan function is striking. Indeed one can provide an alternative proof of (33) by adding together the left-hand sides of (33) and (34) and proving (slightly non-trivially) that the result is, in fact, Slater's (15) [16, p. 153] with q replaced by $-q$.

In fact, it is possible to prove that, instead of (33),

$$\sum_{n=0}^{\infty} \frac{q^{3n^2+4n+1}}{(q;q)_{2n+1}(-q^2;q^2)_n} = \frac{1}{(q^2;q^2)_\infty} \sum_{n=0}^{\infty} q^{4n^2-2n}(1-q^{12n+6}) \sum_{j=-n}^{n} (-1)^j (-q)^{-j(3j-1)/2}. \quad (49)$$

In addition

$$\sum_{n=0}^{\infty} \frac{q^{3n^2}}{(q;q)_{2n}(-q^2;q^2)_n} = \frac{1}{(q^2;q^2)_\infty} \sum_{n=0}^{\infty} q^{4n^2}(1-q^{8n+4}) \sum_{j=-n}^{n} (-1)^j (-q)^{-j(3j-1)/2}. \quad (50)$$

If we denote the left-hand side of (50) by $T(q)$, then Slater's (19) [16, p. 154] asserts

$$T(-q) = \frac{(q^2;q^5)_\infty (q^3;q^5)_\infty (q^5;q^5)_\infty}{(q^2;q^2)_\infty} \quad (51)$$

Identities of this nature combined with the results in Sect. 4 suggest a variety of new Hecke-type series results related to the Rogers-Ramanujan identities.

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Hypergeometric Identities Associated with Statistics on Words

George E. Andrews*, **Carla D. Savage, and Herbert S. Wilf**

From the first two authors to the third in honor of his 80th birthday, in memory of his friendship, and in tribute to his mathematics.

Abstract We show how combinatorial arguments involving a variety of statistics on words can produce nontrivial identities between hypergeometric series in two variables. We establish relationships to the Rogers-Fine identity, Heine's second transformation, and mock theta functions. Finally, we show that any hypergeometric series of a certain form can be interpreted in terms of generalized statistics on words.

Keywords Hypergeometric series • Statistics on words

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1 Introduction

The purpose of this note is to show how combinatorial arguments can produce nontrivial identities between hypergeometric q-series in two variables. This will be illustrated by using as examples

1. The major index of a binary word
2. The Durfee square size of an integer partition
3. The number of inversions in a binary word
4. The number of descents in a binary word
5. The sum of the positions of the 0's in a bitstring
6. "Lecture hall" statistics on words.

Let w be a word of length n over the alphabet $\{0, 1\}$ (a *binary word*). By the *major index* of w we mean the sum of those indices j, $1 \leq j \leq n-1$, for which $w_j > w_{j+1}$, i.e., for which $w_j = 1$ and $w_{j+1} = 0$. Let $f(n,m)$ denote the number of binary words of length n whose major index is m ($f(0,0) = 1$). In Sects. 2 and 3, we find the generating function $F(x,q) = \sum_{n,m} f(n,m)x^n q^m$ in various ways, compare it to the known Mahonian form of this function, and thereby obtain an interesting chain of seven equalities, namely

$$F(x,q) \stackrel{\text{def}}{=} \sum_{n,m \geq 0} f(n,m)x^n q^m \tag{1}$$

$$= \sum_{n,k \geq 0} \begin{bmatrix} n \\ k \end{bmatrix}_q x^n \tag{2}$$

$$= \sum_{n \geq 0} \frac{x^n}{(x;q)_{n+1}} \tag{3}$$

$$= -1 + \sum_{j \geq 0} (1 + (1-2x)q^j) \left(\frac{x^j q^{\binom{j}{2}}}{(x;q)_{j+1}} \right)^2 \tag{4}$$

$$= \sum_{j \geq 0} \left(\frac{x^j q^{j^2/2}}{(x,q)_{j+1}} \right)^2 \tag{5}$$

$$= 1 + \sum_{j \geq 0} \frac{x^{j+1}(1+q^j)}{(x;q)_{j+1}} \tag{6}$$

$$= 1 + 2x + (3+q)x^2 + (4 + 2q + 2q^2)x^3 + \dots . \tag{7}$$

in which the $[\ ]_q$'s are the Gaussian binomial coefficients.

In Sect. 2.5 we highlight the connections between $F(x,q)$ and some third order mock theta functions.

Section 4 deals with words over larger alphabets. In Sect. 5, a related identity is derived by considering the positions of 0's in a bitstring. In Sect. 6 we look at identities arising from some novel statistics on words. In Sect. 7, we consider the process of deriving the generating function $F(x,q) = \sum_{n,k\geq 0} t(n,k)x^n q^k$ when a nice product form for the q-series $\sum_{k\geq 0} t(n,k)q^k$ is known. We show in this case how $F(x,q)$ can be expressed in terms of statistics on words.

2 The Equivalence of (1) Through (5)

For a binary word w of length n, the *blocks* of w are the maximal contiguous subwords whose letters are all the same. The word $w = 11011000$, for example, contains four blocks, namely 11, 0, 11, 000, of lengths 2, 1, 2, 3. The major index of w is then the sum of the indices of the final letters of the blocks of 1's, excepting only a terminal block of 1's. The word w above has major index $2+5=7$.

2.1 *Proof of (1) = (2)*

This follows from MacMahon's result [8] that

$$\begin{bmatrix} n \\ k \end{bmatrix}_q = \sum_w q^{\mathrm{maj}(w)},$$

where the sum is over all binary words w with k ones and $n-k$ zeroes. We refer to (2) as the *Mahonian* form of $F(x,q)$.

2.2 *Proof of (3)*

2.2.1 Via Generatingfunctionology

The q-binomial coefficients satisfy the recurrence

$$\begin{bmatrix} n+1 \\ k \end{bmatrix}_q = q^k \begin{bmatrix} n \\ k \end{bmatrix}_q + \begin{bmatrix} n \\ k-1 \end{bmatrix}_q \qquad (n \geq 0).$$

Let's find their vertical generating function

$$\phi_k(t) \stackrel{\text{def}}{=} \sum_{n\geq 0} t^n \begin{bmatrix} n \\ k \end{bmatrix}_q \qquad (k = 0, 1, 2, \ldots).$$

We find that

$$(1 - tq^k)\phi_k(t) = t\phi_{k-1}(t) \qquad (k \geq 1; \phi_0(t) = 1/(1-t)),$$

and therefore

$$\phi_k(t) = \frac{t^k}{\prod_{j=0}^{k}(1 - tq^j)} \qquad (k = 0, 1, 2, \ldots).$$

Next, the horizontal generating function (= the Gaussian polynomial)

$$\psi_n(x) \stackrel{\text{def}}{=} \sum_{k\geq 0} \begin{bmatrix} n \\ k \end{bmatrix}_q x^k$$

satisfies

$$\psi_{n+1}(x) = \psi_n(qx) + x\psi_n(x) \qquad (n \geq 0; \psi_0 = 1).$$

If we introduce the two variable generating function $\Phi(t, x) = \sum_{n,k\geq 0} \left[\begin{smallmatrix} n \\ k \end{smallmatrix}\right]_q t^n x^k$, then we find that

$$\Phi(t, x)(1 - xt) = t\Phi(t, qx) + 1,$$

which leads to

$$\Phi(t, x) \stackrel{\text{def}}{=} \sum_{n,k\geq 0} \begin{bmatrix} n \\ k \end{bmatrix}_q t^n x^k = \sum_{n\geq 0} \frac{t^n}{\prod_{j=0}^{n}(1 - q^j xt)},$$

as required.

2.2.2 Via *q*-Series

In [2, Theorem 3.3], (3) is derived from (2) using Cauchy's Theorem [2, Theorem 2.1]:

$$\sum_{k\geq 0} \frac{(a; q)_k x^k}{(q; q)_k} = \prod_{k=0}^{\infty} \frac{(1 - axq^k)}{(1 - xq^k)},$$

with $a = q^{n+1}$, after setting $n = n + k$ in (2). In the process we have

$$\sum_{k\geq 0} \begin{bmatrix} n+k \\ k \end{bmatrix}_q x^k = \prod_{k=0}^{\infty} \frac{(1 - xq^{k+n+1})}{(1 - xq^k)} = \frac{1}{(x;q)_{n+1}}, \tag{8}$$

the q-binomial theorem.

2.3 *Proof of (1) = (4)*

To solve the word problem posed in Sect. 1, we split it into four cases, namely words with an even (resp. odd) number of blocks, the first of which is a block of 1's (resp. 0's). We will show all steps of the solution for the first case, and then merely exhibit the results for the other three cases.

Let's do the case of words w, of length n, which have an even number, $2k$, say, of blocks, the first of which is a block of 1's, and suppose that the lengths of these blocks are $a_1, a_2, \ldots, a_{2k}$ (all $a_i \geq 1$). Such a word has descents at the indices $a_1, a_1 + a_2 + a_3, \ldots, a_1 + a_2 + \cdots + a_{2k-1}$, so its major index is

$$\begin{aligned} \text{maj}(w) &= ka_1 + (k-1)a_2 + (k-1)a_3 + \cdots + a_{2k-2} + a_{2k-1} \\ &= \sum_{j=1}^{2k-1} a_{2k-j} \left\lceil \frac{j}{2} \right\rceil. \end{aligned}$$

Let Blocks(w) be the number of blocks of w. It follows that the contribution of all the words whose form is that of the first of the four cases is

$$\begin{aligned} F_1(x,q,t) &= \sum x^{|w|} q^{maj\,(w)} t^{\text{Blocks}(w)} \\ &= \sum_{k\geq 1} \sum_{a_1,\ldots,a_{2k}\geq 1} x^{\sum_{j=1}^{2k} a_j} q^{\sum_{j=1}^{2k-1} a_{2k-j} \lceil j/2 \rceil} t^{2k} \\ &= \sum_{k=1}^{\infty} \frac{x^{2k} q^{k^2} t^{2k}}{(1-x)(1-xq^k)\prod_{j=1}^{k-1}(1-xq^j)^2} \\ &= x^2t^2q + x^3\left(t^2q^2 + t^2q\right) + x^4\left(t^4q^4 + t^2q^3 + t^2q^2 + t^2q\right) + \ldots. \end{aligned}$$

Similarly, in the second case, where the number of blocks is even but the first block consists of 0's, we have

$$\begin{aligned}
F_2(x,q,t) &= \sum x^{|w|} q^{\mathrm{maj}(w)} t^{\mathrm{Blocks}(w)} \\
&= \sum_{k\geq 1} \sum_{a_1,\ldots,a_{2k}\geq 1} x^{\sum_{j=1}^{2k} a_j} q^{\sum_{j=2}^{2k-1} a_{2k-j}\lceil (j-1)/2\rceil} t^{2k} \\
&= \sum_{k\geq 1} \frac{x^{2k} q^{k(k-1)} t^{2k}}{\prod_{j=0}^{k-1}(1-xq^j)^2} \\
&= t^2x^2 + 2t^2x^3 + x^4(3t^2 + t^4q^2) + x^5(4t^2 + 2t^4q^2 + 2t^4q^3) + \ldots
\end{aligned}$$

In the third case the number of blocks is odd, say $2k+1$, with $k \geq 0$, and the first block is all 1's. The major index of such a word is

$$\mathrm{maj}(w) = \sum_{j=1}^{2k-1} a_{2k-j} \left\lceil \frac{j}{2} \right\rceil.$$

Thus,

$$\begin{aligned}
F_3(x,q,t) &= \sum x^{|w|} q^{\mathrm{maj}(w)} t^{\mathrm{Blocks}(w)} \\
&= \sum_{k\geq 0} \sum_{a_1,\ldots,a_{2k+1}\geq 1} x^{\sum_{j=1}^{2k+1} a_j} q^{\sum_{j=1}^{2k-1} a_{2k-j}\lceil j/2\rceil} t^{2k+1} \\
&= \sum_{k\geq 0} \frac{x^{2k+1} q^{k^2} t^{2k+1}}{(1-xq^k)\prod_{j=0}^{k-1}(1-xq^j)^2} \\
&= tx + tx^2 + x^3\left(qt^3 + t\right) + x^4\left(q^2t^3 + 2qt^3 + t\right) \\
&\quad + x^5\left(q^4t^5 + q^3t^3 + 2q^2t^3 + 3qt^3 + t\right) + \ldots
\end{aligned}$$

Finally, if there are $2k+1$ blocks in the word w and the first block is all 0's, the major index is

$$\mathrm{maj}(w) = \sum_{j=0}^{2k-1} a_{2k-j} \left\lceil \frac{j+1}{2} \right\rceil,$$

so

$$\begin{aligned}
F_4(x,q,t) &= \sum x^{|w|} q^{\mathrm{maj}(w)} t^{\mathrm{Blocks}(w)} \\
&= \sum_{k\geq 0} x^{\sum_{j=1}^{2k+1} a_j} q^{\sum_{j=0}^{2k-1} a_{2k-j}\left\lceil \frac{j+1}{2}\right\rceil} t^{2k+1}
\end{aligned}$$

$$= (1-x)\sum_{k\geq 0}\frac{x^{2k+1}q^{k(k+1)}t^{2k+1}}{\prod_{j=0}^{k}(1-xq^j)^2}$$
$$= tx + tx^2 + x^3\left(t^3y^2 + t\right) + x^4\left(2t^3y^3 + t^3y^2 + t\right)$$
$$+x^5\left(t^5y^6 + 3t^3y^4 + 2t^3y^3 + t^3y^2 + t\right) + \dots .$$

Now we compute the desired generating function $F(x,q,t)$ as

$$F(x,q,t) = 1 + \sum_{i=1}^{4} F_i(x,q,t)$$

in which the F_i are explicitly shown above. If we put $t = 1$ we find that

$$\sum x^{|w|}q^{\mathrm{maj}(w)} = 1 + 2x + x^2(q+3) + x^3\left(2q^2 + 2q + 4\right)$$
$$+x^4\left(q^4 + 3q^3 + 4q^2 + 3q + 5\right)$$
$$+x^5\left(2q^6 + 2q^5 + 6q^4 + 6q^3 + 6q^2 + 4q + 6\right) + \dots$$

Observe that if we put $q := 1$, the coefficient of each x^n is indeed 2^n.

On the other hand, the maj statistic is well known to be Mahonian, which implies that its distribution function is

$$\sum_{w} x^{|w|}q^{\mathrm{maj}(w)} = \sum_{n,k}\begin{bmatrix} n \\ k \end{bmatrix}_q x^n,$$

in which the $\begin{bmatrix} n \\ k \end{bmatrix}_q$ are the usual Gaussian polynomials.

It follows that

$$\sum_{n,k\geq 0}\begin{bmatrix} n \\ k \end{bmatrix}_q x^n = 1 + F_1(x,q,1) + F_2(x,q,1) + F_3(x,q,1) + F_4(x,q,1)$$
$$= 1 + \sum_{k=1}^{\infty}\frac{x^{2k}q^{k^2}}{(1-x)(1-xq^k)\prod_{j=1}^{k-1}(1-xq^j)^2} + \sum_{k\geq 1}\frac{x^{2k}q^{k(k-1)}}{\prod_{j=0}^{k-1}(1-xq^j)^2}$$
$$+\sum_{k\geq 0}\frac{x^{2k+1}q^{k^2}}{(1-xq^k)\prod_{j=0}^{k-1}(1-xq^j)^2} + (1-x)\sum_{k\geq 0}\frac{x^{2k+1}q^{k(k+1)}}{\prod_{j=0}^{k}(1-xq^j)^2}$$
$$= 1 + \sum_{k\geq 1}\frac{x^{2k}q^{k^2}}{(x;q)_k^2}\left(\frac{1-x}{1-xq^k} + \frac{1}{q^k}\right)$$

$$+\sum_{k\geq 0}\frac{x^{2k+1}q^{k^2}}{(x;q)_k^2}\left(\frac{1}{1-xq^k}+\frac{(1-x)q^k}{(1-xq^k)^2}\right)$$

$$=-1+\sum_{k\geq 0}\frac{(1+(1-2x)q^k)}{(1-xq^k)^2}\left(\frac{x^kq^{\binom{k}{2}}}{(x;q)_k}\right)^2,$$

as claimed.

2.4 *Proof of (5)*

We prove (5) in four different ways.

2.4.1 Equivalence of (3) and (5) Using the Rogers-Fine Identity

The Rogers-Fine identity is [5], [4, p. 223]:

$$\sum_{n=0}^{\infty}\frac{(\alpha;q)_n}{(\beta;q)_n}\tau^n=\sum_{n=0}^{\infty}\frac{(\alpha;q)_n(\alpha\tau q/\beta;q)_n\beta^n\tau^nq^{n^2-n}(1-\alpha\tau q^{2n})}{(\beta;q)_n(\tau;q)_{n+1}}. \tag{9}$$

Setting $\alpha=0$, $\tau=x$, and $\beta=xq$ in (9) gives

$$\sum_{n=0}^{\infty}\frac{1}{(xq;q)_n}x^n=\sum_{n=0}^{\infty}\frac{x^{2n}q^{n^2}}{(xq;q)_n(x;q)_{n+1}}.$$

Multiply through by $1/(1-x)$ and use the equivalence of (1) and (3) to conclude

$$F(x,q)=\sum_{n=0}^{\infty}\frac{x^n}{(x;q)_{n+1}}=\sum_{n=0}^{\infty}\left(\frac{x^nq^{n^2/2}}{(x;q)_{n+1}}\right)^2.$$

In this form the generating function appears quite similar to, but not identical with (4), though it is of course identical. Consequently, by comparing the two forms, we see that we have proved the small identity

$$\sum_{k\geq 0}\left(\frac{x^kq^{\binom{k}{2}}}{(x,q)_{k+1}}\right)^2(1-2xq^k)=1.$$

We show in the following subsection how to transform (4) into (5).

2.4.2 Direct Proof of (4) = (5)

We would like to prove:

$$-1+\sum_{k\geq 0}(1+(1-2x)q^k)\left(\frac{x^k q^{\binom{k}{2}}}{(x;q)_{k+1}}\right)^2=\sum_{k\geq 0}\left(\frac{x^k q^{k^2/2}}{(x,q)_{k+1}}\right)^2.$$

Using the fact that

$$1+(1-2x)q^k = -x^2q^{2k}+(1-xq^k)(1-xq^k)+q^k,$$

we can transform as follows:

$$\begin{aligned}
-1+\sum_{k\geq 0}&(1+(1-2x)q^k)\left(\frac{x^k q^{\binom{k}{2}}}{(x;q)_{k+1}}\right)^2\\
&=-1-\sum_{k\geq 0}\frac{x^{2k+2}q^{k^2+k}}{(x;q)_{k+1}^2}+\sum_{k\geq 0}\frac{x^{2k}q^{k^2-k}}{(x;q)_k^2}+\sum_{k\geq 0}\frac{x^{2k}q^{k^2}}{(x;q)_{k+1}^2}\\
&=-1-\sum_{k\geq 1}\frac{x^{2k}q^{k^2-k}}{(x;q)_k^2}+\sum_{k\geq 0}\frac{x^{2k}q^{k^2-k}}{(x;q)_k^2}+\sum_{k\geq 0}\frac{x^{2k}q^{k^2}}{(x;q)_{k+1}^2}\\
&=\sum_{k\geq 0}\frac{x^{2k}q^{k^2}}{(x;q)_{k+1}^2}
\end{aligned}$$

2.4.3 Equivalence of (1) and (5) by Recurrence

As an alternative, we can derive (5) directly from the definition of $F(x,q)$ in terms of binary words.

Lemma 1. *Let $f(n,m)$ denote the number of binary words of length n whose major index is m. Then*

$$f(n,m)=2f(n-1,m)-f(n-2,m)+f(n-2,m-n+1)\qquad (n\geq 2; m\geq 0) \tag{10}$$

with initial conditions $f(0,m)=\delta_{m,0}$, $f(1,m)=2\delta_{m,0}$.

Proof. Let $S(n,m)$ be the set of binary words of length n with major index m, so that $f(n,m)=|S(n,m)|$. Let "·" denote concatenation of words and observe that

$$\begin{aligned}\operatorname{maj}(w\cdot 1) &= \operatorname{maj}(w),\\ \operatorname{maj}(w\cdot 10) &= \operatorname{maj}(w) + |w\cdot 1|,\\ \operatorname{maj}(w\cdot 00) &= \operatorname{maj}(w\cdot 0).\end{aligned}$$

Thus

$$\begin{aligned}w\cdot 1 \in S(n,m) &\leftrightarrow w \in S(n-1,m),\\ w\cdot 10 \in S(n,m) &\leftrightarrow w \in S(n-2,m-(n-1)),\\ w\cdot 00 \in S(n,m) &\leftrightarrow w\cdot 0 \in S(n-1,m) - S(n-2,m)\cdot 1.\end{aligned}$$

Since every element of $S(n,m)$ falls into exactly one of the cases above, the result follows. □

As in (1), we define the generating function $F(x,q) = \sum_{n,m\geq 0} f(n,m)x^n q^m$. Next we multiply each of the four terms in (10) by $x^n q^m$ and sum over $n \geq 2$ and $m \geq 0$.

The first term yields $F(x,q) - 2x - 1$, the second gives $2x(F(x,q) - 1)$, the third becomes $x^2 F(x,q)$, and the fourth yields $x^2 qF(xq,q)$. Therefore we have the functional equation

$$F(x,q) = \frac{1 + x^2 qF(xq,q)}{(1-x)^2},$$

whose solution is

$$F(x,q) = \sum_{j\geq 0} \frac{x^{2j} q^{j^2}}{\prod_{\ell=0}^{j}(1-xq^{\ell})^2}.$$

2.4.4 Equivalence of (2) and (5) via Partitions

We can also give a direct proof of the identity

$$\sum_{n,k\geq 0} \begin{bmatrix} n \\ k \end{bmatrix}_q x^n = \sum_{j\geq 0} \frac{x^{2j} q^{j^2}}{((x;q)_{j+1})^2},$$

using partitions. We'll see the value of this after we look at inversions in Sect. 3.

We show that both sides count, for every pair (a,b), the number of partitions λ in an $a \times b$ box, where q keeps track of $|\lambda| = \lambda_1 + \lambda_2 + \ldots + \lambda_a$ and x keeps track of $a + b$. The left-hand side counts all the partitions for fixed (a,b) and then sums over all (a, b). The right-hand side counts all the partitions with Durfee square size j, for every $(j+s)\times(j+t)$ box containing them, and then sums over all j.

Let $P(a, b)$ be the set of partitions whose Ferrers diagram fit in an $a \times b$ box. Let $D(\lambda)$ denote the size of the Durfee square of λ. The argument above actually shows that

$$\sum_{a,b,\geq 0}\sum_{\lambda\in P(a,b)} q^{\lambda} x^{a+b} z^{D(\lambda)} = \sum_{j\geq 0} \frac{x^{2j} q^{j^2}}{((x;q)_{j+1})^2} z^j.$$

We'll return to this at the end of Sect. 3.

2.5 Mock Theta Functions

It was observed in [3] that there is a connection between $F(x, q)$, defined by (1)–(7), and the following two of Ramanujan's third order mock theta functions ([11], cf. p. 62):

$$f(q) = \sum_{j\geq 0} \frac{q^{j^2}}{(-q,q)_j^2}; \tag{11}$$

$$\omega(q) = \sum_{j\geq 0} \frac{q^{2j^2+2j}}{(q,q^2)_{j+1}^2}. \tag{12}$$

Specifically, appealing to (5), note that

$$F(-1, q) = f(q)/4; \tag{13}$$

$$F(q, q^2) = \omega(q). \tag{14}$$

One of the goals of the paper [3] was to develop a methodology for interpreting q-series identities in terms of families of partitions, via an appropriate statistic. After deriving the equivalence of (5) and (3), the appropriate partition statistic was revealed for interpreting $F(x, q)$:

$$\frac{F(x,q)}{1-x} = \sum_{\lambda} q^{|\lambda|} x^{\rho(x)},$$

where the sum is over all partitions, λ, and the statistic $\rho(\lambda)$ is the sum of the number of parts of λ and the largest part of λ. Note that this is equivalent to the interpretation of $F(x, q)$ in the preceding subsection. This was then combined with the observations (13) and (14) to interpret the mock theta functions (11) and (12) as generating functions for certain families of partitions.

In view of (1), (13), and (14), we see that the mock theta functions (11) and (12) can be interpreted in terms of statistics on binary words as:

$$f(q) = \sum_{w} (-1)^{|w|} q^{\mathrm{m}aj};$$

$$\omega(q) = \sum_{w} q^{|w|+2\mathrm{m}aj},$$

where the sum is over all binary words w and $|w|$ denotes the length of w.

3 An "Inversions" View of (5) and (6)

We obtain another identity by carrying out the same sort of analysis on the inversions of a word, rather than the major index. An inversion in a word w is a pair (i, j) such that $i < j$ but $w_i > w_j$ and $\mathrm{inv}(w)$ is the number of inversions in w. The statistic inv is also Mahonian on binary words [8], so its distribution is given by (2).

3.1 Proof of (6)

Let $f(n, k, m)$ be the number of binary strings of length n, containing exactly k 1's, and with m inversions. Then evidently

$$f(n, k, m) = f(n-1, k-1, m) + f(n-1, k, m-k),$$

for $n \geq 2$, with $f(1, k, m) = \delta_{k,0}\delta_{m,0} + \delta_{k,1}\delta_{m,0}$. If we define the generating function $F(x, y, z) = \sum_{n\geq 1, k\geq 0, m\geq 0} f(n, k, m) x^n y^k z^m$, then we find the functional equation

$$F(x, y, z) = \frac{x(1+y) + xF(x, yz, z)}{1-xy},$$

whose solution is

$$F(x, y, z) = \sum_{m\geq 1} \frac{x^m(1+yz^{m-1})}{\prod_{j=0}^{m-1}(1-xyz^j)}.$$

We can now set $y = 1$ and find that the number of binary words of length n with m inversions is equal to the coefficient of $x^n q^m$ in

$$\sum_{m\geq 0} \frac{x^{m+1}(1+q^m)}{(x;q)_{m+1}} = 2x + (3+q)x^2 + (4+2q+2q^2)x^3 + \dots.$$

3.2 The Equivalence of (5) and (6)

Let $g(n,m)$ be the number of binary words of length n with m inversions. The previous subsection showed that (6) is the generating function for $\sum_{n\geq 0, m\geq 0} g(n,m)x^n q^m$.

Because of the equidistribution of maj and inv, $g(n,m) = f(n,m)$, for $f(n,m)$ defined in Sect. 1. But supposing we didn't know that, we show that $g(n,m)$ satisfies the same recurrence as $f(n,m)$ in Lemma 1 of Sect. 2.4.3, and therefore it has the same functional equation, whose solution was shown there to be (5).

Claim. We have the recurrence

$$g(n,m) = 2g(n-1,m) - g(n-2,m) + g(n-2,m-n+1) \quad (n \geq 2; m \geq 0) \tag{15}$$

with initial data $g(0,m) = \delta_{m,0}$, $g(1,m) = 2\delta_{m,0}$.

Proof. Let $R(n,m)$ be the set of binary words of length n with m inversions, so that $g(n,m) = |R(n,m)|$. Observe that

$$\begin{aligned} \mathrm{inv}(1 \cdot w \cdot 0) &= \mathrm{inv}(w) + |w| + 1, \\ \mathrm{inv}(0 \cdot w) &= \mathrm{inv}(w), \\ \mathrm{inv}(w \cdot 1) &= \mathrm{inv}(w) \end{aligned}$$

Words of the form $0 \cdot w \cdot 1$ fall into both of the last two classes above and all other words fall into exactly one of the three classes above. So,

$$|R(n,m)| = |1 \cdot R(n-2, m-(n-1)) \cdot 0| + |0 \cdot R(n-1,m)| + |R(n-1,m) \cdot 1| - |0 \cdot R(n-2,m) \cdot 1|,$$

and the recurrence follows. □

3.3 Revisiting (5)

Recall the notation $P(a,b)$, $D(\lambda)$, and $|\lambda|$ from Sect. 2.4.4 on partitions. View a binary word as a lattice path, where "1" is an east step and "0" is a north step. Then a binary word w with a 0's and b 1's forms the lower boundary of a partition $\lambda \in P(a,b)$. It is not hard to check that

$$\mathrm{inv}(w) = |\lambda|,$$

But also, the Durfee square size, $D(\lambda)$, is interesting, in the following way.

Let ϕ be Foata's "second fundamental transformation" on words [6]. When restricted to binary words w, $\phi(w)$ is a permutation of w, with

$$\mathrm{maj}(w) = \mathrm{inv}(\phi(w)),$$

and ϕ proves bijectively that for any a, b, maj and inv have the same distribution over the binary words with a 0's and b 1's,

Furthermore, if λ is the partition defined by the lattice path associated with $\phi(w)$, then it was shown in [9] that

$$\mathrm{des}(w) = D(\lambda),$$

where des(w) is the number of descents of w. Thus, (maj, des) and (inv, D) have the same joint distribution.

We can combine these observations with the identity from the end of Sect. 2.4.4:

$$\sum_{a,b,\geq 0} \sum_{\lambda \in P(a,b)} q^{\lambda} x^{a+b} z^{D(\lambda)} = \sum_{j\geq 0} \frac{x^{2j} q^{j^2}}{((x;q)_{j+1})^2} z^j$$

to get

$$\begin{aligned} \sum_{j\geq 0} \frac{x^{2j} q^{j^2}}{((x;q)_{j+1})^2} z^j &= \sum_{a,b,\geq 0} \sum_{\lambda \in P(a,b)} q^{\lambda} x^{a+b} z^{D(\lambda)} \\ &= \sum_{w} q^{\mathrm{inv}(w)} x^{|w|} z^{D(\lambda(w))} \\ &= \sum_{w} q^{\mathrm{maj}(w)} x^{|w|} z^{\mathrm{des}(w)}. \end{aligned}$$

So, "des" is something like the "Blocks" statistic used in Sect. 2.3. However, observe that "des" gives rise to (5), whereas "Blocks" gives rise to (4).

4 Larger Alphabets

The above results were all obtained by studying binary words. Now let's look at words over the M-letter alphabet $[M] = \{0, 1, 2, \ldots, M-1\}$.

Let $f(k_0, k_1, \ldots, k_{M-1}; \mu)$ denote the number of words over $[M]$ that contain exactly k_0 0's, k_1 1's,…,k_{M-1} $M-1$'s, and which have major index μ. Of course the length of such a word is $N = \sum_i k_i$. It is known that major index is Mahonian on this set of words [8] and therefore its distribution is given by the q-multinomial coefficient

$$\sum_{\mu\geq 0} f(k_0, k_1, \ldots, k_{M-1}; \mu) q^{\mu} = \begin{bmatrix} N \\ k_0, k_1, \ldots, k_{M-1} \end{bmatrix}_q.$$

See Sloane's sequences A129529, A129531 for the cases $M = 3, 4$. So, if $[M]^*$ denotes the set of all words over $[M]$,

$$F(x,q) = \sum_{w\in[M]^*} q^{\mathrm{maj}(w)} x^{|w|} = \sum_{N\geq 0} \sum_{k_0+\cdots+k_{M-1}=N} \begin{bmatrix} N \\ k_0, k_1, \ldots, k_{M-1} \end{bmatrix}_q x^N. \tag{16}$$

Rewriting the last expression and applying (8), we find
$F(x,q)$

$$\begin{aligned}
&= \sum_{k_0,k_1,\ldots,k_{M-1}\geq 0} \begin{bmatrix} k_0+\cdots+k_{M-1} \\ k_0,\ldots,k_{M-1} \end{bmatrix}_q x^{k_0+\cdots+k_{M-1}} \\
&= \sum_{k_0,k_1,\ldots,k_{M-2}\geq 0} \begin{bmatrix} k_0+\cdots+k_{M-2} \\ k_0,\ldots,k_{M-2} \end{bmatrix}_q x^{k_0+\cdots+k_{M-2}} \sum_{k_{M-1}\geq 0} \begin{bmatrix} k_0+\cdots+k_{M-1} \\ k_{M-1} \end{bmatrix}_q x^{k_{M-1}} \\
&= \sum_{k_0,k_1,\ldots,k_{M-2}\geq 0} \begin{bmatrix} k_0+\cdots+k_{M-2} \\ k_0,\ldots,k_{M-2} \end{bmatrix}_q \frac{x^{k_0+\cdots+k_{M-2}}}{(x;q)_{k_0+\cdots+k_{M-2}}}.
\end{aligned}$$

This generalizes the equivalence of (2) and (3) which is the $M = 2$ case.

We will consider a variation and get a q-difference equation.

Let $f_i(k_0, k_1, \ldots, k_{M-1}; \mu)$ denote the number of words over $[M]$ that contain exactly k_0 0's, k_1 1's,…,k_{M-1} $M-1$'s, and which have major index μ, and whose last letter is i $(i = 0, \ldots, M-1)$.

Of these $f_i(k_0, k_1, \ldots, k_{M-1}; \mu)$ words, the number whose penultimate letter is j is

$$\begin{cases} f_j(k_0, k_1, \ldots, k_i - 1, \ldots, k_{M-1}; \mu - (N-1)), & \text{if } j > i, \\ f_j(k_0, k_1, \ldots, k_i - 1, \ldots, k_{M-1}; \mu), & \text{if } j \leq i. \end{cases}$$

Consequently, for $i = 0 \ldots, M-1$, we have

$$\begin{aligned} f_i(k_0, k_1, \ldots, k_{M-1}; \mu) = \sum_{j>i} f_j(k_0, k_1, \ldots, k_i - 1, \ldots, k_{M-1}; \mu - (N-1)) \\ + \sum_{j\leq i} f_j(k_0, k_1, \ldots, k_i - 1, \ldots, k_{M-1}; \mu). \end{aligned}$$

Now sum both sides over all $\mathbf{k}$ such that $k_0 + \cdots + k_{M-1} = N$, and write $F_i(N, \mu)$ for $\sum_{k_0+\cdots+k_{M-1}=N} f_i(k_0, k_1, \ldots, k_{M-1}; \mu)$. We obtain

$$F_i(N, \mu) = \sum_{j>i} F_j(N-1, \mu - N + 1) + \sum_{j\leq i} F_j(N-1, \mu),$$

with $F_i(1,\mu) = M\delta_{\mu,0}$. In terms of the generating functions

$$\Phi_{N,i} = \sum_{\mu} F_i(N,\mu)q^{\mu},$$

we find that

$$\Phi_{N,i} = q^{N-1}\sum_{j>i}\Phi_{N-1,j} + \sum_{j\le i}\Phi_{N-1,j},$$

with $\Phi_{1,i} = 1$ for all $i = 0,\dots,M-1$.

Finally, if $\Phi_i(x,q) = \sum_{N\ge 1}\Phi_{N,i}x^N$, we find that

$$\Phi_i(x,q) = x + x\sum_{j>i}\Phi_j(qx,q) + x\sum_{j\le i}\Phi_j(x,q). \qquad (i = 0,1,\dots,M-1)$$

5 A Related Identity Based on the Positions of 0's in Bitstrings

If w is a binary string of length n, let $\sigma(w)$ be the sum of the positions that contain 0 bits, the positions being labeled $1,2,\dots,n$. Thus $f(10101) = 2+4 = 6$. We consider the generating function

$$F(x,q) = \sum_{w} x^{|w|}q^{\sigma(w)},$$

the sum extending over all binary words of all lengths.

If we let $T(n,k)$ denote the number of words of length n for which $\sigma(w) = k$, then we have the obvious recurrence $T(n,k) = T(n-1,k) + T(n-1,k-n)$. This leads, in the usual way, to the functional equation

$$F(x,q) = \frac{1 + xqF(xq,q)}{1-x}, \tag{17}$$

which in turn leads, by iteration, to the explicit expression

$$F(x,q) = \sum_{j\ge 0}\frac{x^j q^{\binom{j+1}{2}}}{(x;q)_{j+1}}. \tag{18}$$

On the other hand it is easy to see that

$$\sum_{k} T(n,k)q^k = \prod_{\ell=1}^{n}(1+q^{\ell}), \tag{19}$$

since each position ℓ in w can either be 1, which contributes ℓ to $\sigma(w)$, or 0, which contributes nothing. Thus, we have the identity

$$\sum_{j\geq 0} \frac{x^j q^{\binom{j+1}{2}}}{(x;q)_{j+1}} = \sum_{n\geq 0} x^n \prod_{\ell=1}^{n} (1+q^\ell). \tag{20}$$

Note that (20) is a specialization of Heine's second transformation (Eq. III.2 in Appendix III of [7] with $a = -q, b = q, c = 0, z = x$).

5.1 A Partition Theory View

We can interpret the identity (20) in terms of partitions.

We claim that both sides of the identity count all pairs (λ, n) where λ is a partition into distinct parts and n is greater than or equal to the largest part of λ.

On the right-hand side, $\prod_{\ell=1}^{n}(1+q^\ell)$ is the generating function for partitions into distinct parts, the largest of which is $\leq n$. So, the right-hand side counts all pairs (λ, n) where λ is a partition into distinct parts and n is greater than or equal to the largest part of λ, as claimed.

The left-hand side counts the same quantity by summing over all j the terms $x^n q^{|\lambda|}$ for all pairs (λ, n) where λ is a partition into j positive distinct parts, the largest of which is $\leq n$. To see this, If λ is a partition into j distinct positive parts, then subtracting the staircase partition $(j, j-1, \ldots, 1)$ from λ subtracts $\binom{j+1}{2}$ from the q-weight of λ and subtracts j from the largest part of λ, leaving an ordinary partition λ' with at most j parts. Such λ' are counted in the left-hand-side of (20) by $1/(x;q)_{j+1}$, where x keeps track of the size of the largest part of λ' *plus* an excess corresponding to the number of times the "0" part is selected as the $1/(1-x)$ factor in the product.

5.2 A Generalization

Let w be a word over the K letter alphabet $\{0, 1, \ldots, K-1\}$ and let

$$\sigma(w) = \sum_{i=1}^{n} i w_i .$$

We have $\sigma(10101) = 1 + 3 + 5 = 9$ and $\sigma(120301) = 1 + 4 + 12 + 6 = 23$. We consider the generating function

$$F(x,q) = \sum_{w} x^{|w|} q^{\sigma(w)},$$

the sum extending over all K-ary words of all lengths.

If we let $T(n,k)$ denote the number of words of length n for which $\sigma(w) = k$, then we have the obvious recurrence

$$T(n,k) = \sum_{i=0}^{K-1} T(n-1, k-in). \qquad (n \geq 1; T(0,k) = \delta_{k,0}).$$

If we take our generating function in the form $F(x,q) = \sum_{k,n\geq 0} T(n,k)x^n q^k$, this leads, in the usual way, to the functional equation

$$F(x,q) = \frac{1}{1-x} + \frac{x}{1-x}\sum_{i=1}^{K-1} q^i F(xq^i, q), \tag{21}$$

In the binary case ($K = 2$), this agrees with (17), which has the explicit expression (18).

On the other hand, since a j in position ℓ contributes $j\ell$ to $\sigma(w)$, so

$$\sum_k T(n,k)q^k = \prod_{\ell=1}^{n}(1 + q^\ell + q^{2\ell} + \cdots + q^{(K-1)\ell}) = \prod_{\ell=1}^{n} \frac{1-q^{K\ell}}{1-q^\ell}, \tag{22}$$

and in the case $K = 2$ we have another view of the identity (20).

We would like an explicit solution to the functional equation (21) for $K > 2$, analogous to (20). Recall that (20) was a special case of Heine's second transformation. There is no analog of Heine's second transformation for $K > 2$. However, there is an analog of the first Heine transformation that can be applied. We make use of the following, which is Lemma 1 from [1]:

$$\sum_{n\geq 0} \frac{t^n (a;q^k)_n (b;q)_{kn}}{(q^k;q^k)_n (c;q)_{kn}} = \frac{(b;q)_\infty (at;q^k)_\infty}{(c;q)_\infty (t;q^k)_\infty} \sum_{n\geq 0} \frac{b^n (c/b;q)_n (t;q^k)_n}{(q;q)_n (at;q^k)_n}. \tag{23}$$

Setting $a = c = 0$, $b = x$, $k = K$, and $t = q^k$ in (23) gives

$$F(x,q) = \sum_{n\geq 0} \frac{x^n (q^K;q^K)_n}{(q;q)_n} = \frac{(q^K;q^K)_\infty}{(x;q)_\infty} \sum_{n\geq 0} \frac{q^{Kn}(x;q)_{Kn}}{(q^K;q^K)_n}.$$

6 "Lecture Hall" Statistics on Words

The following statistics arose in [10] in a more general context, but we specialize them here to words. For a K-ary word w of length n, define the following statistics:

$$\text{ASC(w)} = \{i \mid i = 0 \text{ and } w_1 > 0 \text{ or } 1 \leq i < n \text{ and } w_i < w_{i+1}\};$$

$$\mathrm{asc}(w) = |\mathrm{ASC}(w)|;$$

$$\mathrm{lhp}(w) = -(w_1 + w_2 + \cdots + w_n) + \sum_{i \in \mathrm{ASC}(w)} K(n-i);$$

It follows from Theorem 5 in [10] that

$$\sum_{t \geq 0} \sum_{\lambda \in P(n,Kt)} q^{|\lambda|} x^t = \frac{\sum_{w \in [K]^n} q^{\mathrm{lhp}(w)} x^{\mathrm{asc}(w)}}{\prod_{i=0}^{n}(1 - xq^{Ki})},$$

where $[K] = \{0, 1, \ldots, K-1\}$.

As observed in [10], the inner sum on the left is a q-binomial coefficient, so we get the identity:

$$\sum_{t \geq 0} \begin{bmatrix} n+Kt \\ n \end{bmatrix}_q x^t = \frac{\sum_{w \in [K]^n} q^{\mathrm{lhp}(w)} x^{\mathrm{asc}(w)}}{\prod_{i=0}^{n}(1 - xq^{Ki})}.$$

Multiplying both sides by $(1-x)$ and then setting $x = 1$ gives

$$\sum_{t \geq 0} \left(\begin{bmatrix} n+Kt \\ n \end{bmatrix}_q - \begin{bmatrix} n+K(t-1) \\ n \end{bmatrix}_q \right) = \frac{\sum_{w \in [K]^n} q^{\mathrm{lhp}(w)}}{(q;q)_n}.$$

The left-hand side above is just $1/(q;q)_n$, the generating function for partitions into at most n parts. So, simplifying,

$$\sum_{w \in [K]^n} q^{\mathrm{lhp}(w)} = \prod_{\ell=1}^{n} (1 + q^\ell + q^{2\ell} + \cdots + q^{(K-1)\ell}),$$

the same distribution as $\sum_i i w_i$ from Sect. 5.2 (!) We don't have any nice combinatorial explanation for this yet.

Experiments indicate that when $K = 2$, we can actually get the following refinement:

$$\sum_{t \geq 0} \sum_{i=0}^{n} \begin{bmatrix} n+t-i \\ t \end{bmatrix}_{q^2} \begin{bmatrix} t-1+i \\ t-1 \end{bmatrix}_{q^2} (qz)^i x^t = \frac{\sum_{w \in [2]^n} q^{\mathrm{lhp}(w)} x^{\mathrm{asc}(w)} z^{w_1 + w_2 + \cdots + w_n}}{\prod_{i=0}^{n}(1 - xq^{2i})}. \tag{24}$$

To prove this, from the bijective proof of Theorem 5 in [10], it would suffice to verify that the innermost summand on the left is the generating function for partitions in an n by $2t$ box with i odd parts. This was done for us by Christian Krattenthaler as follows, thereby proving (24):

The q-binomial coefficient $\begin{bmatrix} n+t-i \\ n-i \end{bmatrix}_{q^2}$ is the generating function for partitions consisting of $n-i$ even parts, all of which are at most $2t$. On the other hand, the q-binomial coefficient $\begin{bmatrix} t-1+i \\ i \end{bmatrix}$ is the generating function for partitions consisting of i even parts, all of which are at most $2t-2$. Now add 1 to each of the i latter parts. Thereby you get i odd parts, all of which at most $2t$. (This gives a contribution of q^i in the generating function.) Finally shuffle the odd and even parts.

7 The Generating Function of the Terms of a Closed Form q-Series

In trying to find the solution to a combinatorial problem, one often goes through the procedure of finding a recurrence, then a functional equation for the generating function, then by iteration, the solution of that functional equation, and then, with some luck, a nice product form for the coefficients that are of interest.

Here, let's invert that process. Suppose we have a sequence $t(n,k)$ which satisfies

$$\sum_{k\geq 0} t(n,k)q^k = \prod_{j=1}^{n} \frac{a(q^j)}{b(q^j)},$$

where $a(t), b(t)$ are fixed polynomials in t. In other words, we suppose that the sum on the left is a q-hypergeometric term in n. What we would like to know is the generating function

$$F(x,q) = \sum_{n,k} t(n,k)x^n q^k.$$

To do this, put $f(n) = \sum_{k\geq 0} t(n,k)q^k$, and then we have

$$b(q^n)f(n) = a(q^n)f(n-1). \qquad (n \geq 1; f(0) = 1) \tag{25}$$

To simplify the appearance of the following results, let R be the operator that transforms x to xq, i.e., $Rf(x) = f(xq)$, and suppose our polynomials a, b are $a(t) = \sum a_j t^j$ and $b(t) = \sum_j b_j t^j$. Further, take the generating function in the form

$$F(x,q) = \sum_{n,k\geq 0} t(n,k)x^n q^k.$$

Now multiply (25) by x^n and sum over $n \geq 1$, to find that

$$(b(R) - xa(qR))F(x,q) = 1 \tag{26}$$

is the functional equation of the generating function.

7.1 Examples

Example 1. In the case (19) above we have $a(t) = 1 + t$ and $b(t) = 1$. The functional equation (26) now reads as

$$(1 - x(1 + qR))F(x, q) = 1 = (1 - x)F(x, q) - xqF(xq, q),$$

in agreement with (17).

Example 2. Consider the case of the statistic $\sigma(w)$ of Sect. 5.2 on K-ary words when $K = 3$. (This has the same distribution as the statistic lhp from Sect. 6.) Here we have from (22) that $a(t) = 1 + t + t^2$ and $b(t) = 1$. The functional equation (26) takes the form $F(x, q) = 1 + x(F(x, q) + qF(xq, q) + q^2F(xq^2, q))$, i.e.,

$$F(x, q) = \frac{1}{1 - x}\left(1 + xqF(xq, q) + xq^2F(xq^2, q)\right), \tag{27}$$

in agreement with (21). We see by iteration that the solution of this equation is going to be a sum of terms of the form

$$\frac{q^{\alpha}x^{\beta}}{\prod_{i=1}^{n+1}(1 - xq^{s_i})}, \tag{28}$$

for some collection of α, β, s_i to be defined. We want to identify exactly which terms occur. The set T of such terms is defined inductively by the two rules

$$\text{(i)}\ \ \frac{1}{1 - x} \in T;$$

and

$$\text{(ii)}\ \ \text{if}\ \ \frac{q^{\alpha}x^{\beta}}{\prod_{i=1}^{n+1}(1 - xq^{s_i})} \in T,$$

then both of the following terms must be in T :

$$\frac{q^{\alpha+\beta+1}x^{\beta+1}}{(1 - x)\prod_{i=1}^{n+1}(1 - xq^{s_i+1})} \quad \text{and} \quad \frac{q^{\alpha+2\beta+2}x^{\beta+1}}{(1 - x)\prod_{i=1}^{n+1}(1 - xq^{s_i+2})}.$$

It is now straightforward to verify that the inductive rules define T to be:

$$T \;=\; \left\{\frac{q^{\sigma(w)}x^{|w|}}{\prod_{i=1}^{|w|+1}(1 - xq^{w_i+\cdots+w_{|w|}})} \;\middle|\; w \in \{1, 2\}^*\right\}.$$

The generating function is now

$$F(x,q) = \sum_{w\in\{1,2\}^*} \frac{q^{\sigma(w)}x^{|w|}}{\prod_{i=1}^{|w|+1}(1-xq^{w_i+\cdots+w_{|w|}})}.$$

Consequently we have the identity

$$\sum_{w\in\{1,2\}^*} \frac{q^{\sigma(w)}x^{|w|}}{\prod_{i=1}^{|w|+1}(1-xq^{w_i+\cdots+w_{|w|}})} = \sum_{n\geq 0} x^n \prod_{j=1}^{n}(1+q^j+q^{2j}). \qquad (29)$$

We're going to tweak the left side of (29) in the hope of making it prettier.

First we change the alphabet from $\{1,2\}$ to $\{0,1\}$, just because it's friendlier. To do that, define new variables $\{v_i\}_{i=1}^n$ by $v_i = w_i - 1$ $(i = 1,\ldots,n)$, where $n = |w|$. Then the gf becomes

$$\sum_{v\in\{0,1\}^*} \frac{q^{\sigma(w)}x^{|v|}}{\prod_{i=1}^{|v|+1}(1-xq^{w_i+\cdots+w_n})},$$

where we have temporarily used some v's and some w's.

Now introduce yet another set of variables, namely

$$u_i = w_i + \cdots + w_n = v_i + \cdots + v_n + n - i + 1 \quad (i = 1,\ldots,n).$$

Then we have

$$\sigma(w) = \sum_{i=1}^{n} i w_i = (w_1+\cdots+w_n)+(w_2+\cdots+w_n)+\cdots+w_n = u_1+\cdots+u_n = \Sigma(u),$$

say. The generating function now reads as

$$\sum_{u} \frac{q^{\Sigma(u)}x^{|u|}}{\prod_{i=1}^{|u|+1}(1-xq^{u_i})}$$

which is now entirely in terms of the u_i's, but we need to clarify the set of vectors u over which the outer summation extends.

Say that a sequence $\{t_i\}_{i=1}^{n+1}$ of nonnegative integers is *slowly decreasing* if $t_{n+1} = 0$, and we have $t_i - t_{i+1} = 1$ or 2 for all $i = 1,\ldots,n$. Then the outer sum above runs over all slowly decreasing sequences of all lengths, i.e., it is

$$\sum_{u\in\mathrm{sd}} \frac{q^{\Sigma(u)}x^{|u|-1}}{\prod_{i=1}^{|u|}(1-xq^{u_i})}.$$

where sd is the set of all slowly decreasing sequences, $\Sigma(u)$ is the sum of the entries of u, and $|u|$ is the length of u (including the mandatory 0 at the end).

7.2 A Generalization

In the same way we derived (29), we can use the functional equation (26) to derive the following general result.

Suppose $t(n,k)$ satisfies

$$\sum_{k\geq 0} t(n,k)q^k = \prod_{j=1}^{n} \frac{a(q^j)}{b(q^j)},$$

where $a(t), b(t)$ are fixed polynomials in t, $a(t) = \sum_{t=0}^{K-1} a_i t^i$, and $b(t) = \sum_{t=0}^{K-1} b_i t^i$. Then

$$F(x,q) = \sum_{n,k} t(n,k)x^n q^k = \sum_{w\in\{1,2,\ldots,K-1\}^*} \frac{\prod_{i=1}^{|w|}(a_{w_i}xq^{iw_i} - b_{w_i})}{\prod_{i=1}^{|w|+1}(b_0 - a_0xq^{w_i+\cdots+w_{|w|}})}.$$

This shows how the statistics iw_i on words arise naturally in q-series, with the special case of $\sigma(w)$ appearing when the polynomial b is constant.

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Stationary Distribution and Eigenvalues for a de Bruijn Process

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Dedicated to the memory of Herbert S. Wilf.

Abstract We define a de Bruijn process with parameters n and L as a certain continuous-time Markov chain on the de Bruijn graph with words of length L over an n-letter alphabet as vertices. We determine explicitly its steady state distribution and its characteristic polynomial, which turns out to decompose into linear factors. In addition, we examine the stationary state of two specializations in detail. In the first one, the de Bruijn-Bernoulli process, this is a product measure. In the second one, the Skin-deep de Bruin process, the distribution has constant density but nontrivial correlation functions. The two point correlation function is determined using generating function techniques.

1 Introduction

A de Bruijn sequence (or cycle) over an alphabet of n letters and of order L is a cyclic word of length n^L such that every possible word of length L over the alphabet appears once and exactly once. The existence of such sequences and their counting was first given by Camille Flye Sainte-Marie in 1894 for the case $n = 2$, see [10] and the acknowledgement by de Bruijn[8], although the earliest known example comes from the Sanskrit prosodist Pingala's *Chandah Shaastra* (some time between the second century BCE and the fourth century CE [15, 25]). This example is for

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$n = 2$ and $L = 3$ essentially contains the word 0111010001 as a mnemonic for a rule in Sanskrit grammar. Omitting the last two letters (since they are repeating the first two) gives a de Bruijn cycle. Methods for constructing de Bruijn cycles are discussed by Knuth [14].

The number of de Bruijn cycles for alphabet size $n = 2$ was (re-)proven to be $2^{2^{L-1}-L}$ by de Bruijn [7], hence the name. The generalization to arbitrary alphabet size n was first proven to be $n!^{n^{L-1}} \cdot n^{-L}$ by de Bruijn and van Aardenne-Ehrenfest. This result can be seen as an application of the famous BEST-theorem [22–24], which relates the counting of Eulerian tours in digraphs to the evaluation of a Kirchhoff (spanning-tree counting) determinant. The relevant determinant evaluation for the case of de Bruijn graphs (see below) is due to Dawson and Good [6], see also [13].

The (directed) de Bruijn graph $G^{n,L}$ is defined over an alphabet Σ of cardinality n. Its vertices are the words of $u = u_1u_2 \dots u_L \in \sigma^L$, and there is an directed edge or arc between any two nodes $u = u_1u_2 \dots u_L$ and $v = v_1v_2 \dots v_L$ if and only if $t(u) = u_2 \dots u_n = v_1 \dots v_{n-1} = h(v)$, where $h(v)$ ($t(u)$ resp.) stands for the *head* of v (*tail* of u, resp.). This arc is naturally labeled by the word $w = u.v_L = u_1.v$, so that $h(w) = u$ and $t(v) = v$. It is intuitively clear that Eulerian tours in the de Bruijn graph $G^{n,L}$ correspond to de Bruijn cycles for words over Σ of length $L + 1$. de Bruijn graphs and cycles have applications in several fields, e.g. in networking [12] and bioinformatics [17]. For an introduction to de Bruijn graphs, see e.g. [18].

In this article we will study a natural continuous-time Markov chain on $G^{n,L}$ which exhibits a very rich algebraic structure. The transition probabilities are not uniform since they depend on the structure of the vertices as words, and they are symbolic in the sense that variables are attached to the edges as weights. We have not found this in the literature, although there are studies of the uniform random walk on the de Bruijn graph [9]. The hitting times [5] and covering times [16] of this random walk have been studied, as has the structure of the covariance matrix for the alphabet of size $n = 2$ [2] and in general [1]. The spectrum for the undirected de Bruijn graph has been found by Strok [21]. We have also found a similar Markov chain whose spectrum is completely determined in the context of cryptography [11].

After describing our model on $G^{n,L}$ for a de Bruijn process in detail in the next section, we will determine its stationary distribution in Sect. 3 and its spectrum in Sect. 4. In the last section we discuss two special cases, the de Bruijn-Bernoulli process and the Skin-deep de Bruijn process.

2 The Model

We take the de Bruijn graph $G^{n,L}$ as defined above. As alphabet we may take $\Sigma = \Sigma_n = \{1, 2, \dots, n\}$. Matrices will then be indexed by words over Σ_n taken in lexicographical order. Since the alphabet size n will be fixed throughout the article, we will occasionally drop n as super- or subscript if there is no danger of ambiguity.

From each vertex $u = u_1u_2 \dots u_L \in \Sigma^L$ there are n directed edges in $G^{n,L}$ joining u with the vertices $u_2u_3 \dots u_n.a = t(u).a$ for $a \in \Sigma$.

We now give weights to the edges of the graph $G^{n,L}$. Let $X = \{x_{a,k} \,;\, a \in \Sigma, k \geq 1\}$ be the set of weights, to be thought of as formal variables. We will work over Σ^+, the set of all nonempty words over the alphabet Σ (of size n). An *a-block* is a word $u \in \Sigma^+$ which is the repetition of the single letter a so that $u = a^k$ for some $a \in \Sigma$ and $k \geq 1$. Obviously, every word u has a unique decomposition into blocks of maximal length,

$$u = b^{(1)}b^{(2)} \cdots b^{(m)}, \tag{1}$$

where each factor $b^{(i)}$ is a block so that any two neighboring factors are blocks of *distinct* letters. This is the canonical block factorization of u with a minimum number of block-factors.

We now define the function $\beta : \Sigma^+ \to X$ as follows:

- For a block a^k we set $\beta(a^k) = x_{a,k}$;
- For $u \in \Sigma^+$ with canonical block factorization (1) we set $\beta(u) = \beta(b^{(m)})$, i.e., the β-value of the last block of u.

An edge from vertex $u \in \Sigma^L$ to vertex $v \in \Sigma^L$, so that $h(v) = t(u)$ with $v = t(u).a$, say, will then be given the weight $\beta(v)$. This means that

$$\beta(v) = \begin{cases} x_{a,L} & \text{if } \beta(u) = x_{a,L}, \\ x_{a,k+1} & \text{if } \beta(u) = x_{a,k} \text{ with } k < L, \\ x_{a,1} & \text{if } \beta(u) = x_{b,k} \text{ for some } b \neq a. \end{cases} \tag{2}$$

Our *de Bruijn process* will be a continuous time Markov chain derived from the Markov chain represented by the directed de Bruijn graph $G^{n,L}$ with edge weights as defined above. The transition rates are $\beta(v)$ for transitions represented by edges ending in v. We note that these rates can be taken just as variables and not necessarily probabilities. Similarly, expectation values of random variables in this process will be functions in these variables.

The simplest nontrivial example occurs when $n = L = 2$. There are four configurations and the relevant edges are given in the Fig. 1.

Before stating our notation for the transition matrix of a continuous-time Markov chain, our *de Bruijn process*, we need a general notion.

Definition 1. For any $k \times k$ matrix M, let ${}^{\nabla}M$ denote the matrix where the sum of each column is subtracted from the corresponding diagonal element,

$${}^{\nabla}M = M - \mathrm{diag}(1_k \cdot M), \tag{3}$$

where 1_k denotes the all-one row vector of length k and $\mathrm{diag}(m_1, \dots, m_k)$ is a diagonal matrix with entries $m_1, \dots, m_k$ on the diagonal.

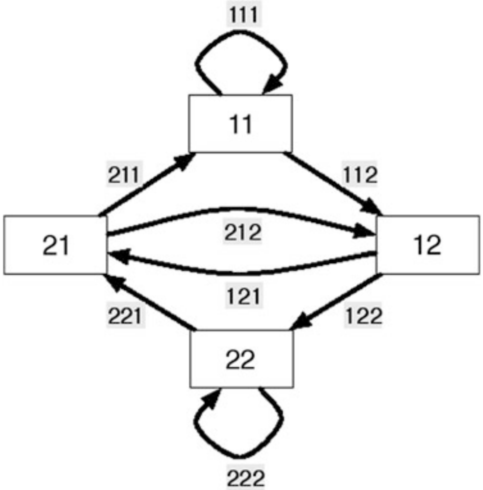

Fig. 1 An example of a de Bruijn graph in two letters and words of length 2

In graph theoretic terms ${}^{\nabla}M$ is the (negative of) the *Kirchhoff* matrix or *Laplacian matrix* of G, if M is the weighted adjacency matrix of a directed graph G. In case M is a matrix representing transitions of a Markov chain, the column (or right) eigenvector of ${}^{\nabla}M$ for eigenvalue zero properly normalized gives the stationary probability distribution of the continuous-time Markov chain.

We note that the graphs $G^{n,L}$ are both irreducible and recurrent, so that the stationary distribution is unique (up to normalization). We will use $M^{n,L}$ to denote the transition matrix of our Markov chain,

$$M^{n,L}_{v,u} = \text{rate}(u \to v) = \beta(v). \tag{4}$$

${}^{\nabla}M^{n,L}$ is then precisely the transition matrix,

$${}^{\nabla}M^{n,L}_{v,u} = \begin{cases} \beta(v) & \text{for } u \neq v, \\ -\sum\limits_{\substack{w \in \Sigma^L \\ u \neq w}} \beta(w) & \text{for } u = v. \end{cases} \tag{5}$$

For the example in Fig. 1, with lexicographic ordering of the states,

$${}^{\nabla}M^{2,2} = \begin{pmatrix} -x_{2,1} & 0 & x_{1,2} & 0 \\ x_{2,1} & -x_{1,1} - x_{2,2} & x_{2,1} & 0 \\ 0 & x_{1,1} & -x_{1,2} - x_{2,1} & x_{1,1} \\ 0 & x_{2,2} & 0 & -x_{1,1} \end{pmatrix}. \tag{6}$$

The stationary distribution is given by probabilities of words, which are to be taken as rational functions in the variables $x_{a,t}$. It is the column vector with eigenvalue zero, which after normalization is then given by

$$\begin{aligned} \Pr[1,1] &= \frac{x_{1,1}x_{1,2}}{(x_{1,2}+x_{2,1})(x_{1,1}+x_{2,1})}, \ \Pr[1,2] = \frac{x_{2,1}x_{1,1}}{(x_{1,1}+x_{2,2})(x_{1,1}+x_{2,1})}, \\ \Pr[2,1] &= \frac{x_{2,1}x_{1,1}}{(x_{1,2}+x_{2,1})(x_{1,1}+x_{2,1})}, \ \Pr[2,2] = \frac{x_{2,2}x_{2,1}}{(x_{1,1}+x_{2,2})(x_{1,1}+x_{2,1})}. \end{aligned} \tag{7}$$

Notice that the probabilities consist of a product of two monomials in the numerator and two factors in the denominator, and that each factor contains two terms. Also, notice that not all the denominators are the same, otherwise the steady state would be a true product measure. Of course, the sums of these probabilities is 1, which is not completely obvious.

It is also interesting to note that the eigenvalues of ${}^{\nabla}M^{2,2}$ are linear in the variables. Other than zero, the eigenvalues are given by

$$-x_{1,1}-x_{2,2}, \quad -x_{1,1}-x_{2,1}, \text{ and } -x_{1,2}-x_{2,1}. \tag{8}$$

Another way of saying this is that the characteristic polynomial of the transition matrix factorizes into linear parts.

3 Stationary Distribution

In this section we determine an explicit expression for the steady state distribution of the de Bruijn process on $G^{n,L}$. Before we do that we will have to set down some notation.

For convenience, we introduce operators which denote the transitions of our Markov chain. Let ∂_a be the operator that adds the letter a to the end of a word and removes the first letter,

$$\partial_a : u \mapsto t(u).a. \tag{9}$$

With β as introduced we introduce the shorthand notation

$$\beta_{a,m} = \sum_{b\in\Sigma} \beta(\partial_b\, a^m) = x_{a,m} + \sum_{b\in\Sigma, b\neq a} x_{b,1}. \tag{10}$$

Note that $\beta_{a,1} = \sum_{b\in\Sigma} x_{b,1}$ does not depend on a. We now define the valuation $\mu(u)$ for $u \in \Sigma^+$ as

$$\mu(u) = \frac{\beta(u)}{\sum_{a\in\Sigma} \beta(\partial_a u)}. \tag{11}$$

Note that the restriction of μ on the alphabet Σ is (formally) a probability distribution. Finally, we define the valuation $\bar{\mu}$, also on Σ^+, as

$$\bar{\mu}(u) = \prod_{i=1}^{L} \mu(u_1 u_2 \dots u_i) = \mu(u_1)\mu(u_1 u_2) \cdots \mu(u_1 u_2 \dots u_L), \tag{12}$$

if $u = u_1 u_2 \dots u_L$. The following result is the key to understanding the stationary distribution.

Proposition 1. *For all $u \in \Sigma^+$,*

$$\sum_{a \in \Sigma} \bar{\mu}(a.u) = \bar{\mu}(u). \tag{13}$$

Proof. As in (1), let us write w in block factorized form:

$$u = b^{(1)} b^{(2)} \cdots b^{(m)} = \tilde{u}.b^{(m)}, \tag{14}$$

where $\tilde{u} = b^{(1)} \dots b^{(m-1)}$ if $m > 1$, and $\tilde{u}$ is the empty word if $m = 1$.

If $b^{(m)} = a^k$, then

$$\mu(u) = \begin{cases} \dfrac{x_{a,k}}{\beta_{a,k}} & \text{if } m = 1, \text{i.e., if } u \text{ is a block,} \\ \dfrac{x_{a,k}}{\beta_{a,k+1}} & \text{if } m > 1, \end{cases} \tag{15}$$

and thus

$$\bar{\mu}(u) = \begin{cases} \displaystyle\prod_{j=1}^{k} \frac{x_{a,j}}{\beta_{a,j}} & \text{if } m = 1, \text{i.e., if } u \text{ is a block,} \\ \bar{\mu}(\tilde{u}) \cdot \displaystyle\prod_{j=1}^{k} \frac{x_{a,j}}{\beta_{a,j+1}} & \text{if } m > 1. \end{cases} \tag{16}$$

We will define another valuation on Σ^+ closely related to $\bar{\mu}$, which we call $\bar{\rho}$. Referring to the factorization (14) we put

$$\bar{\rho}(u) = \begin{cases} \displaystyle\prod_{j=1}^{k} \frac{x_{a,j}}{\beta_{a,j+1}} & \text{if } m = 1, \text{i.e., if } u = a^k \text{ is a block,} \\ \displaystyle\prod_{l=1}^{m} \bar{\rho}(u^{(l)}) & \text{if } m > 1. \end{cases} \tag{17}$$

This new valuation is related to $\bar{\mu}$ by the following properties:

– For blocks $u = a^k$ we have

$$\bar{\rho}(a^k) = \frac{\beta_{a,1}}{\beta_{a,k+1}} \bar{\mu}(a^k), \tag{18}$$

– For u with factorization (14) we have

$$\bar{\mu}(u) = \bar{\mu}(\tilde{u}) \cdot \bar{\rho}(b^{(m)}), \tag{19}$$

– Which, by the obvious induction, implies

$$\bar{\mu}(u) = \bar{\mu}(b^{(1)}) \cdot \prod_{l=2}^{m} \bar{\rho}(b^{(l)}). \tag{20}$$

We are now in a position to prove identity (13). First consider the case where $u = a^k$ is a block.

$$\begin{aligned}
\sum_{b \in \Sigma} \bar{\mu}(b \cdot a^k) &= \bar{\mu}(a^{k+1}) + \sum_{b \neq a} \bar{\mu}(b \cdot a^k) \\
&= \frac{x_{a,k+1}}{\beta_{a,k+1}} \bar{\mu}(a^k) + \sum_{b \neq a} \bar{\mu}(b) \cdot \bar{\rho}(a^k) \\
&= \frac{x_{a,k+1}}{\beta_{a,k+1}} \bar{\mu}(a^k) + \sum_{b \neq a} \frac{x_{b,1}}{\beta_{a,1}} \bar{\rho}(a^k) \\
&= \left(\frac{x_{a,k+1}}{\beta_{a,k+1}} + \sum_{b \neq a} \frac{x_{b,1}}{\beta_{a,k+1}} \right) \bar{\mu}(a^k) \\
&= \bar{\mu}(a^k),
\end{aligned} \tag{21}$$

where we used (18) in the last-but-one step.

The general case is then proven by a simple induction on m.

$$\begin{aligned}
\sum_{a \in \Sigma} \bar{\mu}(a.b^{(1)} b^{(2)} \ldots b^{(m)}) &= \sum_{a \in \Sigma} \bar{\mu}(a.b^{(1)} b^{(2)} \ldots b^{(m-1)}) \cdot \bar{\rho}(b^{(m)}) \\
&= \bar{\mu}(b^{(1)} b^{(2)} \ldots b^{(m-1)}) \cdot \bar{\rho}(b^{(m)}) \\
&= \bar{\mu}(b^{(1)} b^{(2)} \ldots b^{(m)}),
\end{aligned} \tag{22}$$

where we have used property (19) of $\bar{\rho}$ in the last step. □

As a consequence of Proposition 1, we have the following result, which is an easy exercise in induction. The case $L = 1$ was already mentioned immediately after (11).

Corollary 2. *For any fixed length L of words over the alphabet Σ,*

$$\sum_{w\in\Sigma^L} \bar{\mu}(w) = 1. \tag{23}$$

Therefore, the column vector $\bar{\boldsymbol{\mu}}^{n,L} = [\bar{\mu}(u)]_{u\in\Sigma^L}$ can be a seen as a formal probability distribution on Σ^L. We now look at the transition matrix $M^{n,L}$ more closely.

$$M^{n,L}_{v,u} = \delta_{h(v)=t(u)}\,\beta(v). \tag{24}$$

where δ_x is the indicator function for x, i.e., it is 1 if the statement x is true and 0 otherwise. Thus the matrix $M^{n,L}$ is very sparse. It has just n non-zero entries per row and per column. More precisely, the row indexed by v has the entry $\beta(v)$ for the $n\partial$-preimages of v, and the column indexed by u contains $\beta(\partial_a u)$ as the only nonzero entries. In particular, the column sum for the column indexed by u is $\sum_{a\in\Sigma}\beta(\partial_a(u))$. Define the diagonal matrix $\Delta^{n,L}$ as one with precisely these column sums as entries, i.e.

$$\Delta^{n,L}_{v,u} = \begin{cases} \sum_{a\in\Sigma}\beta(\partial_a u) & v=u,\\ 0 & \text{otherwise.}\end{cases} \tag{25}$$

Theorem 3. *The vector $\bar{\boldsymbol{\mu}}^{n,L}$ is the stationary vector for the de Bruijn process on $G^{n,L}$, i.e.,*

$$M^{n,L}\bar{\boldsymbol{\mu}}^{n,L} = \Delta^{n,L}\bar{\boldsymbol{\mu}}^{n,L}. \tag{26}$$

Proof. Consider the row corresponding to word $v = v_1v_2\ldots v_{L-1}v_L = h(v).v_L$ in the equation

$$M\,\overline{\boldsymbol{\mu}} = \Delta\,\overline{\boldsymbol{\mu}}. \tag{27}$$

On the l.h.s. of (27) we have to consider the summation $\sum_{u\in\Sigma^L} M_{v,u}\,\overline{\mu}(u)$, where only those $u\in\Sigma^L$ with $t(u).v_L = v$ contribute. This latter condition can be written as $u = b.h(v)$ for some $b\in\Sigma$, so that this summation can be written as

$$\begin{aligned}\sum_{u\in\Sigma^L} M_{v,u}\,\overline{\mu}(u) &= \sum_{b\in\Sigma} M_{v,b.h(v)}\,\overline{\mu}(b.h(v))\\ &= \beta(v)\sum_{b\in\Sigma}\overline{\mu}(b.h(v)) = \beta(v)\,\overline{\mu}(h(v)),\end{aligned} \tag{28}$$

where the last equality follows from Lemma 6.

On the r.h.s. of (27) we have for the row entry corresponding to the word v:

$$\begin{aligned}\Delta_{v,v}\,\overline{\mu}(v) &= \sum_{a\in\Sigma}\beta(\partial_a v)\,\overline{\mu}(v)\\ &= \sum_{a\in\Sigma}\beta(\partial_a v)\cdot\overline{\mu}(h(v))\,\mu(v) = \beta(v)\,\overline{\mu}(h(v))\end{aligned} \tag{29}$$

in view of the inductive definition of $\overline{\mu}$ in (12) and the definition of μ in (11). ◻

Let $Z^{n,L}$ denote the common denominator of the stationary probabilities of configurations. This is often called, with some abuse of terminology, the *partition function* [4]. The abuse comes from the fact that this terminology is strictly applicable in the sense of statistical mechanics while considering Markov chains only when they are reversible. The de Bruijn process definitely does not fall into this category. Since the probabilities are given by products of μ in (12), one arrives at the following product formula.

Corollary 4. *The partition function of the de Bruijn process on $G^{n,L}$ is given by*

$$Z^{n,L} = \beta_{1,1}\cdot\prod_{m=2}^{L-1}\prod_{a=1}^{n}\beta_{a,m}. \tag{30}$$

Physicists are often interested in properties of the stationary distribution rather than the full distribution itself. One natural quantity of interest in this context is the so-called density distribution of a particular letter, say a, in the alphabet. In other words, they would like to know, for example, how likely it is that a is present at the first site rather than the last site. We can make this precise by defining *occupation variables*. Let $\eta^{a,i}$ denote the occupation variable of species a at site i: it is a random variable which is 1 when site i is occupied by a and zero otherwise. We define the probability in the stationary distribution by the symbol $\langle\ \cdot\ \rangle$. Then $\langle\ \eta^{a,i}\ \rangle$ gives the *density* of a at site i. Similarly, one can ask for joint distributions, such as $\langle\ \eta^{a,i}\eta^{b,j}\ \rangle$, which is the probability that site i is occupied by a and simultaneously that site j is occupied by b. Such joint distributions are known as *correlation functions*.

We will not be able to obtain detailed information about arbitrary correlation functions in full generality, but there is one case in which we can easily give the answer. This is the correlation function for any letters $a_k,\dots,a_2,a_1$ at the last k sites.

Corollary 5. *Let $u = a_k\dots a_2a_1$. Then*

$$\langle\eta^{a_k,L-k+1}\cdots\eta^{a_2,L-1}\eta^{a_1,L}\rangle = \bar{\mu}(u). \tag{31}$$

Proof. By definition of the stationary state,

$$\langle \eta^{a_k,L-k+1} \cdots \eta^{a_2,L-1} \eta^{a_1,L} \rangle = \sum_{v \in \Sigma^{L-k}} \bar{\mu}(v.u). \tag{32}$$

Using Proposition 1 repeatedly $L-k$ times, we arrive at the desired result. □

In particular, Corollary 5 says that the density of species a at the last site is simply

$$\langle \eta^{a,L} \rangle = \frac{x_{a,1}}{\beta_{a,1}}. \tag{33}$$

Formulas for densities at other locations are much more complicated. It would be interesting to find a uniform formula for the density of species a at site k.

4 Characteristic Polynomial of ${}^{\nabla}M^{n,L}$

We will prove a formula for the characteristic polynomial of ${}^{\nabla}M^{n,L}$ in the following. In particular, we will show that it factorizes completely into linear parts. In order to do so, we need to understand the structure of the transition matrices better. We denote by $\chi(M;\lambda)$ the characteristic polynomial of a matrix M in the variable λ.

To begin with, let us recall from the previous section that the transition matrices $M^{n,L}$, taken as mappings defined on row and column indices, are defined by

$$M^{n,L} : \Sigma_n^L \times \Sigma_n^L \to X : (v,u) \mapsto \delta_{h(v)=t(u)} \cdot \beta(v). \tag{34}$$

Lemma 6. *The matrix $M^{n,L}$ can be written as*

$$M^{n,L} = \left[A^{n,L} \mid A^{n,L} \mid \ldots \mid A^{n,L} \right] \ (n \text{ copies of } A^{n,L}), \tag{35}$$

where $A^{n,L}$ is a matrix of size $n^L \times n^{L-1}$ given by

$$A^{n,L} : \Sigma^{n,L} \times \Sigma^{n,L-1} \to X \cup \{0\} : (v,u) \mapsto \delta_{h(v)=u} \cdot \beta(v). \tag{36}$$

We have

$$A^{n,1} = \begin{bmatrix} x_{1,1} \\ x_{2,1} \\ \vdots \\ x_{n,1} \end{bmatrix}, \quad A^{n,L} = \begin{bmatrix} A_1^{n,L-1} & 0^{n,L-1} & \cdots & 0^{n,L-1} \\ 0^{n,L-1} & A_2^{n,L-1} & \cdots & 0^{n,L-1} \\ \vdots & \vdots & \ddots & \vdots \\ 0^{n,L-1} & 0^{n,L-1} & \cdots & A_n^{n,L-1} \end{bmatrix} = \begin{bmatrix} B_1^{n,L-1} \\ B_2^{n,L-1} \\ \vdots \\ B_n^{n,L-1} \end{bmatrix}, \tag{37}$$

where $A_k^{n,L-1}$ is like $A^{n,L-1}$, but with $x_{k,L-1}$ replaced by $x_{k,L}$, and where $0^{n,L-1}$ is the zero matrix of size $n^{L-1} \times n^{L-2}$. The matrices $B_a^{n,L-1}$ are square matrices of size $n^{L-1} \times n^{L-1}$, where for each $a \in \Sigma$ the matrix $B_a^{n,L}$ is defined by

$$B_a^{n,L} : \Sigma^L \times \Sigma^L \to X \cup \{0\} : (v,u) \mapsto \delta_{a.h(v)=u} \cdot \beta(a.v). \tag{38}$$

With these matrices at hand we can finally define the matrix $B^{n,L} = \sum_{a\in\Sigma} B_a^{n,L}$ of size $n^L \times n^L$, so that

$$B^{n,L} : \Sigma^L \times \Sigma^L \to X \cup \{0\} : (v,u) \mapsto \delta_{h(v)=t(u)} \cdot \beta(u_1.v). \tag{39}$$

Lemma 7. *$M^{n,L} - B^{n,L}$ is a diagonal matrix.*

Proof. We have

$$M^{n,L}(v,u) \neq B^{n,L}(v,u) \;\Leftrightarrow\; h(v) = t(u) \text{ and } \beta(u_1.v) \neq \beta(v) \tag{40}$$

But $\beta(u_1.v) \neq \beta(v)$ can only happen if the last block of $u_1.v$ is different from the last block of v, which only happens if v itself is a block, $v = a^L$, and $u_1 = a$, in which case $\beta(v) = x_{a,L}$ and $\beta(u_1.v) = x_{a,L+1}$. So we have

$$(B^{n,L} - M^{n,L})(v,u) = \begin{cases} x_{a,L+1} - x_{a,L} & \text{if } v = u = a^L, \\ 0 & \text{otherwise.} \end{cases} \tag{41}$$

□

We state as an equivalent assertion:

Corollary 8. *For the Kirchhoff matrices of $M^{n,L}$ and $B^{n,L}$ we have equality:*

$$^{\nabla}M^{n,L} =^{\nabla} B^{n,L}. \tag{42}$$

We now prove a very general result about the characteristic polynomial of a matrix with a certain kind of block structure. This will be the key to finding the characteristic polynomial of our transition matrices.

Lemma 9. *Let $P_1, \dots, P_m, Q$ be any $k \times k$ matrices, $P = P_1 + \dots + P_m$ and*

$$R = \begin{bmatrix} P_1 + Q & P_1 & \cdots & P_1 \\ P_2 & P_2 + Q & \cdots & P_2 \\ \vdots & \vdots & \ddots & \vdots \\ P_m & P_m & \cdots & P_m + Q \end{bmatrix}. \tag{43}$$

Then

$$\chi(R;\lambda) = \chi(Q;\lambda)^{m-1} \cdot \chi(P+Q;\lambda). \tag{44}$$

Proof. Multiply R by the block lower-triangular matrix of unit determinant shown to get

$$R \cdot \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ -1 & 1 & 0 & \cdots & 0 \\ 0 & -1 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \\ 0 & 0 & 0 & \cdots & 1 \end{bmatrix} = \begin{bmatrix} Q & 0 & 0 & \cdots & P_1 \\ -Q & Q & 0 & \cdots & P_2 \\ 0 & -Q & Q & \cdots & P_3 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & P_m + Q \end{bmatrix} \tag{45}$$

which has the same determinant as R. Now perform the block row operations which replace row j by the sum of rows 1 through j to get

$$\begin{bmatrix} Q & 0 & 0 & \cdots & P_1 \\ 0 & Q & 0 & \cdots & P_1 + P_2 \\ 0 & 0 & Q & \cdots & P_1 + P_1 + P_3 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & P + Q \end{bmatrix} \tag{46}$$

Since this is now a block upper triangular matrix, the characteristic polynomials is the product of those of the diagonal blocks. □

We will now apply this lemma to the block matrix

$${}^{\nabla}M^{n,L+1} = \begin{bmatrix} B_1^{n,L} - D^{n,L} & B_1^{n,L} & \dots & B_1^{n,L} \\ B_2^{n,L} & B_2^{n,L} - D^{n,L} & \dots & B_2^{n,L} \\ \vdots & \vdots & \ddots & \vdots \\ B_n^{n,L} & B_n^{n,L} & \dots & B_n^{n,L} - D^{n,L} \end{bmatrix} \tag{47}$$

where $D^{n,L}$ is the $(n^L \times n^L)$-diagonal matrix with the column sums of $A^{n,L+1}$ on the main diagonal.

Proposition 10. *The characteristic polynomials* $\chi({}^{\nabla}M^{n,L}; z)$ *satisfy the recursion*

$$\chi({}^{\nabla}M^{n,L+1}; z) = \chi(-D^{n,L}; z)^{n-1} \cdot \chi({}^{\nabla}M^{n,L}; z). \tag{48}$$

Proof. From Corollary 8, Lemma 9, and the easily checked fact ${}^{\nabla}B^{n,L} = B^{n,L} - D^{n,L}$ we get:

$$\begin{aligned} \chi({}^{\nabla}M^{n,L+1}; \lambda) &= \chi(-D^{n,L}; \lambda)^{n-1} \cdot \chi(\textstyle\sum_{a\in\Sigma} B_a^{n,L} - D^{n,L}; \lambda) \\ &= \chi(-D^{n,L}; \lambda)^{n-1} \cdot \chi(B^{n,L} - D^{n,L}; \lambda) \\ &= \chi(-D^{n,L}; \lambda)^{n-1} \cdot \chi({}^{\nabla}B^{n,L}; \lambda) \\ &= \chi(-D^{n,L}; \lambda)^{n-1} \cdot \chi({}^{\nabla}M^{n,L}; \lambda). \end{aligned} \tag{49}$$

□

As a final step, we need a formula for $\chi(-D^{n,L}, \lambda)$.

Lemma 11. *The characteristic polynomial of* $-D^{n,L}$ *is given by*

$$\chi(-D^{n,L},\lambda) = \begin{cases} \lambda + \beta_{1,1} & \text{if } L = 0, \\ \prod_{m=2}^{L} \prod_{a\in\Sigma} (\lambda + \beta_{a,m})^{(n-1)n^{L-m}} \prod_{a\in\Sigma} (\lambda + \beta_{a,L+1}) & \text{if } L > 0. \end{cases} \tag{50}$$

Proof. The case $L = 0$ follows directly from the definition of $A^{n,1}$ in (37). For general L, recall that $A^{n,L+1}$ contains n copies of $A^{n,L}$ with one factor containing $x_{a,L}$ removed and one factor containing $x_{a,L+1}$ added instead, for each $a \in \Sigma$. Thus,

$$\chi(-D^{n,L},\lambda) = \left[\chi(-D^{n,L-1},\lambda)\right]^n \cdot \prod_{a\in\Sigma} \left(\frac{\lambda + \beta_{a,L+1}}{\lambda + \beta_{a,L}} \right), \tag{51}$$

which proves the result. □

We can now put everything together and get from Proposition 10, Lemma 11 and checking the initial case for $L = 1$:

Theorem 12. *The characteristic polynomial of the de Bruijn process on* $G^{n,K}$ *is given by*

$$\chi({}^{\nabla}M^{n,L};\lambda) = \lambda\,(\lambda + \beta_{1,1})^{n-1} \cdot \prod_{m=2}^{L} \prod_{a\in\Sigma} (\lambda + \beta_{a,m})^{(n-1)n^{L-m}}. \tag{52}$$

5 Special Cases

We now consider special cases of the rates where something interesting happens in the de Bruijn process.

5.1 The de Bruijn-Bernoulli Process

There turns out to be a special case of the rates $x_{a,j}$ for which the stationary distribution is a *Bernoulli measure*. That is to say, the probability of finding species a at site i in stationarity is independent, not only of any other site, but also of i itself. This is not obvious because the dynamics at any given site is certainly a priori not independent from what happens at any other site. Since the measure is so simple, all correlation functions are trivial. We denote the single site measure in (11) for this specialized process to be μ_y, and the stationary measure (12) as $\bar{\mu}_y$.

Corollary 13. *Under the choice of rates $x_{a,j} = y_a$ independent of j, the stationary distribution of the Markov chain with transition matrix ${}^{\nabla}M^{n,L}$ is Bernoulli with density*

$$\rho_a = \frac{y_a}{\sum_{b \in \Sigma} y_b}. \tag{53}$$

Proof. The choice of rates simply mean that species a is added with a rate independent of the current configuration. From (11), it follows that for $u = u_1 u_2 \dots u_L$,

$$\mu_y(u) = \frac{y_{u_L}}{\sum_{b \in \Sigma} y_b} = \rho_{u_L}, \tag{54}$$

and using the definition of the stationary distribution $\bar{\mu}$ in (12),

$$\bar{\mu}_y(u) = \prod_{i=1}^{L} \rho_{u_i}, \tag{55}$$

which is exactly the definition of a Bernoulli distribution. □

5.2 *The Skin-Deep de Bruijn Process*

Another tractable version of the de Bruijn process is one where the rate for transforming the word $u = u_1 u_2 \dots u_L$ into $\partial_a u = t(u).a = u_2 \dots u_L.a$ for $a \in \Sigma$ only depends on the occupation of the last site, u_L. Hence, the rates are only *skin-deep*. An additional simplification comes by choosing the rate to be x when $a = u_L$ and 1 otherwise. Namely,

$$x_{a,j} = \begin{cases} x & \text{for } j = 1, \\ 1 & \text{for } j > 1. \end{cases} \tag{56}$$

We first summarize the results. It turns out that any letter in the alphabet is equally likely to be at any site in the skin-deep de Bruijn process. This is an enormous simplification compared to the original process where we do not have a general formula for the density. Further, we have the property that all correlation functions are independent of the length of the words. This is not obvious because the Markov chain on words of length L is not reducible in any obvious way to the one on words of length $L - 1$. This property is quite rare and very few examples are known of such families of Markov chains. One such example is the asymmetric annihilation process [3].

The intuition is as follows. By choosing $x \ll 1$ one prefers to add the same letter as u_L, and similarly, for $x \gg 1$, one prefers to add any letter in Σ other than u_L. Of course, $x = 1$ corresponds to the uniform distribution. Therefore, one expects the average word to be qualitatively different in these two cases. *In the former case, one expects the average word to be the same letter repeated L times, whereas in the latter case, one would expect no two neighboring letters to be the same on average.* Our final result, a simple formula for the two-point correlation function, exemplifies the different in these two cases.

We begin with a formula for the stationary distribution, which we will denote in this specialization by $\bar{\mu}_x$. We will always work with the alphabet Σ on n letters.

Lemma 14. *The stationary probability for a word $u = u_1u_2\dots u_L \in \Sigma^L$ is given by*

$$\bar{\mu}_x(u) = \frac{x^{\gamma(u)-1}}{n(1+(n-1)x)^{L-1}}, \tag{57}$$

where $\gamma(u)$ is the number of blocks of u.

Proof. Analogous to the notation for the stationary distribution, we denote the block function by β_x. From the definition of the model,

$$\beta_x(a^k) = \begin{cases} x & \text{if } k = 1, \\ 1 & \text{if } k > 1. \end{cases} \tag{58}$$

and thus, for any word u the value $\beta_x(u)$ is x if the length of the last block in its block decomposition is 1, and is 1 otherwise. The denominator in (57) is easily explained. For any word u of length L,

$$\sum_{a \in \Sigma} \beta_x(t(u).a) = \begin{cases} 1+(n-1)x & L > 1, \\ nx & L = 1, \end{cases} \tag{59}$$

because for all but one letter in Σ, the size of the last block in $t(u).a$ is going to be 1. The only exception to this argument is, $L = 1$, when $t(u)$ is empty. From (12), we get

$$\bar{\mu}_x(u) = \frac{\beta_x(u_1)\beta_x(u_1u_2)\cdots\beta_x(u_1\dots u_L)}{nx(1+(n-1)x)^{L-1}}. \tag{60}$$

The numerator is $x^{\gamma(u)}$, since we pick up a factor of x every time a new block starts. One factor x is cancelled because $\beta_x(u_1) = x$. □

The formula for the density is essentially an argument about the symmetry of the de Bruijn graph $G^{n,L}$.

Corollary 15. *The probability in the stationary state of $G^{n,L}$ that site i is occupied by letter a is uniform, i.e., for any i s.th. $1 \le i \le L$ we have*

$$\langle \eta^{a,i} \rangle = \frac{1}{n} \; (a \in \Sigma). \tag{61}$$

Proof. Indeed, by Lemma 14 the stationary distribution $\bar{\mu}_x$ is invariant under any permutation of the letters of the alphabet Σ. Hence $\langle \eta^{a,i} \rangle$ does not depend on $a \in \Sigma$ and we have uniformity. □

Since the de Bruijn-Bernoulli process has a product measure, the density of a at site i is also independent of i, but the density is not uniform since it is given by ρ_a (53). The behavior of higher correlation functions here is more complicated than the de Bruijn-Bernoulli process. There is, however, one aspect in which it resembles the former, namely:

Lemma 16. *Correlation functions of $G^{n,L}$ in this model are independent of the length L of the words and they are shift-invariant.*

Proof. We can represent an arbitrary correlation function in the de Bruijn graph $G^{n,L}$ as

$$\langle \eta^{a_1,i_1} \cdots \eta^{a_k,i_k} \rangle_L = \sum_{w^{(0)},\ldots,w^{(k)}} \bar{\mu}_x(w^{(0)} a_1 w^{(1)} \ldots w^{(k-1)} a_k w^{(k)}), \tag{62}$$

where we have sites $1 \le i_1 < i_2 < \ldots < i_k \le L$ and letters $a_1, a_2, \ldots, a_k \in \Sigma$, and where the sum runs over all $(w^{(0)}, w^{(1)}, \ldots, w^{(k)})$ with $w^{(j)} \in \Sigma^{i_{s+1}-i_s-1}$ for $s \in \{0, \ldots, k\}$, and where we put $i_0 = 0$ and $i_{k+1} = L + 1$. Now note that we have from Proposition 1 for any $u \in \Sigma^k$

$$\sum_{w \in \Sigma^L} \bar{\mu}_x(w.u) = \bar{\mu}_x(u). \tag{63}$$

Since $\bar{\mu}_x$, as given in Lemma 14, is also invariant under reversal of words, we also have

$$\sum_{w \in \Sigma^L} \bar{\mu}_x(u.w) = \bar{\mu}_x(u). \tag{64}$$

As a consequence, we can forget about the outermost summations in (62) and get

$$\langle \eta^{a_1,i_1} \cdots \eta^{a_k,i_k} \rangle_L = \sum_{w^{(1)},\ldots,w^{(k-1)}} \bar{\mu}_x(a_1 w^{(1)} \ldots w^{(k-1)} a_k) = \langle \eta^{a_1,j_1} \cdots \eta^{a_k,j_k} \rangle_{i_k - i_1 + 1}, \tag{65}$$

where $j_s = i_s - i_1 + 1$ $(1 \le s \le k)$. Shift-invariance in the sense that

$$\langle \eta^{a_1,i_1} \cdots \eta^{a_k,i_k} \rangle_L = \langle \eta^{a_1,i_1+1} \cdots \eta^{a_k,i_k+1} \rangle_L \tag{66}$$

is an immediate consequence. □

We now proceed to compute the two-point correlation function. This is an easy exercise in generating functions for words according to the number of blocks. The technique is known as "transfer-matrix method", see, e.g., Sect. 4.7 in [20].

For $a, b \in \Sigma$ and $k \ge 1$ we define the generating polynomial in the variable x

$$\alpha_{n,k}(a, b; x) = \sum_{w \in a.\Sigma^{k-1}.b} x^{\gamma(w)-1}, \tag{67}$$

where, as before, $\gamma(w)$ denotes the number of blocks in the block factorization of $w \in \Sigma^+$ (so that $\gamma(w) - 1$ is the number of pairs of adjacent distinct letters in w). Note that

$$\alpha_{n,1}(a, b; x) = \begin{cases} 1 & \text{if } a = b, \\ x & \text{if } a \ne b. \end{cases} \tag{68}$$

The following statement is folklore:

Lemma 17. *Let $\mathbb{I}_n$ denote the identity matrix and $\mathbb{J}_n$ denote the all-one matrix, both of size $n \times n$, and let $K_n(s, t) := s \cdot \mathbb{I}_n + t \cdot \mathbb{J}_n$ for parameters s, t. Then*

$$K_n(s, t)^{-1} = \frac{1}{s(s + nt)} K_n(s + nt, -t). \tag{69}$$

Indeed, this is a very special case of what is known as the Sherman-Morrison formula, see [19, 26].

Consider now the matrix

$$A_n(x) := [\,\alpha_{n,1}(a, b; x)\,]_{a,b\in\Sigma} = (1 - x) \cdot \mathbb{I}_n + x \cdot \mathbb{J}_n = K_n(1 - x, x) \tag{70}$$

which encodes transition in the alphabet Σ. Then, for $k \ge 1$, $A_n(x)^k$ is an $(n \times n)$-matrix which in position (a, b) contains the generating polynomial $\alpha_{n,k}(a, b; x)$:

$$A_n(x)^k = [\,\alpha_{n,k}(a, b; x)\,]_{a.b\in\Sigma}\,. \tag{71}$$

We can get generating functions by summing the geometric series and using Lemma 17:

$$\sum_{k\geq 0} A_n(x)^k z^k = (\mathbb{I}_n - z\cdot A_n(x))^{-1}$$
$$= K_n(1-z+xz,-xz)^{-1} \tag{72}$$
$$= \frac{K_n(1-z-(n-1)xz,xz)}{(1-z+xz)(1-z-(n-1)xz)},$$

which means that for any two distinct letters $a, b \in \Sigma$:

$$\begin{aligned}\sum_{k\geq 0}\alpha_{n,k}(a,a;x)\,z^k &= \frac{1-z-(n-2)xz}{(1-z+xz)(1-z-(n-1)xz)}\\ &= \frac{1}{n}\frac{1}{1-z-(n-1)\,xz}+\frac{n-1}{n}\frac{1}{1-z+xz},\\ \sum_{k\geq 1}\alpha_{n,k}(a,b;x)\,z^k &= \frac{xz}{(1-z+xz)(1-z-(n-1)xz)}\\ &= \frac{1}{n}\frac{1}{1-z-(n-1)\,xz}-\frac{1}{n}\frac{1}{1-z+xz},\end{aligned} \tag{73}$$

or equivalently,

$$\begin{aligned}\alpha_{n,k}(a,a;x) &= \frac{1}{n}\left((1-(n-1)x)^k+(n-1)(1-x)^k\right),\\ \alpha_{n,k}(a,b;x) &= \frac{1}{n}\left((1-(n-1)x)^k-(1-x)^k\right).\end{aligned} \tag{74}$$

We thus arrive at expressions for the two-point correlation functions:

Proposition 18. *For $a, b \in \Sigma$ with $a \neq b$ and $1 \leq i < j \leq L$,*

$$\begin{aligned}\langle \eta^{a,i}\eta^{a,j}\rangle &= \frac{1}{n^2}+\frac{n-1}{n^2}\left(\frac{1-x}{1+(n-1)x}\right)^{j-i},\\ \langle \eta^{a,i}\eta^{b,j}\rangle &= \frac{1}{n^2}-\frac{1}{n^2}\left(\frac{1-x}{1+(n-1)x}\right)^{j-i}.\end{aligned} \tag{75}$$

Proof. By Lemma 16 we may assume $i = 1$ and $j = L$. Comparing Lemma 14 with the definition of the $\alpha_{n,k}(a, b; x)$ in (67) we see that for $a, b \in \Sigma$:

$$\langle \eta^{a,1}\eta^{b,L}\rangle = \frac{\alpha_{n,L-1}(a,b;x)}{n(1+(n-1)x)^{L-1}}, \tag{76}$$

so that the assertion follows from 74. □

The formula (75) is quite interesting because the first term, $1/n^2$, has a significance. From the formula for the density in Corollary 15, we get

$$\langle \eta^{a,1}\eta^{a,L}\rangle - \langle \eta^{a,1}\rangle\langle \eta^{a,L}\rangle = \frac{n-1}{n^2}\left(\frac{1-x}{1+(n-1)x}\right)^{L-1}. \tag{77}$$

The object on the left hand side is called the *truncated* two point correlation function in the physics literature, and its value is an indication of how far the stationary distribution is from a product measure. In the case of a product measure, the right hand side would be zero. Setting

$$\alpha = \frac{1-x}{1+(n-1)x}, \tag{78}$$

we see that $|\alpha| \leq 1$, and so the truncated correlation function goes exponentially to zero as $L \to \infty$. Thus, the stationary measure $\bar{\mu}_x$ behaves like a product measure if we do not look for observables which are close to each other. We can use (77) to understand one of the differences between the values $x < 1$ and $x > 1$, namely in the way this quantity converges. In the former case, the convergence is monotonic, and in the latter, oscillatory.

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Automatic Generation of Theorems and Proofs on Enumerating Consecutive-Wilf Classes

Andrew Baxter, Brian Nakamura, and Doron Zeilberger

To W from Z (et. al.), a gift for his $\frac{2}{3}|S_5|$*-th birthday*

Abstract This article, describes two complementary approaches to enumeration, the positive and the negative, each with its advantages and disadvantages. Both approaches are amenable to automation, and we apply it to the currently active subarea, initiated in 2003 by Sergi Elizalde and Marc Noy, of enumerating consecutive-Wilf classes (i.e. consecutive pattern-avoidance) in permutations.

Keywords Automated enumeration • Consecutive pattern-avoidance

Preface

This article describes two complementary approaches to enumeration, the *positive* and the *negative*, each with its advantages and disadvantages. Both approaches are amenable to *automation*, and when applied to the currently active subarea, initiated in 2003 by Sergi Elizalde and Marc Noy [4], of *consecutive pattern-avoidance* in permutations, were successfully pursued by the first two authors Andrew Baxter [1] and Brian Nakamura [10]. This article summarizes their research and in the case of [10] presents an umbral viewpoint to the same approach. The main purpose of this article is to briefly explain the Maple packages, `SERGI` and `ELIZALDE`, developed by AB-DZ and BN-DZ respectively, implementing the algorithms that enable the computer to "do research" by deriving, *all by itself*, functional equations for the generating functions that enable polynomial-time

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enumeration for any set of patterns. In the case of ELIZALDE (the "negative" approach), these functional equations can be sometimes (automatically!) simplified, and imply "explicit" formulas, that previously were derived by humans using ad-hoc methods. We also get lots of new "explicit" results, beyond the scope of humans, but we have to admit that we still need humans to handle "infinite families" of patterns, but this too, no doubt, will soon be automatable, and we leave this as a challenge to the (human and/or computer) reader.

Consecutive Pattern Avoidance

Inspired by the very active research in pattern-avoidance, pioneered by Herb Wilf, Rodica Simion, Frank Schmidt, Richard Stanley, Don Knuth and others, Sergi Elizalde, in his PhD thesis (written under the direction of Richard Stanley) introduced the study of permutations avoiding *consecutive patterns*.

Recall that an *n-permutation* is a sequence of integers $\pi = \pi_1 \dots \pi_n$ of length n where each integer in $\{1, \dots, n\}$ appears exactly once. It is well-known and very easy to see (today!) that the number of n-permutations is $n! := \prod_{i=1}^{n} i$.

The *reduction* of a list of different (integer or real) numbers (or members of any totally ordered set) $[i_1, i_2, \dots, i_k]$, to be denoted by $R([i_1, i_2, \dots, i_k])$, is the permutation of $\{1, 2, \dots, k\}$ that preserves the relative rankings of the entries. In other words, $p_i < p_j$ iff $q_i < q_j$. For example the reduction of $[4, 2, 7, 5]$ is $[2, 1, 4, 3]$ and the reduction of $[\pi, e, \gamma, \phi]$ is $[4, 3, 1, 2]$.

Fixing a pattern $p = [p_1, \dots, p_k]$, a permutation $\pi = [\pi_1, \dots, \pi_n]$ *avoids* the consecutive pattern p if for all i, $1 \le i \le n - k + 1$, the reduction of the list $[\pi_i, \pi_{i+1}, \dots, \pi_{i+k-1}]$ is *not* p. More generally a permutation π avoids a set of patterns $\mathbb{P}$ if it avoids each and every pattern $p \in \mathbb{P}$.

The central problem is to answer the question: "Given a pattern or a set of patterns, find a 'formula', or at least an efficient algorithm (in the sense of Wilf [12]), that inputs a positive integer n and outputs the number of permutations of length n that avoid that pattern (or set of patterns)".

Human Research

After the pioneering work of Elizalde and Noy [4], quite a few people contributed significantly, including Anders Claesson, Toufik Mansour, Sergey Kitaev, Anthony Mendes, Jeff Remmel, and more recently, Vladimir Dotsenko, Anton Khoroshkin and Boris Shapiro. Also recently we witnessed the beautiful resolution of the Warlimont conjecture by Richard Ehrenborg, Sergey Kitaev, and Peter Perry [3]. The latter paper also contains extensive references.

Recommended Reading

While the present article tries to be self-contained, the readers would get more out of it if they are familiar with [13]. Other applications of the umbral transfer matrix method were given in [5, 14–16].

The Positive Approach vs. the Negative Approach

We will present two *complementary* approaches to the enumeration of consecutive-Wilf classes, both using the Umbral transfer matrix method. The positive approach works better when you have many patterns, and the negative approach works better when there are only a few, and works best when there is only one pattern to avoid.

Outline of the Positive Approach

Instead of dealing with *avoidance* (the number of permutations that have zero occurrences of the given pattern(s)) we will deal with the more general problem of enumerating the number of permutations that have specified numbers of occurrences of *any* pattern of length k.

Fix a positive integer k, and let $\{t_p : p \in S_k\}$ be $k!$ *commuting indeterminates* (alias variables). Define the *weight* of an n-permutation $\pi = [\pi_1, \ldots, \pi_n]$, to be denoted by $w(\pi)$, by:

$$w([\pi_1, \ldots, \pi_n]) := \prod_{i=1}^{n-k+1} t_{R([\pi_i, \pi_{i+1}, \ldots, \pi_{i+k-1}])}.$$

For example, with $k = 3$,

$$\begin{aligned} w([2,5,1,4,6,3]) &:= t_{R([2,5,1])} t_{R([5,1,4])} t_{R([1,4,6])} t_{R([4,6,3])} = \\ &= t_{231} t_{312} t_{123} t_{231} = t_{123} t_{231}^2 t_{312}. \end{aligned}$$

We are interested in an *efficient* algorithm for computing the sequence of polynomials in $k!$ variables

$$P_n(t_{1\ldots k}, \ldots, t_{k\ldots 1}) := \sum_{\pi \in S_n} w(\pi),$$

or equivalently, as many terms as desired in the formal power series

$$F_k(\{t_p, p \in S_k\}; z) = \sum_{n=0}^{\infty} P_n z^n.$$

Note that once we have computed the P_n (or F_k), we can answer *any* question about pattern avoidance by specializing the t's. For example to get the number of n-permutations avoiding the single pattern p, of length k, first compute P_n, and then plug-in $t_p = 0$ and all the other t's to be 1. If you want the number of n-permutations avoiding the set of patterns $\mathbb{P}$ (all of the same length k), set $t_p = 0$ for all $p \in \mathbb{P}$ and the other t's to be 1. As we shall soon see, we will generate *functional equations* for F_k, featuring the $\{t_p\}$ and of course it would be much more efficient to specialize the t_p's to the numerical values already in the functional equations, rather than crank-out the much more complicated $P_n(\{t_p\})$'s and then do the plugging-in.

First let's recall one of the many proofs that the number of n-permutations, let's denote it by $a(n)$, satisfies the recurrence

$$a(n+1) = (n+1)a(n).$$

Given a typical member of S_n, let's call it $\pi = \pi_1 \dots \pi_n$, it can be continued in $n+1$ ways, by deciding on π_{n+1}. If $\pi_{n+1} = i$, then we have to "make room" for the new entry by incrementing by 1 all entries $\geq i$, and then append i. This gives a bijection between $S_n \times [1, n+1]$ and S_{n+1} and taking cardinalities yields the recurrence. Of course $a(0) = 1$, and "solving" this recurrence yields $a(n) = n!$. Of course this solving is "cheating", since $n!$ is just shorthand for the solution of this recurrence subject to the initial condition $a(0) = 1$, but from now on it is considered "closed form" (just by convention!).

When we do *weighted counting* with respect to the weight w with a given pattern-length k, we have to keep track of the last $k-1$ entries of π:

$$[\pi_{n-k+2} \dots \pi_n],$$

and when we append $\pi_{n+1} = i$, the new permutation (let $a' = a$ if $a < i$ and $a' = a+1$ if $a \geq i$)

$$\dots \pi'_{n-k+2} \dots \pi'_n i,$$

has "gained" a factor of $t_{R[\pi'_{n-k+2} \dots \pi'_n i]}$ to its weight.

This calls for the finite-state method, alas, the "alphabet" is indefinitely large, so we need the umbral transfer-matrix method.

We introduce $k-1$ "catalytic" variables $x_1, x_2, \dots, x_{k-1}$, as well as a variable z to keep track of the size of the permutation, and $(k-1)!$ "linear" state variables $A[q]$ for each $q \in S_{k-1}$, to tell us the state that the permutation is in. Define the generalized weight $w'(\pi)$ of a permutation $\pi \in S_n$ to be:

$$w'(\pi) := w(\pi) x_1^{j_1} x_2^{j_2} \dots x_{k-1}^{j_{k-1}} z^n A[q],$$

where $[j_1, \dots, j_{k-1}]$, $(1 \leq j_1 < j_2 < \dots < j_{k-1} \leq n)$ is the *sorted* list of the last $k-1$ entries of π, and q is the reduction of its last $k-1$ entries.

For example, with $k = 3$:

$$\begin{aligned} w'([4,7,1,6,3,5,8,2]) &= t_{231}t_{312}t_{132}t_{312}t_{123}t_{231}x_1^2x_2^8z^8A[21] = \\ &= t_{123}t_{132}t_{231}^2t_{312}^2x_1^2x_2^8z^8A[21]. \end{aligned}$$

Let's illustrate the method with $k = 3$. There are two states: $[1,2],[2,1]$ corresponding to the cases where the two last entries are $j_1 j_2$ or $j_2 j_1$ respectively (we always assume $j_1 < j_2$).

Suppose we are in state $[1,2]$, so our permutation looks like

$$\pi = [\ldots, j_1, j_2],$$

and $w'(\pi) = w(\pi)x_1^{j_1}x_2^{j_2}z^n A[1,2]$. We want to append i $(1 \le i \le n+1)$ to the end. There are three cases.

Case 1: $1 \le i \le j_1$.

The new permutation, let's call it σ, looks like

$$\sigma = [\ldots j_1 + 1, j_2 + 1, i].$$

Its state is $[2,1]$ and $w'(\sigma) = w(\pi)t_{231}x_1^i x_2^{j_2+1}z^{n+1}A[2,1]$.

Case 2: $j_1 + 1 \le i \le j_2$.

The new permutation, let's call it σ, looks like

$$\sigma = [\ldots j_1, j_2 + 1, i].$$

Its state is now $[2,1]$ and $w'(\sigma) = w(\pi)t_{132}x_1^i x_2^{j_2+1}z^{n+1}A[2,1]$.

Case 3: $j_2 + 1 \le i \le n + 1$.

The new permutation, let's call it σ, looks like

$$\sigma = [\ldots j_1, j_2, i].$$

Its state is now $[1,2]$ and $w'(\sigma) = w(\pi)t_{123}x_1^{j_2}x_2^i z^{n+1}A[1,2]$.

It follows that any *individual* permutation of size n, and state $[1,2]$, gives rise to $n+1$ children, and regarding weight, we have the "umbral evolution" (here W is the fixed part of the weight, that does not change):

$$\begin{aligned} Wx_1^{j_1}x_2^{j_2}z^nA[1,2] \to{}& Wt_{231}zA[2,1]\left(\sum_{i=1}^{j_1} x_1^i x_2^{j_2+1}\right)z^n \\ &+Wt_{132}zA[2,1]\left(\sum_{i=j_1+1}^{j_2} x_1^i x_2^{j_2+1}\right)z^n \\ &+Wt_{123}zA[1,2]\left(\sum_{i=j_2+1}^{n+1} x_1^{j_2}x_2^i\right)z^n. \end{aligned}$$

Taking out of the $\sum$-signs whatever we can, we have:

$$Wx_1^{j_1}x_2^{j_2}z^n A[1,2] \to Wt_{231}zA[2,1]\left(\sum_{i=1}^{j_1} x_1^i\right) x_2^{j_2+1}z^n$$
$$+Wt_{132}zA[2,1]\left(\sum_{i=j_1+1}^{j_2} x_1^i\right) x_2^{j_2+1}z^n$$
$$+Wt_{123}zA[1,2]\left(\sum_{i=j_2+1}^{n+1} x_2^i\right) x_1^{j_2}z^n.$$

Now summing up the geometrical series, using the ancient formula:

$$\sum_{i=a}^{b} Z^i = \frac{Z^a - Z^{b+1}}{1-Z},$$

we get

$$Wx_1^{j_1}x_2^{j_2}z^n A[1,2] \to Wt_{231}zA[2,1]\left(\frac{x_1 - x_1^{j_1+1}}{1-x_1}\right) x_2^{j_2+1}z^n$$
$$+Wt_{132}zA[2,1]\left(\frac{x_1^{j_1+1} - x_1^{j_2+1}}{1-x_1}\right) x_2^{j_2+1}z^n$$
$$+Wt_{123}zA[1,2]\left(\frac{x_2^{j_2+1} - x_2^{n+2}}{1-x_2}\right) x_1^{j_2}z^n.$$

This is the same as:

$$Wx_1^{j_1}x_2^{j_2}z^n A[1,2] \to Wt_{231}zA[2,1]\left(\frac{x_1x_2^{j_2+1} - x_1^{j_1+1}x_2^{j_2+1}}{1-x_1}\right) z^n$$
$$+Wt_{132}zA[2,1]\left(\frac{x_1^{j_1+1}x_2^{j_2+1} - x_1^{j_2+1}x_2^{j_2+1}}{1-x_1}\right) z^n$$
$$+Wt_{123}zA[1,2]\left(\frac{x_1^{j_2}x_2^{j_2+1} - x_1^{j_2}x_2^{n+2}}{1-x_2}\right) z^n.$$

This is what was called in [13], and its many sequels, a “pre-umbra”. The above evolution can be expressed for a general *monomial* $M(x_1, x_2, z)$ as:

$$M(x_1,x_2,z)A[1,2] \to t_{231}zA[2,1]\left(\frac{x_1x_2M(1,x_2,z)-x_1x_2M(x_1,x_2,z)}{1-x_1}\right)$$
$$+t_{132}zA[2,1]\left(\frac{x_1x_2M(x_1,x_2,z)-x_1x_2M(1,x_1x_2,z)}{1-x_1}\right)$$
$$+t_{123}zA[1,2]\left(\frac{x_2M(1,x_1x_2,z)-x_2^2M(1,x_1,x_2z)}{1-x_2}\right).$$

But, by *linearity*, this means that the coefficient of $A[1,2]$ (the weight-enumerator of all permutations of state $[1,2]$) obeys the evolution equation:

$$f_{12}(x_1,x_2,z)A[1,2] \to t_{231}zA[2,1]\left(\frac{x_1x_2f_{12}(1,x_2,z)-x_1x_2f_{12}(x_1,x_2,z)}{1-x_1}\right)$$
$$+t_{132}zA[2,1]\left(\frac{x_1x_2f_{12}(x_1,x_2,z)-x_1x_2f_{12}(1,x_1x_2,z)}{1-x_1}\right)$$
$$+t_{123}zA[1,2]\left(\frac{x_2f_{12}(1,x_1x_2,z)-x_2^2f_{12}(1,x_1,x_2z)}{1-x_2}\right).$$

Now we have to do it all over for a permutation in state $[2,1]$. Suppose we are in state $[2,1]$, so our permutation looks like

$$\pi = [\ldots, j_2, j_1],$$

and $w'(\pi) = w(\pi)x_1^{j_1}x_2^{j_2}z^nA[2,1]$. We want to append i $(1 \le i \le n+1)$ to the end. There are three cases.

Case 1: $1 \le i \le j_1$.

The new permutation, let’s call it σ, looks like

$$\sigma = [\ldots j_2+1, j_1+1, i].$$

Its state is $[2,1]$ and $w'(\sigma) = w(\pi)t_{321}x_1^ix_2^{j_1+1}z^{n+1}A[2,1]$.

Case 2: $j_1+1 \le i \le j_2$.

The new permutation, let’s call it σ, looks like

$$\sigma = [\ldots j_2+1, j_1, i].$$

Its state is now $[1,2]$ and
$w'(\sigma) = w(\pi)t_{312}x_1^{j_1}x_2^iz^{n+1}A[1,2]$.

Case 3: $j_2 + 1 \le i \le n + 1$.

The new permutation, let's call it σ, looks like

$$\sigma = [\ldots j_2, j_1, i].$$

Its state is $[1, 2]$ and $w'(\sigma) = w(\pi)t_{213}x_1^{j_1}x_2^{i}z^{n+1}A[1, 2]$.

It follows that any *individual* permutation of size n, and state [2, 1], gives rise to $n + 1$ children, and regarding weight, we have the "umbral evolution" (here W is the fixed part of the weight, that does not change):

$$Wx_1^{j_1}x_2^{j_2}z^n A[2,1] \to Wt_{321}zA[2,1]\left(\sum_{i=1}^{j_1} x_1^i x_2^{j_1+1}\right)z^n$$
$$+Wt_{312}zA[1,2]\left(\sum_{i=j_1+1}^{j_2} x_1^{j_1}x_2^i\right)z^n$$
$$+Wt_{213}zA[1,2]\left(\sum_{i=j_2+1}^{n+1} x_1^{j_1}x_2^i\right)z^n.$$

Taking out of the $\sum$-signs whatever we can, we have:

$$Wx_1^{j_1}x_2^{j_2}z^n A[2,1] \to Wt_{321}zA[2,1]\left(\sum_{i=1}^{j_1} x_1^i\right)x_2^{j_1+1}z^n$$
$$+Wt_{312}zA[1,2]\left(\sum_{i=j_1+1}^{j_2} x_2^i\right)x_1^{j_1}z^n$$
$$+Wt_{213}zA[1,2]\left(\sum_{i=j_2+1}^{n+1} x_2^i\right)x_1^{j_1}z^n.$$

Now summing up the geometrical series, using the ancient formula:

$$\sum_{i=a}^{b} Z^i = \frac{Z^a - Z^{b+1}}{1-Z},$$

we get

$$W x_1^{j_1} x_2^{j_2} z^n A[2,1] \to W t_{321} z A[2,1] \left(\frac{x_1 - x_1^{j_1+1}}{1-x_1} \right) x_2^{j_1+1} z^n$$
$$+ W t_{312} z A[1,2] \left(\frac{x_2^{j_1+1} - x_2^{j_2+1}}{1-x_2} \right) x_1^{j_1} z^n$$
$$+ W t_{213} z A[1,2] \left(\frac{x_2^{j_2+1} - x_2^{n+2}}{1-x_2} \right) x_1^{j_1} z^n.$$

This is the same as:

$$W x_1^{j_1} x_2^{j_2} z^n A[2,1] \to W t_{321} z A[2,1] \left(\frac{x_1 x_2^{j_1+1} - x_1^{j_1+1} x_2^{j_1+1}}{1-x_1} \right) z^n$$
$$+ W t_{312} z A[1,2] \left(\frac{x_1^{j_1} x_2^{j_1+1} - x_1^{j_1} x_2^{j_2+1}}{1-x_2} \right) z^n$$
$$+ W t_{213} z A[1,2] \left(\frac{x_1^{j_1} x_2^{j_2+1} - x_1^{j_1} x_2^{n+2}}{1-x_2} \right) z^n.$$

The above evolution can be expressed for a general *monomial* $M(x_1, x_2, z)$ as:

$$M(x_1,x_2,z) A[2,1] \to t_{321} z A[2,1] \left(\frac{x_1 x_2 M(x_2,1,z) - x_1 x_2 M(x_1 x_2, 1, z)}{1-x_1} \right)$$
$$+ t_{312} z A[1,2] \left(\frac{x_2 M(x_1 x_2, 1, z) - x_2 M(x_1, x_2, z)}{1-x_2} \right)$$
$$+ t_{213} z A[1,2] \left(\frac{x_2 M(x_1, x_2, z) - x_2^2 M(x_1, 1, x_2 z)}{1-x_2} \right).$$

But, by *linearity*, this means that the coefficient of $A[2,1]$ (the weight-enumerator of all permutations of state $[2,1]$) obeys the evolution equation:

$$f_{21}(x_1,x_2,z) A[2,1] \to t_{321} z A[2,1] \left(\frac{x_1 x_2 f_{21}(x_2,1,z) - x_1 x_2 f_{21}(x_1 x_2, 1, z)}{1-x_1} \right)$$
$$+ t_{312} z A[1,2] \left(\frac{x_2 f_{21}(x_1 x_2, 1, z) - x_2 f_{21}(x_1, x_2, z)}{1-x_2} \right)$$
$$+ t_{213} z A[1,2] \left(\frac{x_2 f_{21}(x_1, x_2, z) - x_2^2 f_{21}(x_1, 1, x_2 z)}{1-x_2} \right).$$

Combining we have the "evolution":

$$
\begin{aligned}
&f_{12}(x_1, x_2, z)A[1,2] + f_{21}(x_1, x_2, z)A[2,1] \to \\
&t_{231}zA[2,1]\left(\frac{x_1x_2f_{12}(1, x_2, z) - x_1x_2f_{12}(x_1, x_2, z)}{1-x_1}\right) \\
&+t_{132}zA[2,1]\left(\frac{x_1x_2f_{12}(x_1, x_2, z) - x_1x_2f_{12}(1, x_1x_2, z)}{1-x_1}\right) \\
&+t_{123}zA[1,2]\left(\frac{x_2f_{12}(1, x_1x_2, z) - x_2^2f_{12}(1, x_1, x_2z)}{1-x_2}\right). \\
&+t_{321}zA[2,1]\left(\frac{x_1x_2f_{21}(x_2, 1, z) - x_1x_2f_{21}(x_1x_2, 1, z)}{1-x_1}\right) \\
&+t_{312}zA[1,2]\left(\frac{x_2f_{21}(x_1x_2, 1, z) - x_2f_{21}(x_1, x_2, z)}{1-x_2}\right) \\
&+t_{213}zA[1,2]\left(\frac{x_2f_{21}(x_1, x_2, z) - x_2^2f_{21}(x_1, 1, x_2z)}{1-x_2}\right).
\end{aligned}
$$

Now the "evolved" (new) $f_{12}(x_1, x_2, z)$ and $f_{21}(x_1, x_2, z)$ are the coefficients of $A[1,2]$ and $A[2,1]$ respectively, and since the *initial weight* of both of them is $x_1x_2^2z^2$, we have the established the following system of functional equations:

$$
\begin{aligned}
f_{12}(x_1, x_2, z) &= x_1x_2^2z^2 \\
&+t_{123}z\left(\frac{x_2f_{12}(1, x_1x_2, z) - x_2^2f_{12}(1, x_1, x_2z)}{1-x_2}\right) \\
&+t_{312}z\left(\frac{x_2f_{21}(x_1x_2, 1, z) - x_2f_{21}(x_1, x_2, z)}{1-x_2}\right) \\
&+t_{213}z\left(\frac{x_2f_{21}(x_1, x_2, z) - x_2^2f_{21}(x_1, 1, x_2z)}{1-x_2}\right),
\end{aligned}
$$

and

$$
\begin{aligned}
f_{21}(x_1, x_2, z) &= x_1x_2^2z^2 \\
&+t_{231}z\left(\frac{x_1x_2f_{12}(1, x_2, z) - x_1x_2f_{12}(x_1, x_2, z)}{1-x_1}\right) \\
&+t_{132}z\left(\frac{x_1x_2f_{12}(x_1, x_2, z) - x_1x_2f_{12}(1, x_1x_2, z)}{1-x_1}\right) \\
&+t_{321}z\left(\frac{x_1x_2f_{21}(x_2, 1, z) - x_1x_2f_{21}(x_1x_2, 1, z)}{1-x_1}\right).
\end{aligned}
$$

Let the Computer Do It!

All the above was only done for *pedagogical* reasons. The computer can do it all automatically, much faster and more reliably. Now if we want to find functional equations for the number of permutations avoiding a given set of consecutive patterns $\mathbb{P}$, all we have to do is plug-in $t_p = 0$ for $p \in \mathbb{P}$ and $t_p = 1$ for $p \notin \mathbb{P}$. This gives a polynomial-time algorithm for computing any desired number of terms. This is all done automatically in the Maple package `SERGI`. See the webpage of this article for lots of sample input and output.

Above we assumed that the members of the set P are all of the same length, k. Of course more general scenarios can be reduced to this case, where k would be the largest length that shows up in P. Note that with this approach we end up with a set of $(k-1)!$ functional equations in the $(k-1)!$ "functions" (or rather formal power series) f_p.

The Negative Approach

Suppose that we want to compute quickly the first 100 terms (or whatever) of the sequence enumerating n-permutations avoiding the pattern $[1, 2, \ldots, 20]$. As we have already noted, using the "positive" approach, we have to set-up a *system* of functional equations with 19! equations and 19! unknowns. While the algorithm is still *polynomial* in n (and would give a "Wilfian" answer), it is not very practical! (This is yet another illustration why the ruling paradigm in theoretical computer science, of equating "polynomial time" with "fast" is (sometimes) absurd).

This is analogous to computing words in a *finite* alphabet, say of a letters, avoiding a given word (or words) as *factors* (consecutive subwords). If the word-to-avoid has length k, then the naive transfer-matrix method would require setting up a system of a^{k-1} equations and a^{k-1} unknowns. The elegant and powerful *Goulden-Jackson method* [6, 7], beautifully exposited and extended in [11], and even further extended in [9], enables one to do it by solving one equation in one unknown. We assume that the reader is familiar with it, and briefly describe the analog for the present problem, where the alphabet is "infinite". This is also the approach pursued in the beautiful human-generated papers [2] and [8]. We repeat that the *focus* and *novelty* in the present work is in *automating* enumeration, and the current topic of consecutive pattern-avoidance is used as a *case-study*.

First, some generalities! For ease of exposition, let's focus on a single pattern p (the case of several patterns is analogous, see [2]).

Using the inclusion-exclusion "negative" philosophy for counting, fix a pattern p. For any n-permutation, let $Patt_p(\pi)$ be the set of occurrences of the pattern p in π. For example

$$Patt_{123}(179234568) = \{179, 234, 345, 456, 568\},$$
$$Patt_{231}(179234568) = \{792\},$$
$$Patt_{312}(179234568) = \{923\},$$
$$Patt_{132}(179234568) = Patt_{213}(179234568) = Patt_{321}(179234568) = \emptyset.$$

Consider the much larger set of pairs

$$\{[\pi, S] |\ \pi \in S_n,\ \ S \subset Patt_p(\pi)\},$$

and define

$$weight_p[\pi, S] := (t-1)^{|S|},$$

where $|S|$ is the number of elements of S. For example,

$$weight_{123}[179234568, \{234, 568\}] = (t-1)^2,$$
$$weight_{123}[179234568, \{179\}] = (t-1)^1 = t-1,$$
$$weight_{123}[179234568, \emptyset] = (t-1)^0 = 1.$$

Fix a (consecutive) pattern p of length k, and consider the weight-enumerator of all n-permutations according to the weight

$$w(\pi) := t^{\#occurrences\ of\ pattern\ p\ in\ \pi},$$

let's call it $P_n(t)$. So:

$$P_n(t) := \sum_{\pi \in S_n} t^{|Patt_p(\pi)|}.$$

Now we need the *crucial*, extremely deep, fact:

$$t = (t-1) + 1,$$

and its corollary (for any finite set S):

$$t^{|S|} = ((t-1)+1)^{|S|} = \prod_{s \in S}((t-1)+1) = \sum_{T \subset S}(t-1)^{|T|}.$$

Putting this into the definition of $P_n(t)$, we get:

$$P_n(t) := \sum_{\pi \in S_n} t^{|Patt_p(\pi)|} = \sum_{\pi \in S_n} \sum_{T \subset Patt_p(\pi)} (t-1)^{|T|}.$$

This is the weight-enumerator (according to a different weight, namely $(t-1)^{|T|}$) of a much larger set, namely the set of *pairs*, (π, T), where T is a subset of $Patt_p(\pi)$. Surprisingly, this is much easier to handle!

Consider a typical such "creature" (π, T). There are two cases

Case I: The last entry of π, π_n does not belong to any of the members of T, in which case chopping it off produces a shorter such creature, in the set $\{1, 2, \ldots, n\} \backslash \{\pi_n\}$, and reducing both π and T to $\{1, \ldots, n-1\}$ yields a typical member of size $n-1$. Since there are n choices for π_n, the weight-enumerator of creatures of this type (where the last entry does not belong to any member of T) is $nP_{n-1}(t)$.

Case II: Let's order the members of T by their first (or last) index:

$$[s_1, s_2, \ldots, s_p],$$

where the last entry of π, π_n, belongs to s_p. If s_p and s_{p-1} are disjoint, the ending cluster is simply $[s_p]$. Otherwise s_p intersects s_{p-1}. If s_{p-1} and s_{p-2} are disjoint, then the ending cluster is $[s_{p-1}, s_p]$. More generally, the ending cluster of the pair $[\pi, [s_1, \ldots, s_p]]$ is the unique list $[s_i, \ldots, s_p]$ that has the property that s_i intersects s_{i+1}, s_{i+1} intersects s_{i+2}, ..., s_{p-1} intersects s_p, but s_{i-1} does not intersect s_i. It is possible that the ending cluster of $[\pi, T]$ is the whole T.

Let's give an example: with the pattern 123. The ending cluster of the pair:

$$[157423689, [157, 236, 368, 689]]$$

is $[236, 368, 689]$ since 236 overlaps with 368 (in two entries) and 368 overlaps with 689 (also in two entries), while 157 is disjoint from 236.

Now if you remove the ending cluster of T from T and remove the entries participating in the cluster from π, you get a shorter creature $[\pi', T']$ where π' is the permutation with all the entries in the ending cluster removed, and T' is what remains of T after we removed that cluster. In the above example, we have

$$[\pi', T'] = [1574, [157]].$$

Suppose that the length of π' is r.

Let $C_n(t)$ be the weight-enumerator, according to the weight $(t-1)^{|T|}$, of canonical clusters of length n, i.e., those whose set of entries is $\{1, \ldots, n\}$. Then in Case II we have to choose a subset of $\{1, \ldots, n\}$ of cardinality $n-r$ to be the set of entries of $[\pi', T']$ and then choose a creature of size $n-r$ and a cluster of size r. Combining Cases I and II, we have, $P_0(t) = 1$, and for $n \geq 1$:

$$P_n(t) = nP_{n-1}(t) + \sum_{r=2}^{n} \binom{n}{r} P_{n-r}(t) C_r(t).$$

Now it is time to consider the *exponential generating function*

$$F(z,t) := \sum_{n=0}^{\infty} \frac{P_n(t)}{n!} z^n.$$

We have

$$\begin{aligned}
F(z,t) &:= 1 + \sum_{n=1}^{\infty} \frac{P_n(t)}{n!} z^n = \\
&= 1 + \sum_{n=1}^{\infty} \frac{nP_{n-1}(t)}{n!} z^n + \sum_{n=0}^{\infty} \frac{1}{n!} \left(\sum_{r=2}^{n} \binom{n}{r} P_{n-r}(t) C_r(t) \right) z^n \\
&= 1 + z \sum_{n=1}^{\infty} \frac{P_{n-1}(t)}{(n-1)!} z^{n-1} + \sum_{n=0}^{\infty} \frac{1}{n!} \left(\sum_{r=2}^{n} \frac{n!}{r!(n-r)!} P_{n-r}(t) C_r(t) \right) z^n \\
&= 1 + z \sum_{n=0}^{\infty} \frac{P_n(t)}{n!} z^n + \sum_{n=0}^{\infty} \left(\sum_{r=2}^{n} \frac{1}{r!(n-r)!} P_{n-r}(t) C_r(t) \right) z^n \\
&= 1 + zF(z,t) + \sum_{n=0}^{\infty} \left(\sum_{r=2}^{n} \frac{P_{n-r}(t)}{(n-r)!} C_r(t) r! \right) z^n \\
&= 1 + zF(z,t) + \left(\sum_{n-r=0}^{\infty} \frac{P_{n-r}(t)}{(n-r)!} z^{n-r} \right) \left(\sum_{r=0}^{\infty} \frac{C_r(t)}{r!} z^r \right),
\end{aligned}$$

since $C_0(t) = 0, C_1(t) = 0$, and this equals

$$= 1 + zF(z,t) + F(z,t)G(z,t),$$

where $G(z,t)$ is the exponential generating function of $C_n(t)$:

$$G(z,t) := \sum_{n=0}^{\infty} \frac{C_n(t)}{n!} z^n.$$

It follows that

$$F(z,t) = 1 + zF(z,t) + F(z,t)G(z,t),$$

leading to

$$F(z,t) = \frac{1}{1 - z - G(z,t)}.$$

So if we had a quick way to compute the sequence $C_n(t)$, we would have a quick way to compute the first *whatever* coefficients (in z) of $F(z,t)$ (i.e., as many $P_n(t)$ as desired).

A Fast Way to Compute $C_n(t)$

For the sake of pedagogy let the fixed pattern be 1324. Consider a typical cluster

$$[13254768, [1325, 2547, 4768]].$$

If we remove the last atom of the cluster, we get the cluster

$$[132547, [1325, 2547]],$$

of the set $\{1, 2, 3, 4, 5, 7\}$. Its canonical form, reduced to the set $\{1, 2, 3, 4, 5, 6\}$, is:

$$[132546, [1325, 2546]].$$

Because of the "Markovian property" (chopping the last atom of the clusters and reducing yields a shorter cluster), we can build-up such a cluster, and in order to know how to add another atom, all we need to know is the current last atom. If the pattern is of length k (in this example, $k = 4$), we need only to keep track of the last k entries. Let the sorted list (from small to large) be $i_1 < \cdots < i_k$, so the last atom of the cluster (with r atoms) is $s_r = [i_{p_1}, \ldots, i_{p_k}]$, where $1 \le i_1 < i_2 < \cdots < i_k \le n$ is some increasing sequence of k integers between 1 and n. We introduce k *catalytic* variables $x_1, \ldots, x_k$, and define

$$Weight([s_1, \ldots, s_{r-1}, [i_{p_1}, \ldots, i_{p_k}]]) := z^n (t-1)^r x_1^{i_1} \cdots x_k^{i_k}.$$

Going back to the 1324 example, if we currently have a cluster with r atoms, whose last atom is $[i_1, i_3, i_2, i_4]$, how can we add another atom? Let's call it $[j_1, j_3, j_2, j_4]$. This new atom can overlap with the former one in two possibilities.

(a) If the overlap is of length 2:

$$j_1 = i_2 \quad j_3 = i_4,$$

but because of the "reduction" (making room for the new entries) it is really

$$j_1 = i_2 \quad j_3 = i_4 + 1,$$

(and j_2 and j_4 can be what they wish as long as $i_2 < j_2 < i_4 + 1 < j_4 \le n$).

(b) If the overlap is of length 1:

$$j_1 = i_4$$

(and j_2, j_3, j_4 can be what they wish, provided that $i_4 < j_2 < j_3 < j_4 \le n$).

Hence we have the "umbral-evolution":

$$z^n(t-1)^{r-1}x_1^{i_1}x_2^{i_2}x_3^{i_3}x_4^{i_4} \to z^{n+2}(t-1)^r \sum_{1\le j_1=i_2<j_2<j_3=i_4+1<j_4\le n} x_1^{j_1}x_2^{j_2}x_3^{j_3}x_4^{j_4}$$
$$+z^{n+3}(t-1)^r \sum_{1\le j_1=i_4<j_2<j_3<j_4\le n} x_1^{j_1}x_2^{j_2}x_3^{j_3}x_4^{j_4}.$$

These two iterated geometrical sums can be summed exactly, and from this "pre-umbra" the computer can deduce (automatically!) the umbral operator, yielding a functional equation for the **ordinary** generating function

$$\mathcal{C}(t,z;x_1,\ldots,x_k) = \sum_{n=0}^{\infty} C_n(t;x_1,\ldots,x_k)z^n,$$

of the form

$$\mathcal{C}(t,z;x_1,\ldots,x_k) = (t-1)z^k x_1x_2^2\ldots x_k^k +$$
$$+ \sum\nolimits_{\alpha} R_\alpha(x_1,\ldots,x_k;t,z)\mathcal{C}(t,z;M_1^\alpha,\ldots,M_k^\alpha),$$

where $\{\alpha\}$ is a finite index set, $M_1^\alpha,\ldots,M_k^\alpha$ are specific monomials in $x_1, \ldots, x_k$, z, derived by the algorithm, and R_α are certain rational functions of their arguments, also derived by the algorithm.

Once again, the novelty here is that everything (except for the initial Maple programming) is done *automatically* by the computer. It is the computer doing combinatorial research all on its own!

Post-processing the Functional Equation

At the end of the day we are only interested in $\mathcal{C}(t,z;1,\ldots,1)$. Alas, plugging in $x_1 = 1, x_2 = 1, \ldots, x_k = 1$ would give lots of $0/0$. Taking the limits, and using L'Hôpital, is an option, but then we get a differential equation that would introduce differentiations with respect to the catalytic variables, and we would not gain anything.

But it so happens, in many cases, that the functional operator preserves some of the exponents of the $x_i's$. For example for the pattern 321 the last three entries are always $[3,2,1]$, and one can do a *change of dependent variable*:

$$\mathcal{C}(t,z;x_1,\ldots,x_3) = x_1x_2^2x_3^3g(z;t),$$

and *now* plugging in $x_1 = 1, x_2 = 1, x_3 = 1$ is harmless, and one gets a much simpler functional equation with *no* catalytic variables, that turns out to be (according to S.B. Ekhad) the simple algebraic equation

$$g(z,t) = -(t-1)z^2 - (t-1)(z+z^2)g(z,t),$$

that in this case can be solved in closed-form (reproducing a result that goes back to [EN]). Other times (like the pattern 231), we only get rid of some of the catalytic variables. Putting

$$\mathcal{C}(t,z;x_1,\ldots,x_3) = x_1x_2^2 g(x_3,z;t),$$

(and then plugging in $x_1 = 1, x_2 = 1$) gives a much simplified functional equation, and now taking the limit $x_3 \to 1$ and using L'Hôpital (that Maple does all by itself) one gets a pure differential equation for $g(1,z;t)$, in z, that sometimes can be even solved in closed form (automatically by Maple). But from the point of view of efficient enumeration, it is just as well to leave it at that.

Any pattern p is trivially equivalent to (up to) three other patterns (its reverse, its complement, and the reverse-of-the-complement, some of which may coincide). It turns out that out of these (up to) four options, there is one that is easiest to handle, and the computer finds this one, by finding which ones gives the simplest functional (or, if in luck, differential or algebraic) equation, and goes on to handle only this representative.

The Maple Package ELIZALDE

All of this is implemented in the Maple package `ELIZALDE`, that automatically produces *theorems* and *proofs*. Lots of sample output (including computer-generated theorems and *proofs*) can be found on the webpage of this article:
http://www.math.rutgers.edu/~zeilberg/mamarim/mamarimhtml/auto.html.
In particular, to see all theorems and *proofs* for patterns of lengths 3 through 5 go to (respectively):
http://www.math.rutgers.edu/~zeilberg/tokhniot/sergi/oEP3_200,
http://www.math.rutgers.edu/~zeilberg/tokhniot/sergi/oEP4_60,
http://www.math.rutgers.edu/~zeilberg/tokhniot/sergi/oEP5_40.
If the proofs bore you, and by now you believe Shalosh B. Ekhad, and you only want to see the statements of the *theorems*, for lengths 3 through 6 go to (respectively):
http://www.math.rutgers.edu/~zeilberg/tokhniot/sergi/oET3_200,
http://www.math.rutgers.edu/~zeilberg/tokhniot/sergi/oET4_60,
http://www.math.rutgers.edu/~zeilberg/tokhniot/sergi/oET5_40,
http://www.math.rutgers.edu/~zeilberg/tokhniot/sergi/oET6_30.

Humans, with their short attention spans, would probably soon get tired of even the statements of most of the theorems of this last file (for patterns of length 6).

In addition to "symbol crunching" this package does quite a lot of "number crunching" (of course using the former). To see the "hit parade", ranked by size, together with the conjectured asymptotic growth for single consẽcũtive-pattern

avoidance of lengths between 3 and 6, see, respectively, the output files:
http://www.math.rutgers.edu/~zeilberg/tokhniot/sergi/oE3_200,
http://www.math.rutgers.edu/~zeilberg/tokhniot/sergi/oE4_60,
http://www.math.rutgers.edu/~zeilberg/tokhniot/sergi/oE5_40,
http://www.math.rutgers.edu/~zeilberg/tokhniot/sergi/oE6_30.

Enjoy!

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Watson–Like Formulae for Terminating ${}_3F_2$-Series

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Abstract Several closed formulae are established for terminating Watson–like hypergeometric ${}_3F_2$-series by investigating, through Gould and Hsu's fundamental pair of inverse series relations, the dual relations of Dougall's formula for the very well–poised ${}_5F_4$-series.

1 Introduction and Preliminaries

Following Bailey [1], the classical hypergeometric series, for an indeterminate z and two nonnegative integers p and q, is defined by

$$ {}_{1+p}F_q\left[\begin{matrix} a_0, a_1, \cdots, a_p \\ b_1, \cdots, b_q \end{matrix}\,\middle|\, z\right] = \sum_{k=0}^{\infty} \frac{(a_0)_k (a_1)_k \cdots (a_p)_k}{k!(b_1)_k \cdots (b_q)_k} z^k $$

where the rising shifted–factorial reads as

$$ (x)_0 = 1 \quad \text{and} \quad (x)_n = x(x+1)\cdots(x+n-1) \quad \text{for} \quad n \in \mathbb{N} $$

with its multi–parameter form being abbreviated as

$$ \left[\begin{matrix} \alpha, \ \beta, \ \cdots, \ \gamma \\ A, \ B, \ \cdots, \ C \end{matrix}\right]_n = \frac{(\alpha)_n (\beta)_n \cdots (\gamma)_n}{(A)_n (B)_n \cdots (C)_n}. $$

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When one of numerator parameters $\{a_k\}$ is a negative integer, then the hypergeometric series becomes terminating, which reduces to a polynomial in z.

Around 15 years ago, Chu [3, 4] devised a systematic approach "inversion techniques" to prove terminating hypergeometric series identities. The method is based on a fundamental pair of the inverse series relations discovered by Gould and Hsu [9, 1973]. For its extensions and further applications, the interested reader may refer to the papers [2,5,6]. In order to facilitate the subsequent application, we reproduce Gould and Hsu's inversions as follows. Let $\{a_k, b_k\}_{k\geq 0}$ be two sequences such that the φ-polynomials defined by

$$\varphi(x;0) \equiv 1 \quad \text{and} \quad \varphi(x;n) = \prod_{k=0}^{n-1}(a_k + xb_k) \quad \text{with} \quad n \in \mathbb{N} \tag{1}$$

differ from zero for $x, n \in \mathbb{N}_0$. Then there hold the inverse series relations

$$f(m) = \sum_{k=0}^{m}(-1)^k \binom{m}{k}\varphi(k;m)g(k); \tag{2}$$

$$g(m) = \sum_{k=0}^{m}(-1)^k \binom{m}{k}\frac{a_k + kb_k}{\varphi(m;k+1)}f(k). \tag{3}$$

Among numerous summation formulae for hypergeometric series, Dougall's theorem [8, 1907] (cf. Bailey [1, §4.4]) for the very well–poised ${}_5F_4$–series has been very useful. One of its terminating version can be expressed as

$${}_5F_4\left[\begin{matrix} u, & 1+\frac{u}{2}, & \frac{1}{2}+u-v, & \frac{-m}{2}, & \frac{1-m}{2} \\ & \frac{u}{2}, & \frac{1}{2}+v, & u+\frac{2+m}{2}, & u+\frac{1+m}{2} \end{matrix} \,\middle|\, 1\right] = \left[\begin{matrix} 1+2u, v \\ \frac{1}{2}+u, 2v \end{matrix}\right]_m.$$

By investigating, through the inversion machinery, linear combinations of the last ${}_5F_4$-series with different parameter settings for u, v and m, we shall evaluate the following terminating ${}_3F_2$–series

$$\mathcal{W}_{\varepsilon,\delta}(m|u,v) \;=\; {}_3F_2\left[\begin{matrix} -m, & m+2u, & v \\ & u+\frac{\varepsilon}{2}, & \delta+2v \end{matrix} \,\middle|\, 1\right] \tag{4}$$

where ε and δ are integers. They can be considered as terminating variants of Watson's ${}_3F_2$-series (cf. Bailey [1, §3.3 and §3.4] and [14])

$${}_3F_2\left[\begin{matrix} a, & b, & c \\ \frac{1+a+b}{2}, & 2c & \end{matrix} \,\middle|\, 1\right] = \Gamma\left[\begin{matrix} \frac{1}{2}, & \frac{1+a+b}{2}, & \frac{1}{2}+c, & \frac{1-a-b}{2}+c \\ \frac{1+a}{2}, & \frac{1+b}{2}, & \frac{1-a}{2}+c, & \frac{1-b}{2}+c \end{matrix}\right]$$

because when terminating by $a = -m$ and $b = m + 2u$, this series can be restated equivalently as Watson's original expression [15]

$$ {}_3F_2\left[\begin{matrix}-m,\ m+2u,\ v\\ u+\frac{1}{2},\ 2v\end{matrix}\,\middle|\,1\right]=\begin{cases}\left[\begin{matrix}\frac{1}{2}, & \frac{1}{2}+u-v\\ \frac{1}{2}+u, & \frac{1}{2}+v\end{matrix}\right]_n, & m=2n;\\ 0, & m=2n+1.\end{cases} $$

This identity results in the dual formula of the Dougall sum via Gould and Hsu's inversion pair (2) and (3). To illustrate our approach, this can be confirmed briefly as follows. Write equivalently the foregoing ${}_5F_4$-series in terms of a binomial sum

$$ \mathfrak{D}_m(u,v)=\left[\begin{matrix}2u,v\\ u+\frac{1}{2},2v\end{matrix}\right]_m=\sum_{k\geq 0}\binom{m}{2k}\frac{2u+4k}{(2u+m)_{2k+1}}\left[\begin{matrix}u,u-v+\frac{1}{2}\\ v+\frac{1}{2}\end{matrix}\right]_k\frac{(2k)!}{k!}. \tag{5} $$

Observe that the last equation can be obtained from (3) by specifying

$$ g(m)=\left[\begin{matrix}2u,v\\ u+\frac{1}{2},2v\end{matrix}\right]_m \quad\text{and}\quad \varphi(x;n)=(2u+x)_n $$

as well as

$$ f(2k)=\frac{(2k)!}{k!}\left[\begin{matrix}u,u-v+\frac{1}{2}\\ v+\frac{1}{2}\end{matrix}\right]_k \quad\text{and}\quad f(2k+1)=0. $$

We have the dual relation corresponding to (2) as follows

$$ \sum_{k=0}^{m}(-1)^k\binom{m}{k}(2u+k)_m\left[\begin{matrix}2u,v\\ u+\frac{1}{2},2v\end{matrix}\right]_k=\begin{cases}\frac{(2n)!}{n!}\left[\begin{matrix}u,u-v+\frac{1}{2}\\ v+\frac{1}{2}\end{matrix}\right]_n, & m=2n;\\ 0, & m=2n+1.\end{cases} $$

In terms of hypergeometric series, this becomes Watson's original identity.

This example encourages us to explore further identities for the ${}_3F_2$-series displayed in (4). In the next section, nine identities for $\mathcal{W}_{\varepsilon,\delta}(m|u,v)$ will be shown in detail by applying the Gould–Hsu inversions (2) and (3) to linear combinations of $\mathfrak{D}_m(u,v)$ displayed in (5). The same approach can be employed to demonstrate further identities with 22 selected ones being tabulated in the third section, which cover the formulae for $\mathcal{W}_{\varepsilon,\delta}(m|u,v)$ with ε and δ being small integers.

Fifteen years ago, Lewanowicz [13] succeeded in determining analytical formulae for generalized Watson series, which have further been improved by Chu [7] recently. However, the formulae derived in these both papers are too involved in double sum expressions. Compared with the method utilized in [7, 13], the approach employed here is totally different and more direct as it leads to finding several elegant formulae expressed in terms of factorial quotients by treating directly with the terminating series $\mathcal{W}_{\varepsilon,\delta}(m|u,v)$. To our knowledge, most of the identities proved in this paper do not seem to have explicitly appeared previously except for

Theorem 5 whose particular case has been found by Larcombe and Larsen [12] recently. In order to assure the accuracy of mathematical computations, we have appropriately devised a *Mathematica* package to check all the displayed formulae.

2 Nine Identities and Their Proofs

By utilizing Gould and Hsu's inversion pair (2) and (3) to linear combinations of $\mathfrak{D}_m(u,v)$ displayed in (5), this section will demonstrate nine identities for $\mathcal{W}_{\varepsilon,\delta}(m|u,v)$, which are divided into nine subsections with subsection headers being labeled by (ε,δ) parameters.

2.1 $\varepsilon = 0$ *and* $\delta = 0$

For the following Dougall sum

$$\begin{bmatrix} 2u, v \\ u, 2v \end{bmatrix}_m = \frac{2u+2m}{2u+m}\mathfrak{D}_m(u+\tfrac{1}{2}, v)$$

we can write it explicitly as

$$\begin{bmatrix} 2u, v \\ u, 2v \end{bmatrix}_m = (2u+2m)\sum_{k\geq 0}\binom{m}{2k}\frac{2u+4k+1}{(2u+m)_{2k+2}}\begin{bmatrix} u+\frac{1}{2}, u-v+1 \\ v+\frac{1}{2} \end{bmatrix}_k \frac{(2k)!}{k!}.$$

According to the two–term relation

$$2u+2m = \frac{(2u+m+2k+1)(2u+4k)}{2u+4k+1} + \frac{(m-2k)(2u+4k+2)}{2u+4k+1}$$

we get correspondingly the expression of two binomial sums

$$\begin{bmatrix} 2u, v \\ u, 2v \end{bmatrix}_m = \sum_{k\geq 0}\binom{m}{2k}\frac{(2u+4k)f(2k)}{(2u+m)_{2k+1}} - \sum_{k\geq 0}\binom{m}{2k+1}\frac{(2u+4k+2)f(2k+1)}{(2u+m)_{2k+2}}$$

where $f(k)$ is given explicitly by

$$f(2k) = \frac{(2k)!}{k!}\begin{bmatrix} u+\frac{1}{2}, u-v+1 \\ v+\frac{1}{2} \end{bmatrix}_k,$$

$$f(2k+1) = -\frac{(2k+1)!}{k!}\begin{bmatrix} u+\frac{1}{2}, u-v+1 \\ v+\frac{1}{2} \end{bmatrix}_k.$$

Comparing the last equation with (3) under the specifications

$$g(m) = \begin{bmatrix} 2u, v \\ u, 2v \end{bmatrix}_m \quad \text{and} \quad \varphi(x;n) = (2u+x)_n$$

we find the following dual relation corresponding to (2)

$$\sum_{k=0}^{m} (-1)^k \binom{m}{k} (2u+k)_m \begin{bmatrix} 2u, v \\ u, 2v \end{bmatrix}_k = \begin{cases} f(2n), & m = 2n; \\ f(2n+1), & m = 2n+1. \end{cases}$$

In terms of hypergeometric series, this yields the following identity.

Theorem 1 (Terminating series identity).

$${}_3F_2\left[\begin{matrix} -m, m+2u, & v \\ u, & 2v \end{matrix} \,\middle|\, 1\right] = \begin{cases} \begin{bmatrix} \frac{1}{2}, u-v+1 \\ u, v+\frac{1}{2} \end{bmatrix}_n, & m = 2n; \\ \begin{bmatrix} \frac{3}{2}, u-v+1 \\ u+1, v+\frac{1}{2} \end{bmatrix}_n \frac{-1}{2u}, & m = 2n+1. \end{cases}$$

2.2 $\varepsilon = 2$ and $\delta = 0$

The following Dougall sum

$$\begin{bmatrix} 2u, v \\ u+1, 2v \end{bmatrix}_m = \frac{2u}{2u+m} \mathfrak{D}_m(u+\tfrac{1}{2}, v)$$

can analogously be restated as the equality

$$\begin{bmatrix} 2u, v \\ u+1, 2v \end{bmatrix}_m = 2u \sum_{k \geq 0} \binom{m}{2k} \frac{2u+4k+1}{(2u+m)_{2k+2}} \begin{bmatrix} u+\frac{1}{2}, u-v+1 \\ v+\frac{1}{2} \end{bmatrix}_k \frac{(2k)!}{k!}.$$

Inserting the expression

$$1 = \frac{2u+m+2k+1}{2u+4k+1} - \frac{m-2k}{2u+4k+1}$$

into the binomial sum, we can reformulate it as

$$\begin{aligned}\begin{bmatrix} 2u, v \\ u+1, 2v \end{bmatrix}_m &= \sum_{k\geq 0}\binom{m}{2k}\frac{(2u+4k)f(2k)}{(2u+m)_{2k+1}} \\ &\quad - \sum_{k\geq 0}\binom{m}{2k+1}\frac{(2u+4k+2)f(2k+1)}{(2u+m)_{2k+2}}\end{aligned}$$

where $f(k)$ is given explicitly by

$$\begin{aligned}f(2k) &= \frac{(2k)!}{k!}\begin{bmatrix} u+\frac{1}{2}, u-v+1 \\ v+\frac{1}{2} \end{bmatrix}_k \frac{u}{u+2k}, \\ f(2k+1) &= \frac{(2k+1)!}{k!}\begin{bmatrix} u+\frac{1}{2}, u-v+1 \\ v+\frac{1}{2} \end{bmatrix}_k \frac{u}{u+2k+1}.\end{aligned}$$

This equation matches exactly (3) under the following specifications

$$g(m) = \begin{bmatrix} 2u, v \\ u+1, 2v \end{bmatrix}_m \quad \text{and} \quad \varphi(x;n) = (2u+x)_n.$$

Then the dual relation corresponding to (2) reads as

$$\sum_{k=0}^{m}(-1)^k\binom{m}{k}(2u+k)_m\begin{bmatrix} 2u, v \\ u+1, 2v \end{bmatrix}_k = \begin{cases} f(2n), & m=2n; \\ f(2n+1), & m=2n+1. \end{cases}$$

In terms of hypergeometric series, this gives the following identity.

Theorem 2 (Terminating series identity).

$${}_3F_2\left[\begin{matrix} -m, m+2u, & v \\ u+1, & 2v \end{matrix}\,\middle|\, 1\right] = \begin{cases} \begin{bmatrix} \frac{1}{2}, u-v+1 \\ u, v+\frac{1}{2} \end{bmatrix}_n \dfrac{u}{u+2n}, & m=2n; \\ \begin{bmatrix} \frac{3}{2}, u-v+1 \\ u+1, v+\frac{1}{2} \end{bmatrix}_n \dfrac{1}{2(u+2n+1)}, & m=2n+1. \end{cases}$$

2.3 $\varepsilon = 0$ and $\delta = 1$

According to the linear combination

$$\begin{bmatrix} 2u, v \\ u, 2v+1 \end{bmatrix}_m = \frac{4(u-v)}{2u+m}\mathfrak{D}_m(u+\tfrac{1}{2}, v) - \frac{2(u-2v)(2v+m+1)}{(2u+m)(2v+1)}\mathfrak{D}_m(u+\tfrac{1}{2}, v+1)$$

there holds explicitly the following equality

$$\begin{bmatrix} 2u, v \\ u, 2v+1 \end{bmatrix}_m = \sum_{k\geq 0}\binom{m}{2k}\frac{2u+4k+1}{(2u+m)_{2k+2}}\begin{bmatrix} u+\frac{1}{2}, u-v \\ v+\frac{3}{2} \end{bmatrix}_k \frac{(2k)!}{k!} \times \frac{4(u-v+k)(2v+2k+1)-2(u-2v)(2v+m+1)}{2v+1}.$$

Reformulating the fraction displayed in the last line

$$\frac{(2u+m+2k+1)(2v+2k+1)(2u+4k)}{(2u+4k+1)(2v+1)} - \frac{(m-2k)(2u+4k+2)(2u-2v+2k)}{(2u+4k+1)(2v+1)}$$

we have correspondingly the binomial sum expression

$$\begin{bmatrix} 2u, v \\ u, 2v+1 \end{bmatrix}_m = \sum_{k\geq 0}\binom{m}{2k}\frac{(2u+4k)f(2k)}{(2u+m)_{2k+1}} - \sum_{k\geq 0}\binom{m}{2k+1}\frac{(2u+4k+2)f(2k+1)}{(2u+m)_{2k+2}}$$

where $f(k)$ is given explicitly by

$$f(2k) = \frac{(2k)!}{k!}\begin{bmatrix} u+\frac{1}{2}, u-v \\ v+\frac{1}{2} \end{bmatrix}_k,$$

$$f(2k+1) = \frac{(2k+1)!}{k!}\begin{bmatrix} u+\frac{1}{2}, u-v \\ v+\frac{3}{2} \end{bmatrix}_k \frac{2u-2v+2k}{2v+1}.$$

This equation fits in well with (3) under the following specifications

$$g(m) = \begin{bmatrix} 2u, v \\ u, 2v+1 \end{bmatrix}_m \quad \text{and} \quad \varphi(x;n) = (2u+x)_n.$$

Then the dual relation corresponding to (2) results in

$$\sum_{k=0}^{m}(-1)^k\binom{m}{k}(2u+k)_m\left[\begin{matrix}2u, v\\ u, 2v+1\end{matrix}\right]_k = \begin{cases} f(2n), & m=2n;\\ f(2n+1), & m=2n+1.\end{cases}$$

In terms of hypergeometric series, this becomes the following identity.

Theorem 3 (Terminating series identity).

$${}_3F_2\left[\begin{matrix}-m, m+2u, & v\\ u, & 2v+1\end{matrix}\middle| 1\right] = \begin{cases} \left[\begin{matrix}\frac{1}{2}, u-v\\ u, v+\frac{1}{2}\end{matrix}\right]_n, & m=2n;\\ \left[\begin{matrix}\frac{1}{2}, u-v\\ u, v+\frac{1}{2}\end{matrix}\right]_{n+1}, & m=2n+1.\end{cases}$$

2.4 $\varepsilon = 1$ and $\delta = 1$

From the linear combination

$$\left[\begin{matrix}2u, v\\ u+\frac{1}{2}, 2v+1\end{matrix}\right]_m = \mathfrak{D}_m(u,v) - \frac{2um}{(2u+m)(2v+1)}\mathfrak{D}_{m-1}(u+1, v+1)$$

we can write it explicitly as the following equality

$$\left[\begin{matrix}2u, v\\ u+\frac{1}{2}, 2v+1\end{matrix}\right]_m = \sum_{k\geq 0}\binom{m}{2k}\frac{2u+4k}{(2u+m)_{2k+1}}\left[\begin{matrix}u, u-v+\frac{1}{2}\\ v+\frac{1}{2}\end{matrix}\right]_k\frac{(2k)!}{k!}$$
$$-\frac{2um}{(2u+m)(2v+1)}\sum_{k\geq 0}\binom{m-1}{2k}\frac{2u+4k+2}{(2u+m+1)_{2k+1}}\left[\begin{matrix}u+1, u-v+\frac{1}{2}\\ v+\frac{3}{2}\end{matrix}\right]_k\frac{(2k)!}{k!}.$$

This can be reformulated, in turn, as the binomial sum expression

$$\left[\begin{matrix}2u, v\\ u+\frac{1}{2}, 2v+1\end{matrix}\right]_m = \sum_{k\geq 0}\binom{m}{2k}\frac{(2u+4k)f(2k)}{(2u+m)_{2k+1}}$$
$$-\sum_{k\geq 0}\binom{m}{2k+1}\frac{(2u+4k+2)f(2k+1)}{(2u+m)_{2k+2}}$$

where $f(k)$ is given explicitly by

$$f(2k) = \frac{(2k)!}{k!}\begin{bmatrix} u, u-v+\frac{1}{2} \\ v+\frac{1}{2} \end{bmatrix}_k,$$

$$f(2k+1) = \frac{(2k+1)!}{k!}\begin{bmatrix} u+1, u-v+\frac{1}{2} \\ v+\frac{3}{2} \end{bmatrix}_k \frac{2u}{2v+1}.$$

Comparing the last equation with (3) specified by

$$g(m) = \begin{bmatrix} 2u, v \\ u+\frac{1}{2}, 2v+1 \end{bmatrix}_m \quad \text{and} \quad \varphi(x;n) = (2u+x)_n$$

we can write down the dual relation corresponding to (2) as

$$\sum_{k=0}^{m}(-1)^k\binom{m}{k}(2u+k)_m\begin{bmatrix} 2u, v \\ u+\frac{1}{2}, 2v+1 \end{bmatrix}_k = \begin{cases} f(2n), & m=2n; \\ f(2n+1), & m=2n+1; \end{cases}$$

which is equivalent to the following hypergeometric series identity.

Theorem 4 (Terminating series identity).

$${}_3F_2\left[\begin{matrix} -m, m+2u, & v \\ u+\frac{1}{2}, & 2v+1 \end{matrix}\,\middle|\, 1\right] = \begin{cases} \begin{bmatrix} \frac{1}{2}, u-v+\frac{1}{2} \\ u+\frac{1}{2}, v+\frac{1}{2} \end{bmatrix}_n, & m=2n; \\ \begin{bmatrix} \frac{3}{2}, u-v+\frac{1}{2} \\ u+\frac{1}{2}, v+\frac{3}{2} \end{bmatrix}_n \dfrac{1}{2v+1}, & m=2n+1. \end{cases}$$

2.5 $\varepsilon = 2$ *and* $\delta = 1$

Taking into account of linear combination

$$\begin{bmatrix} 2u+1, v \\ u+1, 2v+1 \end{bmatrix}_m = 2\mathfrak{D}_m(u+\tfrac{1}{2}, v) - \frac{2v+m+1}{2v+1}\mathfrak{D}_m(u+\tfrac{1}{2}, v+1)$$

we have explicitly the following binomial equality

$$\begin{bmatrix} 2u+1, v \\ u+1, 2v+1 \end{bmatrix}_m = \sum_{k\geq 0}\binom{m}{2k}\frac{2u+4k+1}{(2u+m+1)_{2k+1}}\begin{bmatrix} u+\frac{1}{2}, u-v \\ v+\frac{3}{2} \end{bmatrix}\frac{(2k)!}{k!}$$
$$\times\ \frac{2(u-v+k)(2v+2k+1)-(u-v)(2v+m+1)}{(u-v)(2v+1)}.$$

Reformulating the fraction displayed in the last line

$$\frac{(2u+m+2k+1)(2v+2k+1)(u-v+2k)}{(2u+4k+1)(u-v)(2v+1)}-\frac{(m-2k)(u+v+2k+1)(2u-2v+2k)}{(2u+4k+1)(u-v)(2v+1)}$$

we have correspondingly the binomial sum expression

$$\begin{aligned}\left[\begin{matrix}2u, v\\ u+1, 2v+1\end{matrix}\right]_m &= \sum_{k\geq 0}\binom{m}{2k}\frac{(2u+4k)f(2k)}{(2u+m)_{2k+1}}\\ &\quad - \sum_{k\geq 0}\binom{m}{2k+1}\frac{(2u+4k+2)f(2k+1)}{(2u+m)_{2k+2}}\end{aligned}$$

where $f(k)$ is given explicitly by

$$\begin{aligned}f(2k) &= \frac{(2k)!}{k!}\left[\begin{matrix}u+\frac{1}{2}, u-v\\ v+\frac{1}{2}\end{matrix}\right]_k \frac{u(u-v+2k)}{(u-v)(u+2k)},\\ f(2k+1) &= \frac{(2k+1)!}{k!}\left[\begin{matrix}u+\frac{1}{2}, u-v+1\\ v+\frac{3}{2}\end{matrix}\right]_k \frac{2u(u+v+2k+1)}{(2v+1)(u+2k+1)}.\end{aligned}$$

The last equation can be obtained from (3) under the specifications

$$g(m) = \left[\begin{matrix}2u, v\\ u+1, 2v+1\end{matrix}\right]_m \quad \text{and} \quad \varphi(x;n) = (2u+x)_n.$$

Then the dual relation corresponding to (2) reads as

$$\sum_{k=0}^{m}(-1)^k\binom{m}{k}(2u+k)_m\left[\begin{matrix}2u, v\\ u+1, 2v+1\end{matrix}\right]_k = \begin{cases} f(2n), & m=2n;\\ f(2n+1), & m=2n+1.\end{cases}$$

In terms of hypergeometric series, this can be stated as the identity.

Theorem 5 (Terminating series identity).

$${}_3F_2\left[\begin{matrix}-m, m+2u, v\\ u+1, 2v+1\end{matrix}\,\middle|\, 1\right] = \begin{cases}\left[\begin{matrix}\frac{1}{2}, u-v\\ u, v+\frac{1}{2}\end{matrix}\right]_n \dfrac{u(u-v+m)}{(u-v)(u+m)}, & m=2n;\\ \left[\begin{matrix}\frac{3}{2}, u-v+1\\ u+1, v+\frac{3}{2}\end{matrix}\right]_n \dfrac{(u+v+m)}{(2v+1)(u+m)}, & m=2n+1.\end{cases}$$

When $u = 1$, $v = \frac{1}{2}$ and $m = 2n - 1$, this theorem becomes the following identity

$$ {}_3F_2\left[\begin{matrix} \frac{1}{2}, & 1+2n, & 1-2n \\ & 2, & 2 \end{matrix} \,\Big|\, 1\right] = \frac{1+4n}{2n}\left[\begin{matrix} \frac{1}{2}, & \frac{1}{2} \\ 1, & 1 \end{matrix}\right]_n \quad \text{for} \quad n \geq 1. $$

Larcombe and Larsen [12] proved recently its equivalent binomial sum

$$ 16^n \sum_{k=0}^{2n} 4^k \binom{\frac{1}{2}}{k}\binom{-\frac{1}{2}}{k}\binom{-2k}{2n-k} = (1+4n)\binom{2n}{n}^2 $$

which has been the primary motivation for us to investigate $\mathcal{W}_{\varepsilon,\delta}(m|u,v)$. Further different proofs of the last identity can be found in the papers by Gessel–Larcombe [10] and Koepf–Larcombe [11], where generating function approach and computer algebra have respectively been employed.

2.6 $\varepsilon = 0$ *and* $\delta = -1$

The linear combination

$$ \left[\begin{matrix} 2u, v \\ u, 2v-1 \end{matrix}\right]_m = 4\frac{v+m-1}{2u+m}\mathfrak{D}_m(u+\tfrac{1}{2}, v-1) + \frac{2(u-2v+2)(2v+m-1)}{(2u+m)(2v-1)}\mathfrak{D}_m(u+\tfrac{1}{2}, v) $$

is equivalent to the following binomial equality

$$ \left[\begin{matrix} 2u, v \\ u, 2v-1 \end{matrix}\right]_m = \sum_{k\geq 0}\binom{m}{2k}\frac{2u+4k+1}{(2u+m)_{2k+2}}\left[\begin{matrix} u+\frac{1}{2}, u-v+1 \\ v+\frac{1}{2} \end{matrix}\right]_k \frac{(2k)!}{k!} \times\left\{\frac{4(v+m-1)(u-v+k+1)(2v+2k-1)}{(u-v+1)(2v-1)} + \frac{2(u-2v+2)(2v+m-1)}{2v-1}\right\}. $$

Reformulating the fraction inside the braces as

$$ \frac{(2u+m+2k+1)(2u+4k)(2v+2k-1)(u-v+2k+1)}{(2u+4k+1)(u-v+1)(2v-1)} + \frac{2(m-2k)(2u+4k+2)(u+v+2k)(u-v+k+1)}{(2u+4k+1)(u-v+1)(2v-1)} $$

we have correspondingly the binomial sum expression

$$\begin{bmatrix} 2u, v \\ u, 2v-1 \end{bmatrix}_m = \sum_{k\geq 0}\binom{m}{2k}\frac{(2u+4k)f(2k)}{(2u+m)_{2k+1}} - \sum_{k\geq 0}\binom{m}{2k+1}\frac{(2u+4k+2)f(2k+1)}{(2u+m)_{2k+2}}$$

where $f(k)$ is given explicitly by

$$f(2k) = \frac{(2k)!}{k!}\begin{bmatrix} u+\frac{1}{2}, u-v+1 \\ v-\frac{1}{2} \end{bmatrix}_k \frac{u-v+2k+1}{u-v+1},$$

$$f(2k+1) = \frac{(2k+1)!}{k!}\begin{bmatrix} u+\frac{1}{2}, u-v+2 \\ v+\frac{1}{2} \end{bmatrix}_k \frac{2u+2v+4k}{1-2v}.$$

This equation matches exactly (3) under the following specifications

$$g(m) = \begin{bmatrix} 2u, v \\ u, 2v-1 \end{bmatrix}_m \quad \text{and} \quad \varphi(x;n) = (2u+x)_n.$$

Then the dual relation corresponding to (2) give rise to

$$\sum_{k=0}^{m}(-1)^k\binom{m}{k}(2u+k)_m\begin{bmatrix} 2u, v \\ u, 2v-1 \end{bmatrix}_k = \begin{cases} f(2n), & m=2n; \\ f(2n+1), & m=2n+1; \end{cases}$$

which leads to the following hypergeometric series identity.

Theorem 6 (Terminating series identity).

$$ {}_3F_2\left[\begin{matrix} -m, m+2u, v \\ u,\ 2v-1 \end{matrix}\,\middle|\, 1\right] = \begin{cases} \begin{bmatrix} \frac{1}{2}, u-v+1 \\ u, v-\frac{1}{2} \end{bmatrix}_n \dfrac{u-v+2n+1}{u-v+1}, & m=2n; \\ \begin{bmatrix} \frac{1}{2}, u-v+2 \\ u, v-\frac{1}{2} \end{bmatrix}_{n+1} \dfrac{u+v+2n}{v-u-n-2}, & m=2n+1. \end{cases}$$

2.7 $\varepsilon = 1$ *and* $\delta = -1$

For the linear combination

$$\left[\begin{matrix} 2u, v \\ u+\frac{1}{2}, 2v-1 \end{matrix}\right]_m = \mathfrak{D}_m(u, v-1) - \frac{2um}{(2u+m)(1-2v)}\mathfrak{D}_{m-1}(u+1, v)$$

we can state it explicitly the following equality

$$\left[\begin{matrix} 2u, v \\ u+\frac{1}{2}, 2v-1 \end{matrix}\right]_m = \sum_{k\geq 0}\binom{m}{2k}\frac{2u+4k}{(2u+m)_{2k+1}}\left[\begin{matrix} u, u-v+\frac{3}{2} \\ v-\frac{1}{2} \end{matrix}\right]_k \frac{(2k)!}{k!}$$
$$-\frac{2um}{(2u+m)(1-2v)}\sum_{k\geq 0}\binom{m-1}{2k}\frac{2u+4k+2}{(2u+m+1)_{2k+1}}\left[\begin{matrix} u+1, u-v+\frac{3}{2} \\ v+\frac{1}{2} \end{matrix}\right]_k \frac{(2k)!}{k!}.$$

This is, in turn, equivalent to the binomial sum expression

$$\left[\begin{matrix} 2u, v \\ u+\frac{1}{2}, 2v-1 \end{matrix}\right]_m = \sum_{k\geq 0}\binom{m}{2k}\frac{(2u+4k)f(2k)}{(2u+m)_{2k+1}} - \sum_{k\geq 0}\binom{m}{2k+1}\frac{(2u+4k+2)f(2k+1)}{(2u+m)_{2k+2}}$$

where $f(k)$ is given explicitly by

$$f(2k) = \frac{(2k)!}{k!}\left[\begin{matrix} u, u-v+\frac{3}{2} \\ v-\frac{1}{2} \end{matrix}\right]_k,$$
$$f(2k+1) = \frac{(2k+1)!}{k!}\left[\begin{matrix} u+1, u-v+\frac{3}{2} \\ v+\frac{1}{2} \end{matrix}\right]_k \frac{2u}{1-2v}.$$

Comparing this equation with (3) specified by

$$g(m) = \left[\begin{matrix} 2u, v \\ u+\frac{1}{2}, 2v-1 \end{matrix}\right]_m \quad \text{and} \quad \varphi(x; n) = (2u+x)_n$$

we get the dual relation corresponding to (2)

$$\sum_{k=0}^{m}(-1)^k\binom{m}{k}(2u+k)_m\left[\begin{matrix} 2u, v \\ u+\frac{1}{2}, 2v-1 \end{matrix}\right]_k = \begin{cases} f(2n), & m=2n; \\ f(2n+1), & m=2n+1; \end{cases}$$

which results in the following hypergeometric series identity.

Theorem 7 (Terminating series identity).

$$ {}_3F_2\left[\begin{matrix}-m, m+2u, & v\\ u+\frac{1}{2}, & 2v-1\end{matrix}\middle|\,1\right] = \begin{cases} \left[\begin{matrix}\frac{1}{2}, u-v+\frac{3}{2}\\ u+\frac{1}{2}, v-\frac{1}{2}\end{matrix}\right]_n, & m=2n;\\ \left[\begin{matrix}\frac{3}{2}, u-v+\frac{3}{2}\\ u+\frac{1}{2}, v+\frac{1}{2}\end{matrix}\right]_n \dfrac{1}{1-2v}, & m=2n+1.\end{cases} $$

2.8 $\varepsilon = 2$ and $\delta = -1$

The following Dougall sum

$$ \left[\begin{matrix}2u, v\\ u+1, 2v-1\end{matrix}\right]_m = \frac{2u(2v+m-1)}{(2u+m)(2v-1)}\mathfrak{D}_m(u+\tfrac{1}{2}, v) $$

can be expressed in terms of binomial sum

$$ \left[\begin{matrix}2u, v\\ u+1, 2v-1\end{matrix}\right]_m = \frac{2u(2v+m-1)}{2v-1} \times \sum_{k\geq 0}\binom{m}{2k}\frac{2u+4k+1}{(2u+m)_{2k+2}}\left[\begin{matrix}u+\frac{1}{2}, u-v+1\\ v+\frac{1}{2}\end{matrix}\right]_k \frac{(2k)!}{k!}. $$

Substituting the linear factor

$$ 2v+m-1 = \frac{(2u+m+2k+1)(2v+2k-1)}{2u+4k+1} + \frac{2(m-2k)(u-v+k+1)}{2u+4k+1} $$

into the binomial sum, we get

$$ \left[\begin{matrix}2u, v\\ u+1, 2v-1\end{matrix}\right]_m = \sum_{k\geq 0}\binom{m}{2k}\frac{(2u+4k)f(2k)}{(2u+m)_{2k+1}} - \sum_{k\geq 0}\binom{m}{2k+1}\frac{(2u+4k+2)f(2k+1)}{(2u+m)_{2k+2}} $$

where $f(k)$ is given explicitly by

$$ f(2k) = \frac{(2k)!}{k!}\left[\begin{matrix}u+\frac{1}{2}, u-v+1\\ v-\frac{1}{2}\end{matrix}\right]_k \frac{u}{u+2k}, $$

$$ f(2k+1) = \frac{(2k+1)!}{k!}\left[\begin{matrix}u+\frac{1}{2}, u-v+1\\ v+\frac{1}{2}\end{matrix}\right]_k \frac{2u(u-v+k+1)}{(1-2v)(u+2k+1)}. $$

This equation fits in well with (3) under the following specifications

$$g(m) = \left[\begin{matrix} 2u, v \\ u+1, 2v-1 \end{matrix}\right]_m \quad \text{and} \quad \varphi(x;n) = (2u+x)_n.$$

Then the dual relation corresponding to (2) becomes

$$\sum_{k=0}^{m}(-1)^k \binom{m}{k}(2u+k)_m \left[\begin{matrix} 2u, v \\ u+1, 2v-1 \end{matrix}\right]_k = \begin{cases} f(2n), & m=2n; \\ f(2n+1), & m=2n+1. \end{cases}$$

In terms of hypergeometric series, this reads as the following identity.

Theorem 8 (Terminating series identity).

$${}_3F_2\left[\begin{matrix} -m, m+2u, v \\ u+1, 2v-1 \end{matrix}\middle| 1\right] = \begin{cases} \left[\begin{matrix} \frac{1}{2}, u-v+1 \\ u+1, v-\frac{1}{2} \end{matrix}\right]_n \dfrac{u+n}{u+2n}, & m=2n; \\ -\left[\begin{matrix} \frac{1}{2}, u-v+1 \\ u+1, v-\frac{1}{2} \end{matrix}\right]_{n+1} \dfrac{u+n+1}{u+2n+1}, & m=2n+1. \end{cases}$$

2.9 $\varepsilon = 3$ and $\delta = -1$

This is the hardest case we have ever encountered in this research which cannot be treated directly by inverting combinations of Dougall's sum $\mathfrak{D}_m(u,v)$. Therefore we have to consider the rational function defined by

$$h(\tau) = \frac{(1-v-\tau)_{\lfloor \frac{m}{2} \rfloor}}{u+\tau+1/2} = P(\tau) + \frac{(3/2+u-v)_{\lfloor \frac{m}{2} \rfloor}}{u+\tau+1/2}$$

where $P(\tau)$ is polynomial of the degree $\lfloor \frac{m-2}{2} \rfloor$, the greatest integer $\leq \frac{m-2}{2}$. By means of the induction principle, it is not hard to compute its m-th differences

$$\Delta^m h(\tau) = \Delta^m \frac{(3/2+u-v)_{\lfloor \frac{m}{2} \rfloor}}{u+\tau+1/2} = (-1)^m \frac{m!(3/2+u-v)_{\lfloor \frac{m}{2} \rfloor}}{(u+\tau+1/2)_{m+1}}.$$

Recalling the Newton–Gregory formula

$$\Delta^m h(\tau) = \sum_{k=0}^{m}(-1)^{m+k}\binom{m}{k} h(\tau+k)$$

we get the following interesting binomial formula

$$\frac{m!(u-v+3/2)_{\lfloor\frac{m}{2}\rfloor}}{(u+1/2)_{m+1}}=\sum_{k=0}^{m}(-1)^k\binom{m}{k}\frac{(1-v-k)_{\lfloor\frac{m}{2}\rfloor}}{u+k+1/2}.$$

This equation can be identified to (2) with the connecting polynomial being given by $\varphi(x;n)=(1-v-x)_{\lfloor\frac{n}{2}\rfloor}$. The dual relation corresponding to (3) reads as

$$\begin{aligned}\frac{2}{2u+2m+1}&=\sum_{k\geq 0}\binom{m}{2k}\frac{(2k)!}{(1-v-m)_k}\frac{(u-v+3/2)_k}{(u+1/2)_{2k+1}}\\&\quad-\sum_{k\geq 0}\binom{m}{2k+1}\frac{(-v-k)(2k+1)!}{(1-v-m)_{k+1}}\frac{(u-v+3/2)_k}{(u+1/2)_{2k+2}}.\end{aligned}$$

Putting the last two binomial sums together and then applying the relation

$$\begin{aligned}&2(2u+4k+3)(1-v-m+k)+4(m-2k)(v+k)\\&=(2u+4k+3)(2-m-2v)-(m-2k)(2u-4v+3)\end{aligned}$$

we obtain the expression

$$\begin{aligned}1=&\frac{2u+2m+1}{8}\sum_{k\geq 0}\frac{(-m)_{2k}}{(1-v-m)_{k+1}}\frac{(u-v+3/2)_k}{(u+1/2)_{2k+2}}\\&\times\Big\{(2u+4k+3)(2-m-2v)-(m-2k)(2u-4v+3)\Big\}\end{aligned}$$

which can be rewritten in terms of hypergeometric ${}_4F_3$-series as

$$\begin{aligned}1=&\,{}_4F_3\left[\begin{matrix}1,\ \frac{-m}{2},\frac{1-m}{2},u-v+\frac{3}{2}\\2-v-m,\frac{u}{2}+\frac{3}{4},\frac{u}{2}+\frac{5}{4}\end{matrix}\,\middle|\,1\right]\frac{(2u+2m+1)(2v+m-2)}{(2u+1)(2v+2m-2)}\\&+{}_4F_3\left[\begin{matrix}1,\ \frac{1-m}{2},\frac{2-m}{2},u-v+\frac{3}{2}\\2-v-m,\frac{u}{2}+\frac{5}{4},\frac{u}{2}+\frac{7}{4}\end{matrix}\,\middle|\,1\right]\frac{m(2u+2m+1)(2u-4v+3)}{(2u+1)(2u+3)(2v+2m-2)}.\end{aligned}$$

According to the Whipple transformation (cf. Bailey [1, §4.3]), expressing both balanced ${}_4F_3$-series in terms of well–poised ${}_7F_6$-series, we can reformulate the last equation as

$$\begin{aligned}
&\left[\begin{matrix} 2u+1, v \\ u+\frac{3}{2}, 2v-1 \end{matrix}\right]_m \\
&= {}_7F_6\left[\begin{matrix} u, 1+\frac{u}{2}, \frac{u}{2}-\frac{1}{4}, \frac{u}{2}+\frac{1}{4}, u-v+\frac{3}{2}, \frac{1-m}{2}, \frac{-m}{2} \\ \frac{u}{2}, \frac{u}{2}+\frac{5}{4}, \frac{u}{2}+\frac{3}{4}, v-\frac{1}{2}, u+\frac{1+m}{2}, u+\frac{2+m}{2} \end{matrix}\middle| 1\right] \\
&+ \frac{m(2u-4v+3)(2u+2)}{(2u+m+1)(2v-1)(2u+3)} \\
&\times {}_7F_6\left[\begin{matrix} u+1, \frac{3+u}{2}, \frac{u}{2}+\frac{1}{4}, \frac{u}{2}+\frac{3}{4}, u-v+\frac{3}{2}, \frac{2-m}{2}, \frac{1-m}{2} \\ \frac{1+u}{2}, \frac{u}{2}+\frac{7}{4}, \frac{u}{2}+\frac{5}{4}, v+\frac{1}{2}, u+\frac{2+m}{2}, u+\frac{3+m}{2} \end{matrix}\middle| 1\right]
\end{aligned}$$

which can further be stated equivalently as the following binomial sums

$$\begin{aligned}
\left[\begin{matrix} 2u, v \\ u+\frac{3}{2}, 2v-1 \end{matrix}\right]_m &= \sum_{k\geq 0}\binom{m}{2k}\frac{(2u+4k)f(2k)}{(2u+m)_{2k+1}} \\
&- \sum_{k\geq 0}\binom{m}{2k+1}\frac{(2u+4k+2)f(2k+1)}{(2u+m)_{2k+2}}
\end{aligned}$$

where $f(k)$ is given explicitly by

$$f(2k) = \frac{(2k)!}{k!}\left[\begin{matrix} u, u-v+\frac{3}{2} \\ v-\frac{1}{2} \end{matrix}\right]_k \frac{(2u-1)(2u+1)}{(2u+4k-1)(2u+4k+1)},$$

$$\begin{aligned}
f(2k+1) &= \frac{(2k+1)!}{k!}\left[\begin{matrix} u+1, u-v+\frac{3}{2} \\ v+\frac{1}{2} \end{matrix}\right]_k \\
&\times \frac{2u(2u+1)(2u-4v+3)}{(2u+4k+1)(2u+4k+3)(1-2v)}.
\end{aligned}$$

This equation matches exactly (3) under the following specifications

$$g(m) = \left[\begin{matrix} 2u, v \\ u+\frac{3}{2}, 2v-1 \end{matrix}\right]_m \quad \text{and} \quad \varphi(x;n) = (2u+x)_n.$$

Then the dual relation corresponding to (2) reads as

$$\sum_{k=0}^{m}(-1)^k\binom{m}{k}(2u+k)_m\left[\begin{matrix} 2u, v \\ u+\frac{3}{2}, 2v-1 \end{matrix}\right]_k = \begin{cases} f(2n), & m=2n; \\ f(2n+1), & m=2n+1. \end{cases}$$

In terms of hypergeometric series, this yields the following identity.

(ε,δ)	$\mathcal{W}_{\varepsilon,\delta}(2n\|u,v)$	(ε,δ)	$\mathcal{W}_{\varepsilon,\delta}(1+2n\|u,v)$
$(0,2)$	$\left[\begin{matrix}\frac12, u-v\\ u, v+\frac32\end{matrix}\right]_n \frac{v+2n+1}{v+1}$	$(0,2)$	$\left[\begin{matrix}\frac32, u-v\\ u, v+\frac32\end{matrix}\right]_n \frac{u-v/2+n}{(u+n)(v+1)}$
$(-1,1)$	$\left[\begin{matrix}\frac12, u-v+\frac12\\ u+\frac12, v+\frac12\end{matrix}\right]_n$	$(-1,1)$	$\left[\begin{matrix}\frac32, u-v+\frac12\\ u+\frac12, v+\frac32\end{matrix}\right]_n \frac{2u-4v-1}{(2u-1)(2v+1)}$
$(-1,2)$	$\left[\begin{matrix}\frac12, u-v-\frac12\\ u+\frac12, v+\frac32\end{matrix}\right]_n \frac{(2u-1)(v+1)+4n(u+n)}{(2u-1)(v+1)}$	$(-1,2)$	$\left[\begin{matrix}\frac12, u-v-\frac12\\ u-\frac12, v+\frac12\end{matrix}\right]_{n+1} \frac{2v+1}{v+1}$
$(-1,3)$	$\left[\begin{matrix}\frac12, u-v-\frac12\\ u+\frac12, v+\frac32\end{matrix}\right]_n \frac{(2u-1)(v+2)+8n(u+n)}{(2u-1)(v+2)}$	$(-1,0)$	$\left[\begin{matrix}\frac32, u-v+\frac32\\ u+\frac12, v+\frac12\end{matrix}\right]_n \frac{2}{1-2u}$
$(2,-2)$	$\left[\begin{matrix}\frac12, u-v+2\\ u, v-\frac12\end{matrix}\right]_n \frac{u(v+2n-1)}{(u+2n)(v-1)}$	$(2,-2)$	$\left[\begin{matrix}\frac32, u-v+2\\ u+1, v-\frac12\end{matrix}\right]_n \frac{u-v/2+n+1}{(u+2n+1)(1-v)}$
$(-2,2)$	$\left[\begin{matrix}\frac12, u-v\\ u, v+\frac32\end{matrix}\right]_n \frac{(u-1)(v+1)+2n(u-v-1)}{(u-1)(v+1)}$	$(1,2)$	$\left[\begin{matrix}\frac32, u-v+\frac12\\ u+\frac12, v+\frac32\end{matrix}\right]_n \frac{1}{v+1}$

$(-2,3)$	$\left[\begin{matrix}\frac{1}{2}, u-v-1\\ u, v+\frac{3}{2}\end{matrix}\right]_n \frac{(u-1)(v+2)+2n(2u-v+2n-1)}{(u-1)(v+2)}$	$(1,-2)$	$\left[\begin{matrix}\frac{3}{2}, u-v+\frac{5}{2}\\ u+\frac{1}{2}, v-\frac{1}{2}\end{matrix}\right]_n \frac{1}{1-v}$
$(3,-2)$	$\left[\begin{matrix}\frac{1}{2}, u-v+\frac{3}{2}\\ u+\frac{1}{2}, v-\frac{1}{2}\end{matrix}\right]_n \frac{(2u+1)\{(2u-1)(v-1)+4n(u+n)\}}{(2u+4n-1)(2u+4n+1)(v-1)}$	$(3,-2)$	$\left[\begin{matrix}\frac{3}{2}, u-v+\frac{3}{2}\\ u+\frac{1}{2}, v-\frac{1}{2}\end{matrix}\right]_n \frac{(2u-2v+2n+3)(2u+1)}{(2u+4n+1)(2u+4n+3)(1-v)}$
$(3,-3)$	$\left[\begin{matrix}\frac{1}{2}, u-v+\frac{5}{2}\\ u+\frac{1}{2}, v-\frac{3}{2}\end{matrix}\right]_n \frac{(2u+1)\{(2u-1)(v-1)+8n(u+n)\}}{(v-1)(2u+4n-1)(2u+4n+1)}$	$(3,0)$	$\left[\begin{matrix}\frac{3}{2}, u-v+\frac{3}{2}\\ u+\frac{1}{2}, v+\frac{1}{2}\end{matrix}\right]_n \frac{2(2u+1)}{(2u+4n+1)(2u+4n+3)}$
$(4,-2)$	$\left[\begin{matrix}\frac{1}{2}, u-v+2\\ u, v-\frac{1}{2}\end{matrix}\right]_n \frac{(u)_2\{(u-1)(v-1)+2n(u-v+1)\}}{(v-1)(u+2n-1)(u+2n)(u+2n+1)}$	$(3,2)$	$\left[\begin{matrix}\frac{3}{2}, u-v+\frac{1}{2}\\ u+\frac{1}{2}, v+\frac{3}{2}\end{matrix}\right]_n \frac{(2u+1)(2u-2v+4n+1)(2u+2v+4n+3)}{(v+1)(2u-2v+1)(2u+4n+1)(2u+4n+3)}$
$(4,-3)$	$\left[\begin{matrix}\frac{1}{2}, u-v+2\\ u, v-\frac{3}{2}\end{matrix}\right]_n \frac{(u)_2\{(u-1)(v-1)+2n(2u-v+2n+2)\}}{(u+2n-1)(u+2n)(u+2n+1)(v-1)}$	$(3,-4)$	$\left[\begin{matrix}\frac{3}{2}, u-v+\frac{7}{2}\\ u+\frac{1}{2}, v-\frac{3}{2}\end{matrix}\right]_n \frac{(2u+1)(2u-v+2n+3)(2-2v-4n)}{(v-1)(v-2)(2u+4n+1)(2u+4n+3)}$

Theorem 9 (Terminating series identity).

$$
{}_3F_2\left[\begin{matrix}-m, m+2u, v\\ u+\frac{3}{2}, 2v-1\end{matrix}\,\middle|\,1\right]
= \begin{cases}\left[\begin{matrix}\frac{1}{2}, u-v+\frac{3}{2}\\ u+\frac{1}{2}, v-\frac{1}{2}\end{matrix}\right]_n \dfrac{(2u-1)(2u+1)}{(2u+4n-1)(2u+4n+1)}, & m=2n;\\[2ex] \left[\begin{matrix}\frac{3}{2}, u-v+\frac{3}{2}\\ u+\frac{1}{2}, v+\frac{1}{2}\end{matrix}\right]_n \dfrac{(2u+1)(2u-4v+3)}{(2u+4n+1)(2u+4n+3)(1-2v)}, & m=2n+1.\end{cases}
$$

3 Further Hypergeometric Series Identities

Following the same procedure exhibited in the last section, we have systematically examined $\mathcal{W}_{\varepsilon,\delta}(m|u,v)$ for small ε and δ parameters with $-5 \le \varepsilon, \delta \le 5$. It turns out that further 22 formulae have relatively *good* product expressions. They are tabulated in the two previous pages in order for the reader to have an easy access to them.

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Balls in Boxes: Variations on a Theme of Warren Ewens and Herbert Wilf

Shalosh B. Ekhad and Doron Zeilberger

מוקדש להרברט שאול וילף בהגיעו לגבורות

To Herbert Saul Wilf (b. June 13, 1931), on his 80-th birthday

Abstract We discuss, from an experimental mathematics viewpoint, a classical problem in epidemiology recently discussed by Ewens and Wilf, that can be formulated in terms of "balls in boxes", and demonstrate that the "Poission approximation" (usually) suffices.

Keywords Epidemiology • Computer-generated recurrences • Poisson process

Preface

There are r boys and n girls. Each boy must pick *one* girl to invite to be his date in the prom. Although each girl expects to get $R := r/n$ invitations, most likely, many of them would receive less, and many of them would receive more. Suppose that Nilini, the most "popular" girl, got as many as $m + 1$ prom-invitations, is she indeed so popular, or did she just "luck-out"?

Each one of r students has to choose from n different parallel Calculus sections, taught by different professors. Although each professor expects to get $R := r/n$

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students signing-up, most likely, many of them would receive less, and many of them would receive more. Suppose that Prof. Niles, the most "popular" professor got as many as $m + 1$ students, is Prof. Niles justified in assuming that she is more popular than her peers, or did she just "luck-out"?

It is Saturday night, and there are r people who have to decide where to dine, and they have n restaurants to choose from. Although each restaurant expects to get $R := r/n$ diners, most likely, many of them would receive less, and many of them would receive more. Suppose that the Nevada Diner, the most "popular" restaurant, got as many as $m + 1$ diners, can they congratulate themselves for the quality of their food, or ambiance, or location, or can they only congratulate themselves for being lucky?

Each one of r cases of acute lymphocitic leukemia has to choose one of n towns (artificially made all with equal-populations) where to happen. Although each town expects to get $R := r/n$ cases, most likely, many of them would receive less, and many of them would receive more. Suppose that the Illinois town Niles had $m + 1$ cases of that disease, do its people have to be concerned about their environment, or is it only Lady Luck's fault?

Of course all these questions have the same answer, and typically one talks about r balls being placed, uniformly at random, in n boxes, where the largest number of balls that landed at the same box was $m + 1$. Yet another way: A monkey is typing an r-letter word using a keyboard of an alphabet with n letters, and the most frequent letter showed-up $m + 1$ times. Does the typing monkey have a particular fondness for that letter, or is he a truly uniformly-at-random monkey who does not play favorites with the letters?

Asking the Right Question

As Herb Wilf pointed out so eloquently in his wonderful talk at the conference W80 (celebrating his 80th birthday) (based, in part, on [2]), using the depressing disease formulation, the right questions are **not**:

> What is the probability that Nilini would get so many ($m + 1$ of them) prom-invitations?
> What is the probability that Prof. Niles would get so many ($m + 1$ of them) students?
> What is the probability that the Nevada Diner would get so many ($m + 1$ of them) diners?
> What is the probability that Niles, IL would get so many ($m + 1$ of them) cases of acute lymphocitic leukemia?

Even though this is the wrong question (whose answer would make Nilini, Prof. Niles and the Nevada Diner's successes go to their heads, and would make the real-estate prices in Niles, IL, plummet), because it is so tiny, and seemingly extremely unlikely to be "due to chance", let's answer this question anyway.

The a priori probability of Nilini getting $m + 1$ or more prom-invitations, using the *Poisson Approximation* is:

$$e^{-R}(\sum_{i=m+1}^{\infty} \frac{R^i}{i!}) = e^{-R}(e^R - \sum_{i=0}^{m} \frac{R^i}{i!}) = 1 - e^{-R} \sum_{i=0}^{m} \frac{R^i}{i!},$$

indeed very small if m is considerably larger than R.

But a priori we don't know who would be the "lucky champion" (or the unlucky town), the **right** question to ask is:

The Right Question: Given r, n, and m, compute (if possible exactly, but at least approximately):

$P(r, n, m) :=$ the probability that *every* box got $\leq m$ balls.

Getting the Right Answer to the Right Question, as Fast as Possible

In [2], Ewens and Wilf present a beautiful, *fast* ($O(mn)$), algorithm for computing the *exact* value of $P(r, n, m)$, that employs a method that is described in the Nijenhuis-Wilf classic [3] (but that has been around for a long time, and rediscovered several times, e.g. by one of us [5], and before that by J.C.P. Miller, and according to Don Knuth the method goes back to Euler. At any rate, [2] does not claim novelty for the method, only for *applying* it to the present problem).

The *specific* real-life examples given in [2] were:

1. (Niles, IL): $r = 14{,}400, n = 9{,}000$, (so $R = 8/5$), $m = 7$. Using their method, they got (in less than 1 s!) the value

   $$P(14{,}400, 9{,}000, 7) = 0.09539591316713039999715554816 26\ldots,$$

   meaning that the probability that *every* town in the US, of the size of Niles, IL, would get no more than 7 cases is less than 10 %. So with probability 0.9046040868328696000028444518 37, *some* town (of the same size, assuming, artificially that the US has been divided into towns of that size) somewhere, in the US, would get *at least* eight cases. There is (most probably) nothing wrong with their water, or their air-quality, the only one that they may blame is Lady Luck!

   For comparison, the a priori probability that Niles, IL would get eight or more cases is roughly:

   $$1 - e^{-1.6} \sum_{i=0}^{7} \frac{1.6^i}{i!} = 0.00026044\ldots,$$

   a real reason for (unjustified!) concern.

2. (Churchill County, NV): $r = 8{,}000, n = 12{,}000$, (so $R = 2/3$), $m = 11$. Using their method, they got (in less than 1 s!) the value

$$P(8{,}000, 12{,}000, 11) = 0.99999989552964764731072601339 2\ldots,$$

so it is extremely likely that *every* district got at most 11 cases, and the probability that *some* district got 12 or more cases is indeed small, namely

$$1 - P(8{,}000, 12{,}000, 11) = 0.104470 \cdot 10^{-6},$$

so these people should indeed panic.

For comparison, the a priori probability that Churchill County, NV, would get 12 or more cases is roughly:

$$1 - e^{-2/3} \sum_{i=0}^{11} \frac{(2/3)^i}{i!} = 0.870586315 \cdot 10^{-11},$$

in that case people would have been right to be concerned, but for the wrong reason!

The Maple Package `BallsInBoxes`

This article is accompanied by the Maple package `BallsInBoxes` available from: http://www.math.rutgers.edu/~zeilberg/tokhniot/BallsInBoxes.

Lots of sample input and output files can be gotten from: http://www.math.rutgers.edu/~zeilberg/mamarim/mamarimhtml/bib.html.

How to Compute $P(r, n, m)$ Exactly?

Easy! As Ewens and Wilf point out in [2], and Herb Wilf mentioned in his talk, there is an obvious, explicit, "answer"

$$P(r, n, m) = \frac{1}{n^r} \sum \frac{r!}{r_1! r_2! \ldots r_n!},$$

where the sum ranges over the set of n-tuples of integers

$$A(r, n, m) := \{(r_1, r_2, \ldots, r_n) \mid 0 \leq r_1, \ldots, r_n \leq m, r_1 + r_2 + \cdots + r_n = r\}.$$

So "all" we need, in order to get the *exact* answer, is to construct the set $A(r, n, m)$ and add-up all the multinomial coefficients.

Of course, there is a better way. As it is well-known (see [2]), and easy to see, writing

$$P(r,n,m) = \frac{r!}{n^r} \sum_{(r_1,\ldots,r_n)\in A(r,n,m)} \frac{1}{r_1!r_2!\ldots r_n!},$$

the $\sum$ is the coefficient of x^r in the expansion of

$$\left(\sum_{i=0}^{m} \frac{x^i}{i!}\right)^n,$$

so all we need is to go to Maple, and type (once r, n, and m have been assigned numerical values)

```
r!/n**r*coeff(add(x**i/i!,i=0..m)**n,x,r);.
```

This works well for small n and r, but, please, **don't even try** to apply it to the first case of [2], ($r = 14{,}400, n = 9{,}000, m = 7$), Maple would crash!

Ewens and Wilf's brilliant idea was to use the Euler-Miller-(Nijenhuis-Wilf)-Zeilberger-…"quick" method for expanding a power of a polynomial, and get an *answer* in less than a second!

[We implemented this method in Procedure `Prnm(r,n,m)` of `BallsInBoxes`].

While their method indeed takes less than a second (in Maple) for $r = 14{,}400, n = 9{,}000$ (and $7 \le m \le 12$), it takes quite a bit longer for $r = 144{,}000, n = 90{,}000$, and we are willing to bet that for $r = 10^8, n = 10^8$ it would be hopeless to get an *exact answer*, *even* with this fast algorithm.

But why this obsession with *exact* answers? Hello, this is *applied* mathematics, and the epidemiological data is, of course, *approximate* to begin with, and we make lots of unrealistic assumptions (e.g. that the US is divided into 9,000 towns, each exactly the size of Niles, IL). All we need to know is, "are that many diseases likely to be due to pure chance, or is it a cause for concern?", *Yes or No?*, *Ja oder Nein?*, *Oui ou Non?*, *Ken o Lo?*.

Enumeration Digression

It would be nice to get a more compact (than the huge multisum above) (symbolic) "answer", or "formula", in terms of the *symbols* r, n and m. This seems to be hopeless. But fixing, positive integers a, b and m, one can ask for a "formula" (or whatever), in n, for the quantity $P(an, bn, m)$ that can be written as $B(a,b,m;n)/(an)^{bn}$ where

$$B(a,b,m;n) := (an)! \sum_{(r_1,\ldots,r_n)\in A(an,bn;m)} \frac{1}{r_1!r_2!\ldots r_n!},$$

the cardinality of the *natural* combinatorial set consisting of placing an balls in bn boxes in such a way that no box receives more than m balls. Equivalently, all *words* in a bn-letter alphabet, of length an, where no letter occurs more than m times. For example, when $a = b = m = 1$, we have the deep theorem:

$$B(1, 1, 1; n) = n!.$$

Equivalently, $e(n) = B(1, 1, 1; n)$ is a solution of the *linear recurrence equation with polynomial coefficients*

$$e(n + 1) - (n + 1)e(n) = 0, (n \geq 0),$$

subject to the *initial condition* $e(0) = 1$.

It turns out that, thanks to the not-as-famous-as-it-should-be *Almkvist-Zeilberger* algorithm [1] (an important component of the deservedly famous *Wilf-Zeilberger Algorithmic Proof Theory*), one can find similar recurrences (albeit of higher order, so it is no longer "closed-form", in n) for the sequences $B(a, b, m; n)$ for any *fixed* triple of positive integers, a, b, m.
(See Procedures `Recabm` and `RacabmV` in the Maple package `BallsInBoxes`).

Indeed, since $B(a, b, m; n)$ is $(an)!$ times the coefficient of x^{an} in

$$\left(\sum_{i=0}^{m} \frac{x^i}{i!}\right)^{bn},$$

it can be expressed, (thanks to *Cauchy*), as

$$\frac{(an)!}{2\pi i} \oint_{|z|=1} \frac{\left(\sum_{i=0}^{m} \frac{z^i}{i!}\right)^{bn}}{z^{an+1}} \, dz, \qquad (Cauchy)$$

and this is game for the Almkvist-Zeilberger algorithm, that has been incorporated into `BallsInBoxes`. See the web-book
http://www.math.rutgers.edu/~zeilberg/tokhniot/oBallsInBoxes2
for these recurrences for $1 \leq a, b \leq 3$ and $1 \leq m \leq 6$.

Asymptotics

Once the first-named author of the present article computed a recurrence, it can go on, thanks to the *Birkhoff-Trzcinski method* [4, 6], to get very good asymptotics! So now we can get a very precise asymptotic formula (in n) (to any desired order!) for $P(an, bn, m)$, that turns out to be very good for large, and even not-so-large n, and for *any* desired a, b, m. Procedure `Asyabm` in our Maple package `BallsInBoxes`

finds such asymptotic formulas. See
http://www.math.rutgers.edu/~zeilberg/tokhniot/oBallsInBoxes1
for asymptotic formulas, derived by combining Almkvist-Zeilberger with `AsyRec` (also included in `BallsInBoxes` in order to make the latter self-contained.)

This works for *every* m, and *every* a and b, in principle! In practice, as m gets larger than 10, the recurrences become very high order, and take a very long time to derive.

But as long as $m \leq 8$ and even (in fact, especially) when n is very large, this method is much faster than the method of [2] ($O(mn)$ with large n is not that small!). Granted, it does not give you an *exact* answer, but neither do they (in spite of their claim, see below!).

But let's be pragmatic and forget about our purity and obsession with "exact" answers. Since we know from "general nonsense" that the desired probability

$$C(a, b, m; n) := P(an, bn, m) \quad (= B(a, b, m; n)/(an)^{bn})$$

behaves asymptotically as

$$C(a, b, m; n) \asymp \mu^n (c_0 + O(1/n)),$$

for *some* numbers μ and c_0, all we have to do is crank out (e.g.) the 200-th and 201-st term and estimate μ to be $C(a, b, m; 201)/C(a, b, m; 200)$, and then estimate c_0 to be $C(a, b, m; 200)/\mu^{200}$. Using Least Squares one can do even better, and also estimate higher order asymptotics (but we don't bother, enough is enough!).

Procedure `AsyabmEmpir` in our Maple package `BallsInBoxes` uses this method, and gets very good results!

For example, for the Niles, IL, example, in order to get estimates for $P(14{,}400, 9{,}000, m)$, typing

```
evalf(subs(n=1800,AsyabmEmpir(8,5,m,200,n)));
```

for $m = 7, 8, 9, 10, 11, 12$ yields (almost instantaneously)

$m = 7$: 0.09540287131 ... (the exact value being: 0.095395913167 ...),
$m = 8$: 0.664971462304 ... (the exact value being: 0.66495441 ...),
$m = 9$: 0.9378712268719 ... (the exact value being: 0.93786433 ...),
$m = 10$: 0.990845139 ... (the exact value being: 0.9908433 ...),
$m = 11$: 0.998789295 ... (the exact value being: 0.99878892861 ...).

The advantage of the present approach is that we can handle very large n, for example, with the same effort we can compute

```
evalf(subs(n=180000,AsyabmEmpir(8,5,m,200,n)))
```

getting that $P(1{,}440{,}000, 900{,}000, 11)$ is very close to 0.88554890636027. The method used in [2] (i.e. typing

```
Prnm(1440000,900000,11);
```

in `BallsInBoxes`) would take forever!

Caveat Emptor

There is another problem with the $O(mn)$ method described in [2]. Sure enough, it works well for the examples given there, namely $P(14{,}400, 9{,}000, m)$ for $6 \le m \le 12$ and $P(8{,}000, 12{,}000, m)$ for $4 \le m \le 8$.

This is corroborated by our implementation of that method, (Procedure `Prnm(r,n,m)` in `BallsInBoxes`).

Typing (once `BallsInBoxes` has been read onto a Maple session):

```
t0:=time(): Prnm(14400,9000,9) , time()-t0;
```

returns

$0.937864339305858219725360911354, 0.884$

that tells you the desired value (we set `Digits` to be 30), and that it took 0.884 s to compute that value.

But now try:

```
t0:=time(): Prnm(1000,100,15), time()-t0;
```

and get in 0.108 s (real fast!)

$-0.728465229161818857989128673465 \cdot 10^{50}$.

"Something is rotten in the State of Denmark!" We learned in kindergarten that a *probability* has to be between 0 and 1, so a negative probability, especially one with 50 decimal digits, is a bit fishy. Of course, the problem is that [2]'s "exact" result is not really *exact*, as it uses floating-point arithmetic.

Big deal, since we work in Maple, let's increase the system variable `Digits` (the number of digits used in floating-point calculations), and type the following line:

```
evalf(Prnm(1000,100,15),80);
```

getting 5.71860506564981 . . ., a little bit better! (the probability is now less than six, and at least it is positive!), but still nonsense.

`Digits:=83` still gives you nonsense, and it only starts to "behave" at `Digits:=90`.

Now let's multiply the inputs, r and n by 10, and take $m = 22$ and try to evaluate $P(10{,}000, 1{,}000, 22)$. Even `Digits:=250` still gives nonsense! Only Digits:=310 gives you something reasonable and (hopefully) correct.

The way to overcome this problem is to keep upping `Digits` until you get close answers with both `Digits` and, say, `Digits+100`. This is implemented in Procedure `PrnmReliable(r,n,m,k)` in `BallsInBoxes`, if one desires an accuracy of k decimal digits. This is *reliable* indeed, but **not** exact, and *not* rigorous, since it uses numerical heuristics. The exact answer is a *rational number*, that is implemented in Procedure `PrnmExact(r,n,m)` of `BallsInBoxes`.

The Cost of Exactness

If you type

```
t0:=time():PrnmExact(14400,9000,7): time()-t0;
```

you would get in 42 s (no longer that fast!) a *rational number* whose numerator and denominator are *exact* integers with 54,207 digits.
See http://www.math.rutgers.edu/~zeilberg/tokhniot/oBallsInBoxes7a for the outputs (and timings) of `PrnmExact(14400,9000,m);` for m between 6 and 12 and see http://www.math.rutgers.edu/~zeilberg/tokhniot/oBallsInBoxes7b for the outputs (and timings) of `PrnmExact(8000,12000,m);` for m between 4 and 8. No longer fast at all! (2,535 and 248 s respectively).

Let's Keep It Simple: An Ode to the Poisson Approximation

At the end of [2], the authors state:

> A Poisson Approximation is also possible but it may be inaccurate, particularly around the tails of the distribution. Our exact method is fast and does not suffer from any of those problems.

Being curious, we tried it out, to see if it is indeed so bad. Surprise, it is terrific! But let's first review the Poisson approximation as we understand it.

The probability of any particular box (of the n boxes) getting $\leq m$ ball is, roughly, using the Poisson approximation ($R := r/n$):

$$e^{-R} \sum_{i=0}^{m} \frac{R^i}{i!}.$$

Of course the n events are **not** independent, but let's pretend that they are. The probability that *every* box got $\leq m$ balls is approximated by

$$Q(r,n,m) := \left(e^{-R} \sum_{i=0}^{m} \frac{R^i}{i!} \right)^n .$$

($Q(r,n,m)$ is implemented by procedure `PrnmPA(r,n,m)` in `BallsInBoxes`. It is as fast as lightning!)

Ewens and Wilf are very right when they claim that $P(r,n,m)$ and $Q(r,n,m)$ are very far apart around the "tail" of the distribution, but who cares about the tail? Definitely not a scientist and even not an applied mathematician. It turns out, empirically (and we did extensive numerical testing, see Procedure `HowGoodPA1(R0,N0,Incr,M0,m,eps)` in `BallsInBoxes`), that whenever $P(r,n,m)$ is not extremely small, it is very well approximated by $Q(r,n,m)$, and using the latter (it is so much faster!) gives very good approximations, and enables

one to construct the "center" of the probability distribution (i.e. ignoring the tails) very accurately. See
http://www.math.rutgers.edu/~zeilberg/tokhniot/oBallsInBoxes4,
and
http://www.math.rutgers.edu/~zeilberg/tokhniot/oBallsInBoxes5, for comparisons (and timings!, the Poisson Approximation wins!).

In particular, the estimates for the *expectation*, *standard deviation*, and even the higher moments match extremely well!

Another (empirical!) proof of the fitness of the Poisson Approximation can be seen in:
http://www.math.rutgers.edu/~zeilberg/tokhniot/oBallsInBoxes1
where the (rigorous!) asymptotic formulas derived, via `AsyRec`, from the recurrences obtained via the Almkvist-Zeilberger algorithm are very close to those predicted by the Poisson Approximation (except for very small m, corresponding to the "tail").

The Full Probability Distribution of the Random Variable "Maximum Number of Balls in the Same Box"

It would be useful, for given positive integers a and b, to know how the probability distribution "maximum number of balls in the same box when throwing an balls into bn boxes" behaves. One can "empirically" construct (without arbitrarily improbable tail) the distribution of the random variable "maximum number of balls in the same box" when an balls are uniformly-at-random placed in bn boxes (Let's call it $X_n(a,b)$, and X_n for short) using

$$Pr(X_n = m) = P(an, bn, m) - P(an, bn, m-1).$$

First, and foremost, what is the expectation, μ_n, of this random variable? Second, what is the standard deviation, σ_n?, skewness?, kurtosis?, and it would be even nice to know higher α-coefficients (alias moments of $Z_n := (X_n - \mu_n)/\sigma_n$), as asymptotic formulas in n.

For the expectation, μ_n, Procedure `AveFormula(a,b,n,d,L,k)` uses the more accurate "empirical approach" and Maple's built-in Least-Squares command, to obtain the following empirical (symbolic!) estimates for the expectation.

$a = 1, b = 1$: `evalf(AveFormula(1,1,n,1,300,1000,10),10);` yields that μ_n is roughly $2.293850526 + (0.4735983525) \cdot \log n$

$a = 2, b = 1$: `evalf(AveFormula(2,1,n,1,300,1000,10),10);` yields that μ_n is roughly $3.963420618 + (0.5834252496) \cdot \log n$

$a = 1, b = 2$: `evalf(AveFormula(1,2,n,1,300,1000,10),10);` yields that μ_n is roughly $1.640094145 + (0.3873602232) \cdot \log n$.

Note that for $a = 1, b = 1$, the approximation to μ_n can be written $2.293850526 + (1.090500507) \cdot \log_{10} n$, so a "rule-of-thumb" estimate for the expectation when n balls are thrown into n boxes is a bit more than 2 plus the number of (decimal) digits.

Procedure `NuskhaPA1(R,n,K,d)` uses the Poisson Approximation to guess polynomials in $\log n$ of degree d fitting the average, standard deviation, and higher moments, as asymptotic expressions in n, for nR balls thrown into n boxes, where R is now any (numeric) *rational* number. Even $d = 1$ seems to give a fairly good fit, so they all seem to be (roughly) linear in $\log n$.

Procedure `SmallestmPA`

Procedure `SmallestmPA(r,n,conf)` gives you the smallest m for which, with confidence `conf`, you can deduce that the high value of m is **not** due to chance (using the Poisson Approximation). For example

`SmallestmPA(14400,9000,.99);`

yields 10, meaning that if a town the size of Niles, IL got 10 or more cases, then with probability >0.99 it is not just bad luck. If you want to be %99.99-sure of being a victim of the environment rather than of Lady Luck, type:

`SmallestmPA(14400,9000,.9999);`

and get 13, meaning that if you had 13 cases, then with probability larger than 0.9999 it is not due to chance.

The Minimum Number of Balls that Landed in the Same Box, Procedure `LargestmPA`

An equally interesting, and harder to compute, random variable is the *minimum number of balls that landed in the same box*, but the Poisson Approximation handles it equally well. Analogous to `SmallestmPA`, we have, in `BallsInBoxes`, Procedure `LargestmPA(r,n,conf)` that tells you the largest m for which you can't blame luck for getting m or less balls.

For example, if there are 10,000 students that have to decide between 100 different calculus sections,

`LargestmPA(10000,100,.99);`

that happens to be 66, tells you that any section that only has 66 students or less, with probability >0.99, it is because that professor (or time slot, e.g. if it is an 8:00 a.m. class) is not popular, and you can't blame bad luck.

`LargestmPA(10000,100,.9999);`

that outputs 57, tells you that anyone who only had ≤ 57 students enrolled is unpopular with probability $>$%99.99, and can't blame bad luck.

On the other end, going back to the original problem,
`SmallestmPA(10000,100,.99);`
yields 139, telling you that any section for which 139 or more students signed up is *probably* (with prob. >0.99) due to the popularity of that section, while `SmallestmPA(10000,100,.9999);` yields 151.

Final Comments

1. One can possibly (using the *saddle-point method*) get asymptotic formulas from the contour integral (*Cauchy*), but this is not *our* cup-of-tea, so we leave it to other people.
2. Another "back-of-the-envelope" "Poisson Approximation" is to argue that since the probability of any individual box getting strictly more than m balls is roughly (recall that $R = r/n$)

$$e^{-R} \sum_{i=m+1}^{\infty} \frac{R^i}{i!} = e^{-R}(e^R - \sum_{i=0}^{m} \frac{R^i}{i!}) = 1 - e^{-R} \sum_{i=0}^{m} \frac{R^i}{i!},$$

by the *linearity of expectation*, the expected number of *lucky* (or *unlucky* if the balls are diseases) boxes exceeding m balls is roughly

$$n \left(1 - e^{-R} \sum_{i=0}^{m} \frac{R^i}{i!} \right).$$

In the case of Niles, IL, the expected number of towns that would get eight or more cases is:

$$9{,}000 \left(1 - e^{-1.6} \sum_{i=0}^{7} \frac{(1.6)^i}{i!} \right) = 2.343961376410372,$$

so it is not at all surprising that at least one town got as many as eight cases. On the other hand, in the other example $r = 8{,}000, n = 12{,}000, m = 12$, the expected number of unfortunate counties is:

$$12{,}000 \left(1 - e^{-(2/3)} \sum_{i=0}^{12} \frac{(2/3)^i}{i!} \right) = 0.533706802 \cdot 10^{-8},$$

so it is indeed a reason for concern.

Conclusion

We completely agree with Ewens and Wilf that simulation takes way too long, and is not that accurate, and that *their* method is far superior to it. But we strongly disagree with their dismissal of the Poisson Approximation. In fact, we used their ingenious method to conduct extensive empirical (numerical) testing that established that the Poisson Approximation, that they dismissed as “inaccurate”, is, as a matter of fact, sufficiently accurate, and far more reliable, in addition to being yet-much-faster! It is much safer to use the Poisson Approximation than to use their “exact” method (in floating-point arithmetic), and when one uses *truly* exact calculations, in rational arithmetic, their “fast” method becomes *anything but*.

Even when the floating-point problem is addressed by using multiple precision (`PrnmReliable` discussed above), their fast algorithm becomes slow for very large r and n, while the Poisson Approximation is almost instantaneous even for very large r and n, and *any* m.

So while we believe that the algorithm in [2] is not as *useful* as the Poisson Approximation, it sure was *meta-useful*, since it enabled us to conduct extensive numerical testing that showed, *once and for all*, that it is far less useful then the latter.

Additional evidence comes from our own symbolic approach (fully rigorous for $m \leq 9$ and semi-rigorous for higher values of m), that establishes the adequacy of the Poisson Approximation for *symbolic* n.

Finally, as we have already pointed out, since the data that one gets in applications is always *approximate* to begin with, insisting on an “exact” answer, even when it is easy to compute, is unnecessary.

Coda: But We, Enumerators, Do Care About Exact Results!

Our point, in this article, was that for *applications* to statistics, the Poisson Approximation suffices. But *we* are *not* statisticians. We are *enumerators*, and we do like exact results! The approach of [2] enables us to know, for example, in less than 1 s the **exact** number of ways that 1,001 balls can be placed in 1,001 boxes such that no box received more than 7 balls. Just type (in `BallsInBoxes`) `(1001**1001)*PrnmExact(1001,1001,7);` and get a beautiful **exact** integer with 3,004 digits!
Typing `(1001**1001)*PrnmPA(1001,1001,7);` will give you something fairly close (the ratio being $0.9997852\ldots$) but for a **pure** enumerator, this is very unsatisfactory. So long live exact answers!, but *not* in statistics.

Acknowledgements We wish to thank Eugene Zima for helpful corrections. Accompanied by Maple package http://www.math.rutgers.edu/~zeilberg/tokhniot/BallsInBoxes. Sample input and output can be gotten from: http://www.math.rutgers.edu/~zeilberg/mamarim/mamarimhtml/bib.html. Supported in part by the National Science Foundation of the United States of America.

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Beating Your Fractional Beatty Game Opponent and: What's the Question to Your Answer?

Aviezri S. Fraenkel

To Herb Wilf on his 80th birthday: He shall be as a CW (Calkin-Wilf) tree planted by the waters that spreads out its roots by the river, shall not see when heat comes, its leaf shall remain green, shall not be anxious in the year of drought, nor shall it cease from bearing fruit (adapted from Jeremiah 17, 8). What was to be a celebratory volume unfortunately turned into a commemorative one. Yet the above dedication remains valid, since Herb's heritage lives on, spreads its roots and continues to bear rich fruit.

Abstract Given a subtraction game on two piles of tokens, the usual question is to characterize its P-positions. These normally split the positive integers into two complementary sequences for Wythoff-like games. Here we invert the problem: We are given two sequences, and the challenge is to find appropriate succinct game rules for a game having the given P-positions. The main additional challenge in this work is that the given sequences do not split the positive integers. We present two solutions for a seemingly first such problem, the second in terms of two exotic numeration systems. Both characterizations lead to linear-time winning strategies for the game induced by the two sequences.

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1 Prologue

Preliminary Thoughts. *Subtraction games*, also called *take-away games*, are games on m piles of tokens, where each of two players playing alternately, selects one or more piles and removes from them a number of tokens according to the specified game rules.[1] In this paper we consider impartial subtraction games.

A game is *impartial* if for every game position, all moves one player can do also the opponent can do, unlike the *partizan* chess, where the black player cannot touch a white piece and conversely.

A P-position in a game is a position such that the player moving from it loses whatever his move is; an N-position is a position from which a player has a winning move. Notice that every move from a P-position lands in an N-position; from an N position there is a (winning) move to a P-position. In *normal* play the player making the last move wins; in *misère* play the player making the last move loses. Throughout we are concerned solely with normal play.

Nim is a subtraction game played on a finite number of tokens. A move consists of selecting a (nonempty) pile and removing from it any positive number of tokens, up to and including the entire pile (a *Nim move*). *Wythoff* is a subtraction game played on two piles of tokens. There are two types of moves: a Nim move or taking the *same* number of tokens from both piles. The latter is a *Wythoff move*.

For $m \geq 2$, the P-positions of games typically split the positive integers into m disjoint sets $A^1, \ldots, A^m$: $\cup_{i=1}^m A^i = \mathbb{Z}_{\geq 1}$, $A^i \cap A^j = \emptyset$ for all $i \neq j$ for Wythoff-like games. Two of many examples: [3, 6]. There are only a few studies where this splitting does not hold. In [2] and [8] the Nim move is restricted to taking any positive multiple of b tokens from a single pile, where b is an a priori given positive integer parameter (and there is a restricted Wythoff move in [8]). The P-positions there constitute b pairs of integers and there are omissions and repetitions of integers in some of the pairs. Sequences that jointly cover every positive integer precisely m times for any given $m \geq 1$ were given by O'Bryant [17] using a generating function approach; and Graham and O'Bryant [11] used them for generalizing a conjecture about splitting sets. They were constructed by elementary means by Larsson and applied there to combinatorial game theory [15]. More recently, Gurvich [12] considered a generalization of Wythoff's game where, for $m = 2$, $A^1 \cap A^2 = \emptyset$, but $|\mathbb{Z}_{\geq 1} \setminus (A^1 \cup A^2)| = \infty$. In [10] games are analyzed for which both $A^1 \cap A^2 \neq \emptyset$ and $|\mathbb{Z}_{\geq 1} \setminus (A^1 \cup A^2)| = \infty$. But exceptions they are.

In the present paper we consider a case, also for $m = 2$, apparently a first of its kind, where the P-positions constitute a single pair (A^1, A^2) of integers, $|A^1 \cap A^2| = \infty$, but $A^1 \cup A^2 = \mathbb{Z}_{\geq 1}$ for a Wythoff-like game. The easy part is to construct A^1, A^2 with such properties; the hard part is to formulate appropriate succinct game rules

[1] They can equivalently be modeled as games played on a collection of nonnegative integers, which are reduced by the players to 0 according to the game rules.

Table 1 Excerpts of the first few terms of the sequences A and B

n	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27
a_n	0	1	2	3	4	5	6	7	8	9	10	11	12	14	15	16	17	18	19	20	21	22	23	24	25	26	28	29
b_n	0	1	3	5	6	8	10	12	13	15	17	19	20	22	24	26	27	29	31	33	34	36	38	40	41	43	45	47

n	28	35	36	37	38	39	40	41	49	50	51	52	60	61	62	63	64	65	66	67	68
a_n	30	37	38	39	40	42	43	44	52	53	55	56	64	65	66	67	69	70	71	72	73
b_n	48	61	62	64	66	68	69	71	85	87	89	90	104	106	108	109	111	113	115	116	118

for a game whose P-positions are such non-complementary sequences. We seek a question for a given answer!

2 The Game, Main Theorem and Examples

Denote by $\varphi = (1 + \sqrt{5})/2$ the golden section. Then $\varphi^2 = (3 + \sqrt{5})/2$, and $\varphi^{-1} + \varphi^{-2} = 1$. Multiplying by $3/2$, we get

$$\alpha^{-1} + \beta^{-1} = 3/2, \tag{1}$$

where

$$\alpha = \frac{2\varphi}{3} = \frac{1+\sqrt{5}}{3} = 1.0786893\ldots, \quad \beta = \frac{2\varphi^2}{3} = \frac{3+\sqrt{5}}{3} = 1.745356\ldots,$$

and $\beta - \alpha = 2/3$. For $n \geq 0$, let $a_n = \lfloor n\alpha \rfloor$, $b_n = \lfloor n\beta \rfloor$. These are *Beatty* sequences: the floor of the multiples of a positive number. For $\alpha > 0$ irrational, the two Beatty sequences are *complementary* if and only if $\alpha^{-1} + \beta^{-1} = 1$. Complementarity means that every positive integer appears exactly once in exactly one of the two sequences. Let

$$A := \cup_{n \geq 0} a_n, \quad B := \cup_{n \geq 0} b_n, \quad \mathcal{T} := \cup_{n \geq 0} (a_n, b_n),\ a_n \in A,\ b_n \in B.$$

We denote by $\overline{\mathcal{T}} = \mathbb{Z}_{\geq 0} \setminus \mathcal{T}$ the complement of $\mathcal{T}$, that is, all pairs $(x, y) \in \mathbb{Z}_{\geq 0} \times \mathbb{Z}_{\geq 0}$ not in $\mathcal{T}$. The first few terms of A and B are displayed in Table 1.

In the game FREAK there are two piles of finitely many tokens. We denote the piles by the number of tokens they contain, i.e.,

$$(x, y), \text{ with } 0 \leq x \leq y. \tag{2}$$

Two players alternate in reducing the piles. Play ends when the piles are empty. Recall that the player first unable to move loses and the opponent wins (normal play).

Remark 1. In a move from a position (x, y) subject to (2) where x is unchanged, but $y \to y - t$ with $t > 0$, we may have $x \leq y - t$ or $y - t < x$. To be consistent with (2) we write $(x, y) \to (x, y - t)$ in the former case, and $(x, y) \to (y - t, x)$ in the latter case.

The P-positions of FREAK are given, namely $\mathcal{P} = \mathcal{T}$. What are succinct game rules of FREAK such that it has precisely these P-positions? We chose this particular set $\mathcal{T}$ since it seems like the simplest case in which the two Beatty sequences are not complementary.

We claim that at each stage a FREAK player has the choice of making one of the following two types of moves:

(I) (Restricted Wythoff move.) $(x, y) \to (x - t, y - t)$ for every $t \in \{1, \dots, x\}$, except that this move is blocked if $t \in \{1, 2, 3\}$ and $x \in A$ and $y \in B$.

(II) (Restricted Nim move.)

(a) $(x, y) \to (x - t, y)$ for any $0 < t \le x$; or
(b) $(x, y) \to (x, y - t)$ for any $0 < t \le y$; or
(c) $(x, y) \to (y - t, x)$ for any $0 < t \le y$, except that this move is blocked if $x \in A \cap B$ and $y \in B$.

Theorem 1. *For the game* FREAK, $\mathcal{P} = \mathcal{T}$.

Example 1. We refer the reader to Table 1.

- The moves from $\mathcal{T}$ to $\mathcal{T}(4, 6) \to (3, 5)$, $(12, 20) \to (11, 19)$ are blocked because $4, 12 \in A$ and $6, 20 \in B$ ((I), $t = 1$).
- Similarly, the moves $(14, 22) \to (12, 20)$, $(28, 45) \to (26, 43)$ are blocked ((I), $t = 2$).
- Also $(14, 22) \to (11, 19)$, $(43, 69) \to (40, 66)$ are blocked ((I), $t = 3$).
- $(12, 20) \to (7, 12)$ and $(19, 31) \to (11, 19)$ are blocked by (II)(c), since $12 \in A \cap B$, $19 \in A \cap B$; and $20, 31 \in B$.
- For every $s > 13$, $(13, s) \to (8, 13)$ is not blocked by (II)(c), since $13 \notin A$.
- Notice that moves from the complement $\overline{\mathcal{T}}$ to $\mathcal{T}$ such as $(15, 34) \to (15, 24)$, $(15, 22) \to (14, 22)$ or $(10, 17)$, $(11, 16) \to (8, 13)$ are not blocked.

It should be clear that a winning strategy for FREAK can be effected by means of the P-positions. Given any game position (x, y) subject to (2), we have only to find out to which sequence, A or B, x and y belong. The complexity of the implied computation will be discussed later on.

3 Preliminaries

For proving Theorem 1, we begin by collecting a few facts about the sequences A and B.

For any number $r \in \mathbb{R}_{>0}$ and $n \in \mathbb{Z}_{\ge 0}$, let $\Delta\lfloor nr \rfloor = \lfloor (n + 1)r \rfloor - \lfloor nr \rfloor$.

Lemma 1. (i) *Each of the sequences A and B is strictly increasing.*
(ii) *For every $n \ge 0$, $\Delta\lfloor n\alpha \rfloor = 2 \implies \Delta\lfloor n\beta \rfloor = 2$.*

Proof. Note that $1 < \alpha < \beta < 2$. These inequalities imply:

$$\Delta\lfloor n\alpha\rfloor \in \{1,2\}, \quad \Delta\lfloor n\beta\rfloor \in \{1,2\} \quad \text{for all } n \in \mathbb{Z}_{\geq 1}. \tag{3}$$

Also note that $\Delta\lfloor n\alpha\rfloor = 2$ if and only if $(n+1)\alpha = i+1+\delta_1$, $n\alpha = i-\delta_2$ for some integer $i = i(n)$, and $0 < \delta_1, \delta_2 < \alpha - 1 < 0.08$. For such n we have, $(n+1)\beta = (n+1)(\alpha+2/3) = i+1+\delta_1+2(n+1)/3$; $n\beta = n(\alpha+2/3) = i-\delta_2+2n/3$. Put $n = 3k+i$, $i \in \{0,1,2\}$. Then $(n+1)\beta = i+1+\delta_1+2k+2(i+1)/3$, $n\beta = i-\delta_2+2k+2i/3$. We consider three cases:

1. $i = 0$. Then $\Delta\lfloor n\beta\rfloor = (i+2k+1)-(i-1+2k) = 2$.
2. $i = 1$. Then $\Delta\lfloor n\beta\rfloor = (i+2k+2)-(i+2k) = 2$.
3. $i = 2$. Then $\Delta\lfloor n\beta\rfloor = (i+2k+3)-(i+2k+1) = 2$.Thus $\Delta\lfloor n\alpha\rfloor = 2 \implies \Delta\lfloor n\beta\rfloor = 2$. This implies,

$$\lfloor n\beta\rfloor - \lfloor n\alpha\rfloor \text{ is a nondecreasing function of } n. \tag{4}$$

The properties (3) immediately imply (i). Let $\lfloor n\alpha\rfloor = K$, $\lfloor n\beta\rfloor = L$. If $\Delta\lfloor n\alpha\rfloor = 2$, then $\lfloor (n+1)\alpha\rfloor = K+2$, $\lfloor (n+1)\beta\rfloor = L+\delta$, where $\delta \in \{1,2\}$ by (3). Now $\lfloor n\beta\rfloor - \lfloor n\alpha\rfloor = L-K$, $\lfloor (n+1)\beta\rfloor - \lfloor (n+1)\alpha\rfloor = L-K+\delta-2$. By (4), $L-K+\delta-2 \geq L-K$, so $\delta \geq 2$. By (3), $\delta = 2$, establishing (ii). □

Corollary 1. *For every $n \geq 0$, $\Delta\lfloor n\beta\rfloor = 1 \implies \Delta\lfloor n\alpha\rfloor = 1$.*

Proof. In view of (3), this is the contrapositive statement of Lemma 1(ii). □

Lemma 2. *We have,*

(i) $A \cup B = \mathbb{Z}_{\geq 0}$ *(every nonnegative integer appears in $A \cup B$).*
(ii) Every nonnegative integer N is assumed at most twice in $A \cup B$. If N appears twice, it appears once in A and once in B.
(iii) $b_m = a_n \implies m \leq n$.
(iv) $|A \cap B| = \infty$.

Proof. (i) It is convenient to put $\xi_1 = \alpha^{-1}$, $\xi_2 = \beta^{-1}$. Consider the sequence $\zeta = \{\alpha, \beta, 2\alpha, 2\beta, 3\alpha, 3\beta, \ldots\}$. It suffices to show that if $M \geq 1$ is any integer and there are N_M members of $\zeta < M$, then $N_{M+1} \geq N_M + 1$. The number of $n > 0$ satisfying $n\alpha < M$ is $\lfloor M\xi_1\rfloor$, and the number of $n > 0$ satisfying $n\beta < M$ is $\lfloor M\xi_2\rfloor$. So $N_M = \lfloor M\xi_1\rfloor + \lfloor M\xi_2\rfloor$. Now

$$M\xi_1 - 1 < \lfloor M\xi_1\rfloor < M\xi_1, \quad M\xi_2 - 1 < \lfloor M\xi_2\rfloor < M\xi_2.$$

Adding, $(3M/2)-2 < N_M < 3M/2$. If $M = 2t$ is even, then $3t-2 < N_M < 3t$, so $N_M = 3t-1$, and then $3t-1/2 < N_{M+1} < 3t+3/2$, so $N_{M+1} \in \{3t, 3t+1\}$. Thus $N_{M+1} - N_M \in \{1,2\}$. If $M = 2t+1$, $M+1 = 2t+2$, we obviously also get $N_{M+1} - N_M \in \{1,2\}$, proving (i).

(ii) Since each of A and B is strictly increasing, N can appear at most once in each.

(iii) Follows immediately from the fact that $\alpha < \beta$.

(iv) We have to show that $N_{M+1} - N_M = 2$ is assumed for infinitely many $M \in \mathbb{Z}_{\geq 0}$. If $N_{M+1} - N_M = 1$ for all large M then a simple density argument shows that $\xi_1 + \xi_2 = 1$, a contradiction. □

Lemma 3. $\Delta\lfloor n\beta \rfloor = 1$ *implies*

$$\Delta\lfloor (n-2)\beta \rfloor = \Delta\lfloor (n-1)\beta \rfloor = \Delta\lfloor (n+1)\beta \rfloor = \Delta\lfloor (n+2)\beta \rfloor = 2.$$

Proof. We have $\Delta\lfloor n\beta \rfloor = 1$ if and only if $N < n\beta < N+1 < (n+1)\beta < N+2$ for some $N \in \mathbb{Z}_{\geq 0}$. Since the fractional parts $\{n\beta\}_{n\geq 1}$ are dense in the reals (Kronecker's Theorem), this inequality holds for infinitely many pairs of integers (n, N). Since $1.74 < \beta < 1.75$, we then have $N+3 < (n+2)\beta < N+4 < N+5 < (n+3)\beta < N+6$. Then $\Delta\lfloor (n+1)\beta \rfloor = \Delta\lfloor (n+2)\beta \rfloor = 2$. We also have $\Delta\lfloor n\beta \rfloor = 1$ if and only if $N-1 > (n-1)\beta > N-2 > N-3 > (n-2)\beta > N-4$, so $\Delta\lfloor (n-2)\beta \rfloor = \Delta\lfloor (n-1)\beta \rfloor = 2$. □

Lemma 4. *If* $\Delta\lfloor n\alpha \rfloor = 2$*, then* $\Delta\lfloor (n+i)\alpha \rfloor = 1$ *for at least all* $i \in \{1, \ldots, 11\}$.

Proof. Follows from the fact that $\lfloor \{\alpha\}^{-1} \rfloor = 12$, where $\{x\}$ denotes the fractional part of x. □

Definition 1. For any real number x and any $n \in \mathbb{Z}_{\geq 0}$, $\Delta\lfloor nx \rfloor$ is called an x-*difference*.

Lemma 5. *For* $n, r \in \mathbb{Z}_{\geq 1}$*, let*

$$\lfloor (n+r)\beta \rfloor - \lfloor n\beta \rfloor = \lfloor (n+r)\alpha \rfloor - \lfloor n\alpha \rfloor = t. \tag{5}$$

Then $r \leq 2$*,* $t \leq 3$*; and* $r = 2$ *with* $t = 3$ *is achieved.*

Proof. We wish to maximize r. If any two consecutive β-differences are 2, then the corresponding α-differences cannot be 2 by Lemma 4. So one of the two consecutive β-differences must be 1. The corresponding α-difference is then also 1 by Corollary 1. The next β-difference is then necessarily 2 (Lemma 3), and the next α-difference can be 2. Then the next β-difference is still 2, but the corresponding α-difference is 1. Thus $r \leq 2$, $t \leq 3$; and $r = 2$ with $t = 3$ in (5) is achieved, for example for $n = 11$. □

Lemma 6. *Let* $(a_n, b_n) \in \mathcal{T}$*. Then* $(a_n - t, b_n - t) = (a_m, b_m) \in \mathcal{T}$ *for no* $t > 3$.

Proof. Follows immediately from Lemmas 3 to 5. □

4 Proof of the Main Theorem

We need to show $\mathcal{P} = \mathcal{T}$. Since FREAK is acyclic, it suffices to show two things: Any move from any position in $\mathcal{T}$ results in a position in $\overline{\mathcal{T}}$; and from any position in $\overline{\mathcal{T}}$, there exists a move to a position in $\mathcal{T}$.

We precede these two aspects with a notation and a proposition.

Notation 1. For every $n \in \mathbb{Z}_{\geq} 0$, let $d_n := b_n - a_n$.

Lemma 7. *(i) For every* $n \in \mathbb{Z}_{\geq} 0$, $d_{n+1} - d_n \in \{0, 1\}$.
(ii) d_n *is a nondecreasing function of* n.
(iii) $\cup_{n\geq 0} d_n = \mathbb{Z}_{\geq 0}$.

Proof. (i) We have, $d_{n+1} - d_n = \Delta\lfloor n\beta\rfloor - \Delta\lfloor n\alpha\rfloor$. By (3), $\Delta\lfloor n\alpha\rfloor \in \{1, 2\}$. If $\Delta\lfloor n\alpha\rfloor = 1$, then $\Delta\lfloor n\beta\rfloor \in \{1, 2\}$. If $\Delta\lfloor n\alpha\rfloor = 2$, then $\Delta\lfloor n\beta\rfloor = 2$ by Lemma 1.
(ii) It follows immediately from (i) that d_n is nondecreasing.
(iii) The fact that the multiset $\cup_{n\geq 0} d_n$ contains every nonnegative integer also follows immediately from (i). □

Any move from any position in $\mathcal{T}$ results in a position in $\overline{\mathcal{T}}$. Let $(a_n, b_n) \in \mathcal{T}$, $n \geq 1$. We have to show that $(a_n, b_n) \to (a_m, b_m) \in \mathcal{T}$ for no $m \geq 0$. For $t \in \{1, 2, 3\}$, $(a_n, b_n) \to (a_n - t, b_n - t)$ is blocked by (I). For $t > 3$, $(a_n - t, b_n - t) \to (a_m, b_m)$ is impossible (Lemma 6). Since A and B are strictly increasing, a move of type B cannot lead from $\mathcal{T}$ to $\mathcal{T}$.

From any position in $\overline{\mathcal{T}}$, there exists a move to a position in $\mathcal{T}$. Suppose $(x, y) \in \overline{\mathcal{T}}$, $0 \leq x \leq y$. We first deal with the case $x = y := t$. For $t = 1$, $(t, t) = (1, 1)$ is in $\mathcal{T}$; $(2, 2) \to (0, 0)$ is not blocked since $2 \notin B$. Also $(3, 3) \to (2, 3) \in \mathcal{T}$ is not blocked: it is a move of the form (II)(a). For $t > 3$, taking (t, t) is never blocked. Moreover, $(0, y) \to (0, 0)$ and $(1, y) \to (1, 1)$ are not blocked. We may thus assume $1 < x < y$. Then $x = a_n = b_m$ implies $n > m$, since $\beta > \alpha$, so B increases at least as fast as A (CF Lemma 2(iii)).

Since A, B cover the nonnegative integers (Lemma 2(i)), we have either (i) $x = a_n$ or (ii) $x = b_n$ for some $n \in \mathbb{Z}_{\geq 0}$. Of course Lemma 2(iv) implies that $x = a_n = b_m$ for infinitely many $n > m > 1$.

(i) $x \in B$, say $x = b_m$.
(i1) $x \notin A$. Then the Nim move $y \to a_m$ is a non blocked move of the form (II)(c).
(i2) $x \in A$, say $x = a_n$. We have $1 < m < n$.
(i21) $y > b_n$. Then do $y \to b_n$. This move is of the form (II)(b). It is not blocked, since $b_n > x = a_n$.
(i22) $y < b_n$. We consider two cases.
1. $y \in B$, say $y = b_k$. Then $k < n$, so can make the (II)(a) move $x \to a_k$.
2. $y \notin B$. Then move $y \to x_m$. It is an unblocked move of the form (II)(c).
(ii) $x \in A$, say $x = a_n$. The case where also $x \in B$, say $x = b_m$, was dealt with in (i2) above, so we may assume $x \notin B$.
(ii1) $y > b_n$. Then move $y \to b_n$. This Nim move is not blocked, since $b_n > a_n = x$. The move is of the form (II)(b).
(ii2) $y < b_n$. If $y \in B$, say $y = b_k$, then we have $k < n$, so we can move $x \to a_k$, as in (i22)1. So we may assume $y \notin B$. We have $1 < a_n = x < y < b_n$. Let $d := y - x = y - a_n < b_n - a_n = d_n$. By Lemma 7(iii), there exists $k < n$

such that $d_k = d$, that is, $b_k - a_k = y - a_n$, so $y - b_k = a_n - a_k := t$. Then the Wythoff move $(x, y) \to (a_n - t, y - t) = (a_k, b_k) \in \mathcal{T}$ is not blocked, even if $t \in \{1, 2, 3\}$, since $y \notin B$. □

5 A Linear Winning Strategy

Given any game position (x, y) of FREAK subject to (2), it obviously suffices to know whether $x \in A$, $x \in B$, $y \in A$, $y \in B$. The proof of Theorem 1 then enables us to win if $(x, y) \in \overline{\mathcal{T}}$.

Theorem 2. *The computations to determine whether or not any of* $x \in A$, $x \in B$, $y \in A$, $y \in B$ *holds is linear in the succinct input size* $\log x + \log y = \log xy$ *of any input game position* (x, y), $1 \le x \le y$.

Proof. Since α is irrational and $1 < \alpha < 2$,

$$x = \lfloor n\alpha \rfloor \iff x < n\alpha < x + 1 \iff \frac{x}{\alpha} < n < \frac{x+1}{\alpha} \iff \left\lfloor \frac{x+1}{\alpha} \right\rfloor = \left\lfloor \frac{x}{\alpha} \right\rfloor + 1.$$

Therefore either $x = \lfloor n\alpha \rfloor = a_n$, where $n = \lfloor (x+1)/\alpha \rfloor$, or else, by Lemma 2(i), $x = \lfloor n\beta \rfloor = b_n$, where $n = \lfloor (x+1)/\beta \rfloor$.

Since also $1 < \beta < 2$, we can compute the same way whether $y = \lfloor n\beta \rfloor$, together with the multiplier n and/or whether $y = \lfloor n\alpha \rfloor$ with its multiplier n. These computations require that α and β be computed to a precision of only $O(\log y)$ digits. Once we made these linear computations, we make the appropriate move prescribed in sub-steps of (i) or (ii) of the proof of Theorem 1. □

6 An Alternate Linear Winning Strategy

We now present a strategy that depends on two exotic numeration systems. Recall that any positive irrational α can be expanded in a *simple continued fraction*:

$$\alpha = a_0 + \cfrac{1}{a_1 + \cfrac{1}{a_2 + \cfrac{1}{a_{3\ldots}}}} := [a_0, a_1, a_2, a_3 \ldots],$$

where $a_0 \in \mathbb{Z}_{\ge 0}$, $a_i \in \mathbb{Z}_{\ge 1}$, $i \ge 1$. The *convergents* of the continued fraction are the rationals $p_n/q_n = [a_0, \ldots, a_n]$, and they satisfy the recurrences (see e.g., [13], Chap. 10):

$$p_{-1} = 1,\ p_0 = a_0,\ p_n = a_n p_{n-1} + p_{n-2} \quad (n \ge 1),$$

$$q_{-1} = 0,\ q_0 = 1,\ q_n = a_n q_{n-1} + q_{n-2} \qquad (n \geq 1).$$

For the case $a_0 = 1$ (then $1 < \alpha < 2$), one of the numeration systems, the p-system, is spawned by the numerators of the convergents (see [5,9]): Every positive integer N can be written uniquely in the form

$$N = \sum_{i \geq 0} s_i p_i,\ 0 \leq s_i \leq a_{i+1},\ s_{i+1} = a_{i+2} \implies s_i = 0 \quad (i \geq 0).$$

Denote by S, T, the numeration systems based on the numerators of the convergents of the simple continued fraction expansion of α, β, respectively. For any positive integer N, let $R_S(N)$, $R_T(N)$ denote the representations of N in the S, T numeration systems, respectively. We say that N is S*-vile*, T*-vile* if $R_S(N)$, $R_T(N)$ respectively ends in an even number (possibly 0) of 0s. Analogously, N is S*-dopey*, T*-dopey* if $R_S(N)$, $R_T(N)$ respectively ends in an odd number of 0s.

Note 1. The names "evil" and "dopey" are inspired by the *evil* and *odious* numbers, those that have an even and an odd number of 1's in their binary representation respectively. To indicate that we count 0s rather than 1s, and only at the tail end, the "ev" and "od" are reversed to "ve" and "do" in "vile" and "dopey". "Evil" and "odious" were coined by Elwyn Berlekamp, John Conway and Richard Guy [1].

We notice that

$$\alpha = [1, 12, 1, 2, 2, 2, \alpha], \quad \beta = [1, 1, 2, \alpha].$$

The periodicities are of course a manifestation of Lagrange's Theorem ([13, Chap. 10]). For α we have $p_0 = 1$, $p_1 = 13$, $p_2 = 14$, $p_3 = 41$, $p_4 = 96, \ldots$. For β, $p_0 = 1$, $p_1 = 2$, $p_2 = 5$, $p_3 = 7$, $p_4 = 89, \ldots$. Also $s_0 \leq a_1 = 1$, so $s_0 \in \{0, 1\}$ for both numeration systems. In Table 2 we exhibit $R_S(N)$ on the left-hand side and $R_T(N)$ on the right-hand side for the first few positive integers N.

Comparing Tables 1 and 2, notice that, at least for the range $n \in [1, 20]$: $n \in A$ if and only if n is S-vile; $n \in B$ if and only if n is T-vile. This property holds in general – see [5], Sect. 5. It follows immediately that the game rules of FREAK, in terms of the S- and T-numeration systems, can be stated as follows:

(I) (Restricted Wythoff move.) $(x, y) \to (x - t, y - t)$ for every $t \in \{1, \ldots, x\}$, except that this move is blocked if the following three conditions hold: (a) $t \in \{1, 2, 3\}$, (b) x is S-vile, (c) y is T-vile.

(II) (Restricted Nim move.)

(a) $(x, y) \to (x - t, y)$ for any $0 < t \leq x$; or
(b) $(x, y) \to (x, y - t)$ for any $0 < t \leq y$; or
(c) $(x, y) \to (y - t, x)$ for any $0 < t \leq y$ except that this move is blocked if x is both S-vile and T-vile and y is T-vile.

Table 2 Representation of $1 \le n \le 15$ in the S- (left) and T-system (right)

14	13	1	n	7	5	2	1
0	0	1	1	0	0	0	1
0	0	2	2	0	0	1	0
0	0	3	3	0	0	1	1
0	0	4	4	0	0	2	0
0	0	5	5	0	1	0	0
0	0	6	6	0	1	0	1
0	0	7	7	1	0	0	0
0	0	8	8	1	0	0	1
0	0	9	9	1	0	1	0
0	0	10	10	1	0	1	1
0	0	11	11	1	0	2	0
0	0	12	12	1	1	0	0
0	1	0	13	1	1	0	1
1	0	0	14	2	0	0	0
1	0	1	15	2	0	0	1
1	0	2	16	2	0	1	0
1	0	3	17	2	0	1	1
1	0	4	18	2	0	2	0
1	0	5	19	2	1	0	0
1	0	6	20	2	1	0	1

The computation whether x or y is S-vile or T-vile can obviously be done in linear-time in the input size $\log xy$ of any game position (x, y). It follows that also the winning strategy based on the two numeration systems is linear. It has the advantage of avoiding the floor function and division, both of which are needed for our first winning strategy.

7 Epilogue

Preliminary Thoughts. We presented two linear winning strategies for a game on $m = 2$ piles of tokens for which the P-positions constitute a *single* pair of integers (A^1, A^2) (in contrast to [2] and [8]), (A^1, A^2) satisfy $|A^1 \cap A^2| = \infty$, but $|A^1 \cup A^2| = \mathbb{Z}_{\ge 1}$. It appears to be a first such case for a Wythoff-like game.

FREAK, the name of the game, derives from FRactional BEAtty game. The terminology "vile" and "dopey" is inspired by the evil and odious numbers, those that have an even and an odd number of 1's in their binary representation respectively. To indicate that we count 0s rather than 1s, and only at the tail end, the "ev" and "od" are reversed to "ve" and "do" in "vile" and "dopey". "Evil" and "odious" were coined by Elwyn Berlekamp, John Conway and Richard Guy while composing their famous book *Winning Ways* [1]. Urban Larsson suggested the particular values of α, β used in this work. A "fractional Beatty theorem" was recently proved by Peter Hegarty [14] (following a suggestion of mine). In previous

Table 3 The first few terms of the P-positions (a_n, b_n)

n	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27
a_n	0	0	1	2	3	4	5	6	6	7	8	9	10	11	12	13	13	14	15	16	17	18	19	19	20	21	22	23
b_n	0	2	5	8	11	14	17	20	22	25	28	31	34	37	40	43	45	48	51	54	57	60	63	65	68	71	74	77

papers we have shown that a judicious choice of numeration systems can improve the efficiency of winning strategies of various games, much as data structures in Computer Science. In the present paper, numeration systems are the tool used uniformly for both formulating and analyzing FREAK.

Further questions

(1) Extend the above results to an infinite set of fractional Beatty games, for example, for $\alpha = \ell\varphi/(2k+1)$, $\beta = \ell\varphi^2/(2k+1)$, k, ℓ any fixed positive integers.
(2) Are there "simpler" game rules for the same set of P-positions considered here?
(3) A move $R = (r_1, \ldots, r_m) \neq (0, \ldots, 0)$ in an m-pile subtraction game is *invariant* if R can be made from every game position $(s_1, \ldots, s_m)$ for which $s_i - r_i \geq 0$ for $i = 1, \ldots, m$. An m-pile subtraction game is *invariant* if all its moves are invariant. Otherwise the game is *variant*. The move rules for FREAK are obviously variant. Duchêne and Rigo [4] conjectured that for $m = 2$, given any two *complementary* Beatty sequences A, B, there exists an invariant game with $(A, B) \cup \{(0, 0)\}$ as its P-positions. This conjecture was proved in [16]. Is there an invariant game with the P-positions presented in Sect. 2 above?
(4) More generally, can the invariance theorem proved in [16] be extended in the following sense: Is there a nontrivial subset of non-complementary Beatty sequences A, B, for which there always exists an invariant game with $(A, B) \cup \{(0, 0)\}$ as its P-positions?
(5) Let $r, t \in \mathbb{R}_{>0}$. The equation $\alpha^{-1} + (\alpha + t)^{-1} = r$ has the positive solution $\alpha = (2r^{-1} - t + \sqrt{t^2 + 4r^{-2}})/2$. For every set of values $(r, t) \in \mathbb{R}^2_{>0}$ for which α is irrational one can define, in principle, an (r, t)-Beatty game. So there is a continuum of such games. If r and t are restricted to be rational we get a denumerable number of games. (One can even consider such games when α is rational, see [7].) For example, for $r = 3/2$, $t = 2$, $\alpha = (\sqrt{13} - 1)/3$ (so $2/3 < \alpha < 1$), and $\beta = \alpha + 2 = (\sqrt{13} + 5)/3$. It may be of interest to formulate game rules for a game whose P-positions are $\cup_{n \geq 0}(a_n, b_n)$, where $a_n = \lfloor n\alpha \rfloor$, $b_n = \lfloor n\beta \rfloor$. In this game there are infinitely many integers that are repeated (at most twice) in $\{a_n\}_{n \geq 0}$, in addition to $|A \cap B| = \infty$. But there is the nice property that $b_n = a_n + 2n$ for all $n \geq 0$, as can be seen in Table 3 below.
(6) Investigate the Sprague-Grundy function of fractional Beatty games in an attempt to give a poly-time winning strategy for playing them in a sum.
(7) Consider take-away games on $m > 2$ piles, where the m sequences $A^1, \ldots, A^m$ constituting the P-positions do not split $\mathbb{Z}_{\geq 1}$.

(8) Consider partizan take-away games where the P-positions do not split $\mathbb{Z}_{\geq 1}$.
(9) Investigate Fractional Beatty games for misère play.

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WZ-Proofs of "Divergent" Ramanujan-Type Series

Jesús Guillera

Dedicated to the memory of Herb Wilf, who was part of the commitee of my PhD thesis

Abstract We prove some "divergent" Ramanujan-type series for $1/\pi$ and $1/\pi^2$ applying a Barnes-integrals strategy of the WZ-method. In addition, in the last section, we apply the WZ-duality technique to evaluate some convergent related series.

Keywords Hypergeometric series • WZ-method • Ramanujan-type series for $1/\pi$ and $1/\pi^2$ • Barnes integrals

1 Wilf-Zeilberger's Pairs

We recall that a function $A(n,k)$ is *hypergeometric* in its two variables if the quotients

$$\frac{A(n+1,k)}{A(n,k)} \quad \text{and} \quad \frac{A(n,k+1)}{A(n,k)}$$

are rational functions in n and k, respectively. Also, a pair of hypergeometric functions in its two variables, $F(n,k)$ and $G(n,k)$, is said to be a *Wilf and Zeilberger (WZ) pair* [13, Chap. 7] if

$$F(n+1,k) - F(n,k) = G(n,k+1) - G(n,k). \tag{1}$$

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In this case, H. S. Wilf and D. Zeilberger [17] have proved that there exists a rational function $C(n,k)$ such that

$$G(n,k) = C(n,k)F(n,k). \tag{2}$$

The rational function $C(n,k)$ is the so-called *certificate* of the pair (F,G). To discover WZ-pairs, we use Zeilberger's Maple package EKHAD [13, Appendix A]. If EKHAD certifies a function, we have found a WZ-pair! We will write the functions $F(n,k)$ and $G(n,k)$ using rising factorials, also called Pochhammer symbols, rather than the ordinary factorials. The rising factorial is defined by

$$(x)_n = \begin{cases} x(x+1)\cdots(x+n-1), & n \in \mathbb{Z}^+, \\ 1, & n = 0, \end{cases} \tag{3}$$

or more generally by $(x)_t = \Gamma(x+t)/\Gamma(x)$. For $t \in \mathbb{Z} - \mathbb{Z}^-$, this last definition coincide with (3). But it is more general because it is also defined for all complex x and t such that $x + t \in \mathbb{C} - (\mathbb{Z} - \mathbb{Z}^+)$.

2 A Barnes-Integrals WZ Strategy

If we sum (1) over all $n \geq 0$, we get

$$\sum_{n=0}^{\infty} G(n,k) - \sum_{n=0}^{\infty} G(n,k+1) = -F(0,k) + \lim_{n\to\infty} F(n,k) \tag{4}$$

whenever the series above are convergent and the limit is finite. D. Zeilberger was the first to apply the WZ-method to prove a Ramanujan-type series for $1/\pi$ [4]. Following his idea, in a series of papers [5,6,9,10] and in the author's thesis [8], we use WZ-pairs together with formula (4) to prove a total of 11 Ramanujan-type series for $1/\pi$ and 4 Ramanujan-like series for $1/\pi^2$. However, while we discovered those pairs we also found some WZ-pairs corresponding to "divergent" Ramanujan-type series [12], like the following pair:

$$F(n,k) = A(n,k)\frac{(-1)^n}{\Gamma(n+1)}\left(\frac{16}{9}\right)^n, \quad G(n,k) = B(n,k)\frac{(-1)^n}{\Gamma(n+1)}\left(\frac{16}{9}\right)^n,$$

where

$$A(n,k) = U(n,k)\frac{-n(n-2)}{3(n+2k+1)}, \quad B(n,k) = U(n,k)(5n+6k+1),$$

and

$$U(n,k) = \frac{\left(\frac{1}{2}\right)_n \left(\frac{1}{4}+\frac{3k}{2}\right)_n \left(\frac{3}{4}+\frac{3k}{2}\right)_n}{(1+k)_n(1+2k)_n} \frac{\left(\frac{1}{6}\right)_k \left(\frac{5}{6}\right)_k}{(1)_k^2}.$$

We cannot use formula (4) with this pair because the series is divergent and the limit is infinite, due to the factor $(-16/9)^n$. To deal with this kind of WZ-pairs we will proceed as follows: First we replace the factor $(-1)^n$ with $\Gamma(n+1)\Gamma(-n)$. By doing it we again get a WZ-pair, because $(-1)^n$ and $\Gamma(n+1)\Gamma(-n)$ transform formally in the same way under the substitution $n \to n+1$; namely, the sign changes. To fix ideas, the modified version of the WZ-pair above is

$$\tilde{F}(s,t) = A(s,t)\Gamma(-s)\left(\frac{16}{9}\right)^s, \quad \tilde{G}(s,t) = B(s,t)\Gamma(-s)\left(\frac{16}{9}\right)^s.$$

Then, integrating from $s = -i\infty$ to $s = i\infty$ along a path $\mathcal{P}$ (curved if necessary) which separates the poles of the form $s = 0, 1, 2\ldots$ from all the other poles, we obtain

$$\frac{1}{2\pi i}\int_{-i\infty}^{i\infty} B(s,t)\Gamma(-s)(-z)^s ds = \sum_{n=0}^{\infty} B(n,t)\frac{z^n}{n!}, \quad |z| < 1, \tag{5}$$

where we have used the Barnes integral theorem, which is an application of Cauchy's residues theorem using a contour which closes the path with a right side semicircle of center at the origin and infinite radius. The Barnes integral gives the analytic continuation of the series to $z \in \mathbb{C} - [1, \infty)$. Integrating along the same path the identity $\tilde{G}(s,t+1) - \tilde{G}(s,t) = \tilde{F}(s+1,t) - \tilde{F}(s,t)$, we obtain

$$\int_{-i\infty}^{i\infty} \tilde{G}(s,t+1)ds - \int_{-i\infty}^{i\infty} \tilde{G}(s,t)ds = \int_{-i\infty}^{i\infty} \tilde{F}(s+1,t)ds - \int_{-i\infty}^{i\infty} \tilde{F}(s,t)ds \tag{6}$$

$$= \int_{1-i\infty}^{1+i\infty} \tilde{F}(s,t)ds - \int_{-i\infty}^{i\infty} \tilde{F}(s,t)ds = -\int_{\mathcal{C}} \tilde{F}(s,t)ds,$$

where $\mathcal{C}$ is the contour limited by the path $\mathcal{P}$, the same path but moved one unit to the right, and the lines $y = -\infty$ and $y = +\infty$. As the only pole inside this contour is at $s = 0$ and the residue at this point is zero, the last integral is zero and we have

$$\int_{-i\infty}^{i\infty} \tilde{G}(s,t)ds = \int_{-i\infty}^{i\infty} \tilde{G}(s,t+1)ds. \tag{7}$$

This implies, by Weierstrass's theorem [16], that

$$\frac{1}{2\pi i}\int_{-i\infty}^{i\infty} \tilde{G}(s,t)ds = \lim_{t\to\infty}\frac{1}{2\pi i}\int_{-i\infty}^{i\infty} \tilde{G}(s,t)ds = \frac{1}{2\pi i}\int_{-i\infty}^{i\infty} \lim_{t\to\infty} \tilde{G}(s,t)ds$$

$$= \frac{1}{2\pi i}\int_{-i\infty}^{i\infty} \frac{3}{\pi}\left(\frac{1}{2}\right)_s \Gamma(-s)2^s ds = \frac{\sqrt{3}}{\pi},$$

where the last equality holds because

$$\frac{1}{2\pi i}\int_{-i\infty}^{i\infty}\left(\frac{1}{2}\right)_s \Gamma(-s)(-z)^s ds = \sum_{n=0}^{\infty}\frac{\left(\frac{1}{2}\right)_n}{(1)_n}z^n = \frac{1}{\sqrt{1-z}}, \quad |z|<1,$$

implies that

$$\frac{1}{2\pi i}\int_{-i\infty}^{i\infty}\left(\frac{1}{2}\right)_s \Gamma(-s)(-z)^s ds = \frac{1}{\sqrt{1-z}}, \quad z\in\mathbb{C}-[1,\infty).$$

Hence, we have

$$\frac{1}{2\pi i}\int_{-i\infty}^{i\infty}\frac{\left(\frac{1}{2}\right)_s\left(\frac{1}{4}+\frac{3t}{2}\right)_s\left(\frac{3}{4}+\frac{3t}{2}\right)_s}{(1+t)_s(1+2t)_s}\frac{\left(\frac{1}{6}\right)_t\left(\frac{5}{6}\right)_t}{(1)_t^2}(5s+6t+1)\Gamma(-s)\left(\frac{4}{3}\right)^{2s}ds = \frac{\sqrt{3}}{\pi},$$

or equivalently

$$\frac{1}{2\pi i}\int_{-i\infty}^{i\infty}\frac{\left(\frac{1}{2}\right)_s\left(\frac{1}{4}+\frac{3t}{2}\right)_s\left(\frac{3}{4}+\frac{3t}{2}\right)_s}{(1+t)_s(1+2t)_s}(5s+6t+1)\Gamma(-s)\left(\frac{4}{3}\right)^{2s}ds = \frac{\sqrt{3}}{\pi}\frac{(1)_t^2}{\left(\frac{1}{6}\right)_t\left(\frac{5}{6}\right)_t}.$$

Finally, substituting $t=0$, we see that

$$\frac{1}{2\pi i}\int_{-i\infty}^{i\infty}\frac{\left(\frac{1}{2}\right)_s\left(\frac{1}{4}\right)_s\left(\frac{3}{4}\right)_s}{(1)_s^2}(5s+1)\Gamma(-s)\left(\frac{4}{3}\right)^{2s}ds = \frac{\sqrt{3}}{\pi}. \tag{8}$$

It is very convenient to write the Barnes integral in hypergeometric notation. By the definition of hypergeometric series, we see that for $-1\le z<1$, we have

$$\sum_{n=0}^{\infty}\frac{\left(\frac{1}{2}\right)_n(s)_n(1-s)_n}{(1)_n^3}z^n = {}_3F_2\left(\left.\begin{matrix}\frac{1}{2}, & s, & 1-s\\ & 1, & 1\end{matrix}\right| z\right)$$

and

$$\sum_{n=0}^{\infty}\frac{\left(\frac{1}{2}\right)_n(s)_n(1-s)_n}{(1)_n^3}nz^n = \frac{1}{2}s(1-s)z\,{}_3F_2\left(\left.\begin{matrix}\frac{3}{2}, & 1+s, & 2-s\\ & 2, & 2\end{matrix}\right| z\right),$$

where the notation on the right side stands for the analytic continuation of the series on the left. Hence, we can write (8) in the form

$${}_3F_2\left(\left.\begin{matrix}\frac{1}{2}, & \frac{1}{4}, & \frac{3}{4}\\ & 1, & 1\end{matrix}\right| \frac{-16}{9}\right) - \frac{5}{6}\,{}_3F_2\left(\left.\begin{matrix}\frac{3}{2}, & \frac{5}{4}, & \frac{7}{4}\\ & 2, & 2\end{matrix}\right| \frac{-16}{9}\right) = \frac{\sqrt{3}}{\pi}.$$

If, instead of integrating to the right side, we integrate (8) along a contour which closes the path $\mathcal{P}$ with a semicircle of center $s = 0$ taken to the left side with an infinite radius, then we have poles at $s = -n - 1/2$, at $s = -n - 1/4$ and at $s = -n - 3/4$ for $n = 0, 1, 2, \ldots$, and we obtain

$$\frac{\sqrt{3}}{2}\sum_{n=0}^{\infty}\frac{\left(\frac{1}{2}\right)_n^3}{(1)_n\left(\frac{3}{4}\right)_n\left(\frac{5}{4}\right)_n}(10n+3)(-1)^n\left(\frac{3}{4}\right)^{2n}$$
$$-\frac{\sqrt{2}\,\pi^2}{8\,\Gamma\left(\frac{3}{4}\right)^4}\sum_{n=0}^{\infty}\frac{\left(\frac{1}{4}\right)_n^3}{(1)_n\left(\frac{1}{2}\right)_n\left(\frac{3}{4}\right)_n}(20n+1)(-1)^n\left(\frac{3}{4}\right)^{2n}$$
$$-\frac{3\sqrt{2}\,\Gamma\left(\frac{3}{4}\right)^4}{16\,\pi^2}\sum_{n=0}^{\infty}\frac{\left(\frac{3}{4}\right)_n^3}{(1)_n\left(\frac{3}{2}\right)_n\left(\frac{5}{4}\right)_n}(20n+11)(-1)^n\left(\frac{3}{4}\right)^{2n}=1.$$

which is an identity relating three convergent series.

3 Other Examples

In a similar way we can prove other identities of the same kind, for example,

$$\frac{1}{2\pi i}\int_{-i\infty}^{i\infty}\frac{\left(\frac{1}{2}+t\right)_s^3\left(\frac{1}{2}\right)_s^2}{(1+t)_s^3(1+2t)_s}(10s^2+6s+1+14st+4t^2+4t)\Gamma(-s)2^{2s}ds=\frac{4}{\pi^2}\frac{(1)_t^4}{\left(\frac{1}{2}\right)_t^4},$$

$$\frac{1}{2\pi i}\int_{-i\infty}^{i\infty}\frac{\left(\frac{1}{2}\right)_s\left(\frac{1}{2}+t\right)_s^2}{(1)_s(1+2t)_s}(3s+2t+1)\Gamma(-s)2^{3s}ds=\frac{1}{\pi}\frac{(1)_t}{\left(\frac{1}{2}\right)_t},$$

and

$$\frac{1}{2\pi i}\int_{-i\infty}^{i\infty}\frac{\left(\frac{1}{2}\right)_s\left(\frac{1}{2}+2t\right)_s\left(\frac{1}{3}+t\right)_s\left(\frac{2}{3}+t\right)_s}{\left(\frac{1}{2}+\frac{t}{2}\right)_s\left(1+\frac{t}{2}\right)_s(1+t)_s}$$
$$\times\frac{(15s+4)(2s+1)+t(33s+16)}{2s+t+1}\Gamma(-s)2^{2s}ds=\frac{3\sqrt{3}}{\pi}\frac{1}{2^{6t}}\frac{(1)_t^2}{\left(\frac{1}{4}\right)_t\left(\frac{3}{4}\right)_t}.$$

In the two last examples the hypothesis of Weierstrass theorem fail and hence we cannot apply it, but we obtain the sum using Meurman's periodic version of Carlson's theorem [2, p. 39] which asserts that if $H(z)$ is a periodic entire function of period 1 and there is a real number $c < 2\pi$ such that $H(z) = \mathcal{O}(\exp(c|Im(z)|))$ for all $z \in \mathbb{C}$, then $H(z)$ is constant [1, Appendix] and [11, Theorem 2.3]. In the second and third examples we determine the constants $1/\pi$ and $3\sqrt{3}/\pi$ taking $t = 1/2$ and $t = -1/3$ respectively. Substituting $t = 0$ in the above examples, we obtain respectively

$$\frac{1}{2\pi i}\int_{-i\infty}^{i\infty}\frac{\left(\frac{1}{2}\right)_s^5}{(1)_s^4}(10s^2+6s+1)\Gamma(-s)2^{2s}ds = \frac{4}{\pi^2}, \tag{9}$$

$$\frac{1}{2\pi i}\int_{-i\infty}^{i\infty}\frac{\left(\frac{1}{2}\right)_s^3}{(1)_s^2}(3s+1)\Gamma(-s)2^{3s}ds = \frac{1}{\pi}, \tag{10}$$

and

$$\frac{1}{2\pi i}\int_{-i\infty}^{i\infty}\frac{\left(\frac{1}{2}\right)_s\left(\frac{1}{3}\right)_s\left(\frac{2}{3}\right)_s}{(1)_s^2}(15s+4)\Gamma(-s)2^{2s}ds = \frac{3\sqrt{3}}{\pi}. \tag{11}$$

Using hypergeometric notation, we can write (9), (10) and (11) respectively in the following forms:

$$ {}_5F_4\left(\left.\begin{matrix}\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\\ 1, 1, 1, 1\end{matrix}\right| -4\right) - \frac{3}{4}\,{}_5F_4\left(\left.\begin{matrix}\frac{3}{2}, \frac{3}{2}, \frac{3}{2}\ \frac{3}{2}\ \frac{3}{2}\\ 2, 2, 2, 2\end{matrix}\right| -4\right)$$
$$-\frac{5}{4}\,{}_5F_4\left(\left.\begin{matrix}\frac{3}{2}, \frac{3}{2}, \frac{3}{2}\ \frac{3}{2}\ \frac{3}{2}\\ 2, 2, 2, 1\end{matrix}\right| -4\right) = \frac{4}{\pi^2},$$

$$ {}_3F_2\left(\left.\begin{matrix}\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\\ 1, 1\end{matrix}\right| -8\right) - 3\,{}_3F_2\left(\left.\begin{matrix}\frac{3}{2}, \frac{3}{2}, \frac{3}{2}\\ 2, 2\end{matrix}\right| -8\right) = \frac{1}{\pi},$$

and

$$4\,{}_3F_2\left(\left.\begin{matrix}\frac{1}{2}, \frac{1}{3}, \frac{2}{3}\\ 1, 1\end{matrix}\right| -4\right) - \frac{20}{3}\,{}_3F_2\left(\left.\begin{matrix}\frac{3}{2}, \frac{4}{3}, \frac{5}{3}\\ 2, 2\end{matrix}\right| -4\right) = \frac{3\sqrt{3}}{\pi}.$$

Related applications of the WZ-method for Barnes-type integrals are for example in [3, Sect. 5.2] and [14].

4 The Dual of a "Divergent" Ramanujan-Type Series

The WZ duality technique [13, Chap. 7] allows to transform pairs which lead to divergences into pairs which lead to convergent series. To get the dual $\hat{G}(n,k)$ of $G(-n,-k)$, we make the following changes:

$$(a)_{-n} \to \frac{(-1)^n}{(1-a)_n}, \quad (1)_{-n} \to \frac{n(-1)^n}{(1)_n}, \quad (a)_{-k} \to \frac{(-1)^k}{(1-a)_k}, \quad (1)_{-k} \to \frac{k(-1)^k}{(1)_k}.$$

4.1 Example 1

The package EKHAD certifies the pair

$$F(n,k) = U(n,k)\frac{2n^2}{2n+k}, \qquad G(n,k) = U(n,k)\frac{6n^2+2n+k+4nk}{2n+k}, \quad (12)$$

where

$$U(n,k) = \frac{\left(\frac{1}{2}\right)_n^2 \left(1+\frac{k}{2}\right)_n \left(\frac{1}{2}+\frac{k}{2}\right)_n}{(1)_n^2 (1+k)_n^2} \frac{\left(\frac{1}{2}\right)_k}{(1)_k} 4^n = \frac{(2n)!^2(2n+k)!(2k)!}{n!^4 k!(n+k)!^2} \frac{1}{16^n 4^k}.$$

We cannot use this WZ-pair to obtain a Ramanujan-like evaluation because, as $z > 1$, the corresponding series and also the corresponding Barnes integral are both divergent. However, we will see how to use it to evaluate a related convergent series. What we will do is to apply the WZ duality technique. Thus, if we take the dual of $G(-n,-k)$ and replace k with $k-1$, we obtain

$$\hat{G}(n,k) = \frac{1}{U(n,k)} \frac{2(2k-1)(2n+k)}{n^2(n+k)^2(n+k-1)^2}(6n^2-6n+1-k+4nk),$$

and EHKAD finds its companion

$$\hat{F}(n,k) = \frac{1}{U(n,k)} \frac{-2(2n+k)(2n+k-1)(2n-1)^2}{n^2(n+k)^2(n+k-1)^2}.$$

Applying Zeilberger’s formula

$$\sum_{n=j}^{\infty}(\hat{F}(n+1,n)+\hat{G}(n,n)) = \sum_{n=j}^{\infty}\hat{G}(n,j)$$

with $j = 1$, we obtain

$$\sum_{n=1}^{\infty} \left(\frac{16}{27}\right)^n \frac{(1)_n^3}{\left(\frac{1}{2}\right)_n \left(\frac{1}{3}\right)_n \left(\frac{2}{3}\right)_n} \frac{11n-3}{n^3} = 16 \sum_{n=1}^{\infty} \frac{1}{4^n} \frac{(1)_n^3}{\left(\frac{1}{2}\right)_n^3} \frac{3n-1}{n^3}. \quad (13)$$

The series in (13) are dual to Ramanujan-type “divergent” series, and in [7, p. 221] we proved that the series on the right side is equal to $\pi^2/2$. Hence

$$\sum_{n=1}^{\infty} \left(\frac{16}{27}\right)^n \frac{(1)_n^3}{\left(\frac{1}{2}\right)_n \left(\frac{1}{3}\right)_n \left(\frac{2}{3}\right)_n} \frac{11n-3}{n^3} = 8\pi^2. \quad (14)$$

Formula (14), as well as other similar formulas, was conjectured in [15, Conjecture 1.4] by Zhi-Wei Sun.

4.2 Example 2

The package EKHAD certifies the pair

$$F(n,k) = U(n,k)\frac{64n^3}{(2k+1)(2n-2k+1)},$$

$$G(n,k) = U(n,k)\frac{(2n+1)^2(11n+3) - 12k(2n^2+3nk+n+k)}{(2n+1)^2},$$

where

$$U(n,k) = \frac{\left(\frac{1}{2}-k\right)_n \left(\frac{1}{2}+k\right)_n^2 \left(\frac{1}{3}\right)_n \left(\frac{1}{3}\right)_n}{(1)_n^3 \left(\frac{1}{2}\right)_n^2} \left(\frac{27}{16}\right)^n.$$

Taking the dual $\hat{G}(n,k)$ of $G(-n,-k)$, replacing n with $n+x$ and applying Zeilberger's theorem

$$\sum_{n=0}^{\infty} \hat{G}(n+x,0) = \lim_{k\to\infty} \sum_{n=0}^{\infty} \hat{G}(n+x,k) + \sum_{k=0}^{\infty} \hat{F}(x,k),$$

where $\hat{F}(n,k)$ is the companion of $\hat{G}(n,k)$, we obtain

$$\sum_{n=0}^{\infty} \frac{(1+x)_n^3}{\left(\frac{1}{2}+x\right)_n \left(\frac{1}{3}+x\right)_n \left(\frac{2}{3}+x\right)_n} \left(\frac{16}{27}\right)^n \frac{11(n+x)-3}{(n+x)^3}$$
$$= \frac{6(3x-1)(3x-2)}{x^3(2x-1)} \sum_{k=0}^{\infty} \frac{\left(\frac{1}{2}\right)_k \left(\frac{3}{2}-x\right)_k}{\left(\frac{1}{2}+x\right)_k^2}.$$

Taking $x = 1$ we again obtain (14).

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Smallest Parts in Compositions

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Dedicated to Herbert Wilf on the occasion of his 80-th birthday.

Abstract By analogy with recent Work of Andrews on smallest parts in partitions of integers, we consider smallest parts in compositions (ordered partitions) of integers. In particular, we study the number of smallest parts and the sum of smallest parts in compositions of n as well as the position of the first smallest part in a random composition of n.

1 Introduction

A composition of an integer $n > 0$ is a representation of n as an ordered sum of positive integers $n = a_1 + a_2 + \cdots + a_m$. It is well known that there are 2^{n-1} compositions of n, and $\binom{n-1}{k-1}$ compositions of n with exactly k summands or parts, which will also be referred to as k-compositions.

The subject of integer compositions has engaged the attention of Herbert Wilf on several occasions (see for example [3] and [5]).

In this note we undertake an enumerative study of compositions with respect to the smallest summand. Our inspiration came mostly from the work of G. Andrews which considered smallest parts in integer partitions [2]. He proved that the number $spt(n)$ of smallest parts in partitions of n is given by

$$spt(n) = np(n) - \frac{1}{2}N_2(n),$$

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where $p(n)$ is the number of partitions of n and $N_2(n)$ is the second Atkin-Garvan moment of ranks.

We will consider both the number and sum of smallest parts in all compositions. It turns out that, in the case of compositions, we are availed of both elementary and advanced techniques for discussing the two statistics. We will compute explicit formulas, and asymptotic estimates, for the total number of smallest parts in all compositions of n, and for the sum of smallest parts in all compositions of n.

In this context we find the following sequence in the Encyclopedia of Integer Sequences:

Total number of smallest parts in compositions of $n \geq 1$ ([6, A097941]):
1, 3, 6, 15, 31, 72, 155, 340, 738, 1,595, 3,424, 7,335, 15,642, 33,243, 70,432, 148,808, ...

In Sect. 2 we use elementary constructive arguments to derive the necessary exact formulas. Then in Sect. 3 we use generating function techniques to obtain the formulas, leading naturally to asymptotic enumeration of compositions for large n. The final section is devoted to the enumeration of compositions with respect to the first position of the smallest parts.

2 Constructive Proofs

We will need the following known result (see for example [1, p. 63]):

Lemma 1. *The number of k-compositions of $[n]$ in which each part $\geq m$ is given by*

$$\binom{n-(m-1)k-1}{k-1}.$$

Let $c_j(n,k,r) \stackrel{\text{def}}{=}$ number of k-compositions of n with smallest part j such that j appears r times in each composition.
Then

Proposition 1. *If $n = kj$ then $c_j(n,k,r) = \delta_{kr}$, and*

$$c_j(n,k,r) = \binom{k}{r}\binom{n-jk-1}{k-r-1}, \quad n > kj, \tag{1}$$

where δ_{ij} is the Kronecker delta.

Proof. The case $n = jk$ gives the unique composition $(\frac{n}{k}, \ldots, \frac{n}{k})$. So we assume $n > jk$ and construct a composition enumerated by $c_j(n,k,r)$.

Fix any r of the k positions to hold the j's, in $\binom{k}{r}$ ways. Then the remaining $k-r$ positions can be filled with a composition of $n-rj$, into $k-r$ parts, each $\geq j+1$, such that the ith part occupies the ith available position, from left to right. The number of such compositions, by Lemma 1, is $\binom{n-rj-j(k-r)-1}{k-r-1} = \binom{n-jk-1}{k-r-1}$. Hence

$$c_j(n,k,r) = \binom{k}{r}\binom{n-jk-1}{k-r-1}. \qquad \square$$

Corollary 1. *The number $c_j(n,k)$ of k-compositions of n with smallest part j is given by*

$$c_j(n,k) = \binom{n-(j-1)k-1}{k-1} - \binom{n-jk-1}{k-1}. \tag{2}$$

Proof. If compositions with parts $\geq j+1$ are deleted from the set of compositions with parts $\geq j$, we obtain the set of compositions with smallest part j. Now apply Lemma 1. $\square$

2.1 The Number of Smallest Parts

Corollary 2. *The number $f_j(n,k)$ of all occurrences of a fixed smallest part j among all k-compositions of n is given by.*

$$f_j(n,k) = k\binom{n-(j-1)k-2}{k-2}. \tag{3}$$

Proof. Since there are $c_j(n,k,r)$ k-compositions of n with smallest part j such that j appears r times in each composition, the frequency $f_j(n,k,r)$ of j among all compositions in which it appears r times is given by $f_j(n,k,r) = rc_j(n,k,r)$. Thus

$$f_j(n,k,r) = rc_j(n,k,r) = r\binom{k}{r}\binom{n-jk-1}{k-r-1},$$

and

$$f_j(n,k) = \sum_{r\geq 1} f_j(n,k,r) = \sum_{r\geq 1} r\binom{k}{r}\binom{n-jk-1}{k-r-1}$$

Then we apply the rule $\frac{k}{n}\binom{n}{k} = \binom{n-1}{k-1}$, and note that the Vandermonde convolution gives:

$$\sum_{r\geq 1}\binom{k-1}{r-1}\binom{n-jk-1}{k-r-1} = \binom{n-(j-1)k-2}{k-2}.$$

□

Since the set of smallest parts among all k-compositions of n is $\{1, 2, \ldots, \lfloor n/k \rfloor\}$, we can use Corollary 2 to obtain:

Corollary 3. *The number $sp(n,k)$ of smallest parts among all k-compositions of n is given by*

$$sp(n,k) = k\sum_{j=1}^{\lfloor n/k \rfloor}\binom{n-(j-1)k-2}{k-2}. \tag{4}$$

It is easily verified that the sum $\sum_k sp(n,k)$, $n > 0$, agrees with the Sloane sequence [6, A097941] mentioned earlier.

2.2 The Sum of Smallest Parts

The following corollaries are immediate consequences of Corollaries 2 and 3.

Corollary 4. *The sum $s(n,k,j)$ of all copies of a fixed smallest part j among all k-compositions of n is given below.*

$$s(n,k,j) = jk\binom{n-(j-1)k-2}{k-2}. \tag{5}$$

Corollary 5. *The sum $s(n,k)$ of all smallest parts among all k-compositions of n is given below.*

$$s(n,k) = k\sum_{j=1}^{\lfloor n/k \rfloor} j\binom{n-(j-1)k-2}{k-2}. \tag{6}$$

The sequence for the sum of smallest parts in all compositions of an integer $n > 0$ is not yet in Sloane [6]:

$$\sum_k s(n,k),\ n > 0,:\ 1, 4, 8, 20, 37, 56, 173, 372, 788, 1{,}680, 3{,}550, 7{,}554, \ldots$$

3 An Approach via Generating Functions

3.1 The Number of Compositions of n with Smallest Part j

Let $c_j(n,m)$ denote the number of compositions of n with m parts and with smallest part j and let $c_j(n)$ denote the number of compositions of n with smallest part j. We use the following decomposition of the set C_j of compositions of n with smallest part j.

$$\begin{aligned} C_j &= \{\text{a composition with all parts} \geq j+1\} \\ &\quad \times \{\text{a part equal to } j\} \times \{\text{a composition with all parts} \geq j\}. \end{aligned} \tag{7}$$

Translating to generating functions in the style of Wilf [7], where z marks the size of a composition and y marks the number of parts, gives

$$\begin{aligned} C_j(z,y) = \sum_{n\geq 1}\sum_{m\geq 1} c_j(n,m) z^n y^m &= \frac{yz^j}{\left(1-\frac{yz^j}{1-z}\right)\left(1-\frac{yz^{j+1}}{1-z}\right)} \\ &= \frac{y(z-1)^2 z^j}{(yz^j+z-1)(yz^{j+1}+z-1)}. \end{aligned}$$

Setting $y=1$ the generating function for compositions with smallest part j is

$$\sum_{n\geq 1} c_j(n) z^n = \frac{(z-1)^2 z^j}{(z^j+z-1)(z^{j+1}+z-1)}.$$

The generating function for $c_j(n)$ is a rational function of z and the asymptotic growth of the coefficients will depend on the smallest positive zero ρ of the denominator polynomials z^j+z-1 and $z^{j+1}+z-1$. Since $\rho<1$, it satisfies the equation $1-\rho-\rho^j=0$. By singularity analysis

$$c_j(n) \sim [z^n]\frac{(\rho-1)^2\rho^j}{(j\rho^{j-1}+1)(\rho^{j+1}+\rho-1)(z-\rho)}.$$

After some simplification this leads to the asymptotic estimate

$$c_j(n) \sim \frac{\rho^{2j-n-1}}{(1-\rho)(j\rho^{j-1}+1)}.$$

In the case $j = 1$ we have the exact result $c_j(n) = 2^{n-1} - F_n$ where F_n is the n-th Fibonacci number with $F_0 = 0$ and $F_1 = 1$. Consequently *almost all compositions of n have smallest part* 1.

For $j = 2$ we find $\rho = \frac{1}{2}\left(\sqrt{5}-1\right) = 0.618034\ldots$ and for $n = 50$ our asymptotic estimate for $c_2(50)$ is 7,778,742,049 as compared the exact value 7,739,952,337. Similarly, For $j = 3$ we find $\rho = 0.682327803\ldots$ and for $n = 50$ our asymptotic estimate for $c_3(50)$ is 38,789,712 as compared the exact value 37,287,157.

For a fixed number m of parts we can obtain explicit formulas for $c_j(n, m)$ in the spirit of Sect. 1. We can write

$$C_j(z, y) = yz^j \left(\sum_{k=0}^{\infty} \frac{y^k z^{(j+1)k}}{(1-z)^k}\right) \sum_{k=0}^{\infty} \frac{y^k z^{jk}}{(1-z)^k}.$$

Then

$$[y^m]C_j(z, y) = \frac{z^j}{(1-z)^{m-1}} \sum_{k=0}^{m-1} z^{(j+1)k} z^{j(-k+m-1)} = (1-z)^{-m}\left(z^{jm} - z^{(j+1)m}\right).$$

Consequently

$$c_j(n, m) = \binom{n-(j-1)m-1}{m-1}[[n \geq jm]] - \binom{n-jm-1}{m-1}[[n \geq (j+1)m]]$$

and hence

$$c_j(n) = \sum_{m=1}^{n}\left(\binom{n-(j-1)m-1}{m-1}[[n \geq jm]] - \binom{n-jm-1}{m-1}[[n \geq (j+1)m]]\right),$$

where the Iverson notation $[[P]]$ takes the value 1 if the condition P is satisfied and 0 otherwise.

3.2 The Number of Smallest Parts in Compositions of n

Again we use the decomposition (7). We mark with u all the smallest parts, getting the bivariate generating function for the number of smallest parts of compositions of n with smallest part j as

$$\frac{uz^j}{\left(1 - \frac{z^{j+1}}{1-z}\right)\left(1 - uz^j - \frac{z^{j+1}}{1-z}\right)} = \frac{u(z-1)^2 z^j}{(1 - z^{j+1} - z)\left((u-1)z^{j+1} - uz^j - z + 1\right)}.$$

Summing over j we find that the generating function for compositions of n according to number of smallest parts is

$$S(z,u) := \sum_{j\geq 1} \frac{u(z-1)^2 z^j}{(1-z^{j+1}-z)\left((u-1)z^{j+1}-uz^j-z+1\right)}.$$

In particular, the total number of smallest parts in compositions of n has generating function

$$S'(z,1) = \sum_{j\geq 1} \frac{(z-1)^2 z^j}{(1-z-z^j)^2}.$$

We find this is

$$z+3z^2+6z^3+15z^4+31z^5+72z^6+155z^7+340z^8+738z^9+1595z^{10}+3424z^{11}$$

$$+7335z^{12}+15642z^{13}+33243z^{14}+70432z^{15}+148808z^{16}+313571z^{17}+O[z]^{18}.$$

The coefficients are sequence $A097941$ in Sloane. For asymptotic purposes the dominant pole comes from the $j = 1$ term whose coefficient is $2^{-3+n}(2+n)$.

Thus the average number of smallest parts in compositions of n is $\frac{n+2}{4} + O(\left(\frac{\sqrt{5}+1}{4}\right)^n)$.

3.3 The Sum of Smallest Parts in Compositions of n

We mark with u^j all the smallest parts, getting the bivariate generating function for the sum of smallest parts of compositions of n with smallest part j as

$$\frac{u^j z^j}{\left(1-\frac{z^{j+1}}{1-z}\right)\left(1-u^j z^j-\frac{z^{j+1}}{1-z}\right)} = \frac{u^j(z-1)^2 z^j}{(1-z^{j+1}-z)\left((u^j-1)z^{j+1}-u^j z^j-z+1\right)}.$$

Summing over j we find that the generating function for compositions of n according to the sum of smallest parts is

$$S2(z,u) := \sum_{j\geq 1} \frac{u^j(z-1)^2 z^j}{(1-z^{j+1}-z)\left((u^j-1)z^{j+1}-u^j z^j-z+1\right)}.$$

In particular, the total sum of smallest parts in compositions of n has generating function

$$S2'(z,1) = \sum_{j\geq 1} \frac{(z-1)^2 j z^j}{(1-z-z^j)^2}.$$

We find this is

$$z + 4z^2 + 8z^3 + 20z^4 + 37z^5 + 86z^6 + 173z^7 + 372z^8 + 788z^9 + 1680z^{10} + 3550z^{11}$$

$$+7554z^{12} + 15994z^{13} + 33820z^{14} + 71374z^{15} + 150376z^{16} + 316151z^{17} + O[z]^{18}.$$

The coefficients are sequence $A097940$ in Sloane. For asymptotic purposes the dominant pole again comes from the $j = 1$ term whose coefficient is $2^{-3+n}(2+n)$.

Thus the average sum of smallest parts in compositions of n is $\frac{n+2}{4} + O(\left(\frac{\sqrt{5}+1}{4}\right)^n)$. We can make this more precise by considering the $j = 2$ term more carefully. From this we find that
the total sum of smallest parts in compositions of n exceeds the total number of smallest parts in compositions of n by

$$\frac{1}{50}\left(-25 + 13\sqrt{5} + \left(35 - 15\sqrt{5}\right)n\right)\left(\frac{1}{2} + \frac{\sqrt{5}}{2}\right)^n \text{ as } n \to \infty.$$

For example, for $n = 50$ the exact difference is 43,618,840,751 and the asymptotic result is 43,351,455,601.

4 First Position of Smallest Parts

In this section we consider the related idea of counting compositions with respect to the first position of their smallest parts. We denote the result of Lemma 1 by

$$c(n,k)_{\geq m} = \binom{n-(m-1)k-1}{k-1},$$

thus making the notation $c(n,k)_{>m}$ clear as well.

Let $w(n,k,p)$ denote the number of k-compositions of n in which the smallest parts occur for the first time in the p-th position, and let $w_s(n,k,p)$ be the number of compositions enumerated by $w(n,k,p)$ such that the smallest part is s, $1 \leq p \leq k \leq n,\ 1 \leq s \leq n$. Thus $w(n,k,p) = \sum_s w_s(n,k,p)$.

Then the following special values are immediate

$$w_s(n,k,1) = c(n-s,k-1)_{\geq s};\ w_s(n,k,k) = c(n-s,k-1)_{>s};$$

Thus

$$w_n(n,k,1) = \delta_{1k} = w_n(n,k,k).$$

In general, when $1 < p < k$, a composition enumerated by $w_s(n,k,p)$ consists of the concatenation of three strings namely:

$((p-1)$-composition of m with parts $> s)$,(s),$((k-p)$-composition of $n-m$ with parts $\geq s)$,
where $1 \leq m \leq n-s-1$.

Hence Lemma 1 gives, for $1 < p < k$,

$$w_s(n,k,p) = \sum_m c(m,p-1)_{>s} \cdot 1 \cdot c(n-s-m,k-p)_{\geq s},$$

that is,

$$w_s(n,k,p) = \sum_m \binom{m-s(p-1)-1}{p-2}\binom{n-s-m-(s-1)(k-p)-1}{k-p-1}, \quad (8)$$

and when $1 \leq s < n,\ k > 1$, we have

$$w_s(n,k,1) = \binom{n-s-(s-1)(k-1)-1}{k-2}, \quad w_s(n,k,k) = \binom{n-s-s(k-1)-1}{k-2}.$$

4.1 First Position of Smallest Parts via Generating Functions

Let $v_j(n,m,l)$ denote the number of compositions of n with m parts and with smallest part j and l positions prior to the first smallest part. As previously we use the decomposition (7) of the set C_j of compositions of n with smallest part j.

Translating to generating functions, where z marks the size of a composition, y the number of parts and x the number of positions prior to the first smallest part, gives

$$V_j(z,y,x) = \sum_{n\geq 1}\sum_{m\geq 1}\sum_{\ell\geq 0} v_j(n,m,l)z^n y^m x^\ell = \frac{yz^j}{\left(1-\frac{yz^j}{1-z}\right)\left(1-\frac{xyz^{j+1}}{1-z}\right)}$$

$$= \frac{y(z-1)^2 z^j}{(yz^j+z-1)(xyz^{j+1}+z-1)}.$$

Setting $y = 1$ the generating function for compositions with smallest part j and l positions prior to the first smallest part is

$$V_j(z, 1, x) = \frac{(z-1)^2 z^j}{(z^j + z - 1)(xz^{j+1} + z - 1)}.$$

Summing over j and differentiating with respect to x gives

$$V'(z, 1, 1) = \sum_{j \geq 1} \frac{(z-1)^2 z^{2j+1}}{(1 - z - z^j)(z^{j+1} + z - 1)^2}.$$

This is

$$z^3 + 2z^4 + 7z^5 + 15z^6 + 36z^7 + 80z^8 + 174z^9 + 371z^{10} + 787z^{11} + 1644z^{12} + 3410z^{13}$$

$$+7031z^{14} + 14423z^{15} + 29455z^{16} + 59948z^{17} + O\left(z^{18}\right),$$

which is not in Sloane. The dominant pole again comes from the $j = 1$ term, with $[z^n]V'(z, 1, 1) \sim 2^{n-1}$. It follows that the average position of the first smallest part is 2.

We can also determine the asymptotic distribution of the position of the first smallest part. The generating function for compositions in which the first smallest part occurs in position k is

$$V_{(k)}(z) = \sum_{j \geq 1} \left(\frac{z^{j+1}}{1-z}\right)^{k-1} \frac{z^j(1-z)}{1-z-z^j} = \frac{1}{(1-z)^{k-2}} \sum_{j \geq 1} \frac{z^{kj+k-1}}{1-z-z^j}.$$

The dominant pole again comes from the $j = 1$ term, with $[z^n]V_{(k)}(z) \sim 2^{-k}2^{n-1}$. Thus the position of the first smallest part follows a geometric distribution with parameter $1/2$. In particular, asymptotically half of all compositions of n will have the first smallest part in position 1.

4.2 The First Position of the Part Equal to k

The distribution of part sizes in a random composition is well known to be geometric with parameter $1/2$ as discussed for instance in [4]. In the same spirit we briefly consider the average position of the first part equal to k, any fixed k, in a composition of n. We use the following decomposition of the set of compositions of n with at least one occurrence of k.

$$\{\text{a composition with no } k\} \times \{k\} \times \{\text{any composition}\}.$$

We mark with x the positions to the left of the first k obtaining the generating function

$$\frac{1}{1-x\left(\frac{z}{1-z}-z^k\right)}\frac{z^k}{1-2z}=\frac{z^k(1-z)^2}{1-z-xz+xz^k(1-z)}.$$

Differentiating with respect to x gives

$$\frac{z^k(1-z)^2(z-z^k(1-z)}{(1-2z)(1-2z+z^k(1-z))^2}.$$

From the dominant pole at $z=1/2$ we find that the coefficient of z^n is asymptotic to $(2^k-1)2^{n-1}$.

Asymptotically almost all compositions of n have one or more parts k, so the average position of the first part equal to k is therefore 2^k, as is to be expected from the essentially geometric distribution of the part sizes.

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Cyclic Sieving for Generalised Non-crossing Partitions Associated with Complex Reflection Groups of Exceptional Type

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Dedicated to the memory of Herb Wilf

Abstract We prove that the generalised non-crossing partitions associated with well-generated complex reflection groups of exceptional type obey two different cyclic sieving phenomena, as conjectured by Armstrong, and by Bessis and Reiner. The computational details are provided in the manuscript *"Cyclic sieving for generalised non-crossing partitions associated with complex reflection groups of exceptional type—the details"* [arχiv:1001.0030].

1 Introduction

In his memoir [3], Armstrong introduced *generalised non-crossing partitions* associated with finite (real) reflection groups, thereby embedding Kreweras' non-crossing partitions [22], Edelman's m-divisible non-crossing partitions [12], the

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non-crossing partitions associated with reflection groups due to Bessis [7] and Brady and Watt [11] into one uniform framework. Bessis and Reiner [10] observed that Armstrong's definition can be straightforwardly extended to *well-generated complex reflection groups* (see Sect. 2 for the precise definition). These generalised non-crossing partitions possess a wealth of beautiful properties, and they display deep and surprising relations to other combinatorial objects defined for reflection groups (such as the generalised cluster complex of Fomin and Reading [13], or the extended Shi arrangement and the geometric multichains of filters of Athanasiadis [5,6]); see Armstrong's memoir [3] and the references given therein.

On the other hand, *cyclic sieving* is a phenomenon brought to light by Reiner, Stanton and White [29]. It extends the so-called "(-1)-phenomenon" of Stembridge [35, 36]. Cyclic sieving can be defined in three equivalent ways (cf. [29, Proposition 2.1]). The one which gives the name can be described as follows: given a set S of combinatorial objects, an action on S of a cyclic group $G = \langle g \rangle$ with generator g of order n, and a polynomial $P(q)$ in q with non-negative integer coefficients, we say that the triple (S, P, G) *exhibits the cyclic sieving phenomenon*, if the number of elements of S fixed by g^k equals $P(e^{2\pi i k/n})$. In [29] it is shown that this phenomenon occurs in surprisingly many contexts, and several further instances have been discovered since then, see the recent survey [32].

In [3, Conjecture 5.4.7] (also appearing in [10, Conjecture 6.4]) and [10, Conjecture 6.5], Armstrong, respectively Bessis and Reiner, conjecture that generalised non-crossing partitions for irreducible well-generated complex reflection groups exhibit two different cyclic sieving phenomena (see Sects. 3 and 7 for the precise statements).

According to the classification of these groups due to Shephard and Todd [33], there are two infinite families of irreducible well-generated complex reflection groups, namely the groups $G(d,1,n)$ and $G(e,e,n)$, where n,d,e are positive integers, and there are 26 exceptional groups. For the infinite families of types $G(d,1,n)$ and $G(e,e,n)$, the two cyclic sieving conjectures follow from the results in [19].

The purpose of the present article is to present a proof of the cyclic sieving conjectures of Armstrong, and of Bessis and Reiner, for the 26 exceptional types, thus completing the proof of these conjectures. Since the generalised non-crossing partitions feature a parameter m, from the outset this is *not* a finite problem. Consequently, we first need several auxiliary results to reduce the conjectures for each of the 26 exceptional types to a *finite* problem. Subsequently, we use Stembridge's *Maple* package `coxeter` [37] and the *GAP* package `CHEVIE` [14,27] to carry out the remaining *finite* computations. The details of these computations are provided in [21]. In the present paper, we content ourselves with exemplifying the necessary computations by going through some representative cases. It is interesting to observe that, for the verification of the type E_8 case, it is essential to use the decomposition numbers in the sense of [17, 18, 20] because, otherwise, the necessary computations would not be feasible in reasonable time with the currently available computer facilities. We point out that, for the special case where the aforementioned parameter m is equal to 1, the first cyclic sieving conjecture has been proven in a uniform fashion by Bessis and Reiner in [10]. The crucial result on which this proof is based is (14) below, and it plays an important role in our reduction of the conjectures for the 26 exceptional groups to a finite problem. A—non-uniform—proof of cyclic sieving for non-crossing partitions associated with *real* reflection groups under the action of the so-called Kreweras map—a special case of the second cyclic sieving phenomenon discussed in the present paper—is given by Armstrong, Stump and Thomas in [4]. Just recently, Rhoades proposed a uniform approach to prove the first cyclic sieving conjecture for *real* reflection groups (but for generic m), see [30, Theorem 3.7].

Our paper is organised as follows. In the next section, we recall the definition of generalised non-crossing partitions for well-generated complex reflection groups and of decomposition numbers in the sense of [17, 18, 20], and we review some basic facts. The first cyclic sieving conjecture is subsequently stated in Sect. 3. In Sect. 4, we outline an elementary proof that the q-Fuß–Catalan number, which is the polynomial P in the cyclic sieving phenomena concerning the generalised non-crossing partitions for well-generated complex reflection groups, is always a polynomial with non-negative integer coefficients, as required by the definition of cyclic sieving. (Full details can be found in [21, Sect. 4]. The reader is referred to the first paragraph of Sect. 4 for comments on other approaches for establishing polynomiality with non-negative coefficients.) Section 5 contains the announced auxiliary results which, for the 26 exceptional types, allow a reduction of the conjecture to a finite problem. In Sect. 6, we discuss a few cases which, in a representative manner, demonstrate how to perform the remaining case-by-case verification of the conjecture. For full details, we refer the reader to [21, Sect. 6]. The second cyclic sieving conjecture is stated in Sect. 7. Section 8 contains the auxiliary results which, for the 26 exceptional types, allow a reduction of the conjecture to a finite problem, while in Sect. 9 we discuss some representative cases of the remaining case-by-case verification of the conjecture. Again, for full details we refer the reader to [21, Sect. 9].

2 Preliminaries

A *complex reflection group* is a group generated by (complex) reflections in $\mathbb{C}^n$. (Here, a reflection is a non-trivial element of $GL_n(\mathbb{C})$ which fixes a hyperplane pointwise and which has finite order.) We refer to [24] for an in-depth exposition of the theory complex reflection groups.

Shephard and Todd provided a complete classification of all *finite* complex reflection groups in [33] (see also [24, Chap. 8]). According to this classification, an arbitrary complex reflection group W decomposes into a direct product of *irreducible* complex reflection groups, acting on mutually orthogonal subspaces of the complex vector space on which W is acting. Moreover, the list of irreducible complex reflection groups consists of the infinite family of groups $G(m, p, n)$, where m, p, n are positive integers, and 34 exceptional groups, denoted $G_4, G_5, \ldots, G_{37}$ by Shephard and Todd.

In this paper, we are only interested in finite complex reflection groups which are *well-generated*. A complex reflection group of rank n is called *well-generated* if it is generated by n reflections.[1] Well-generation can be equivalently characterised by a duality property due to Orlik and Solomon [28]. Namely, a complex reflection group of rank n has two sets of distinguished integers $d_1 \le d_2 \le \cdots \le d_n$ and $d_1^* \ge d_2^* \ge \cdots \ge d_n^*$, called its *degrees* and *codegrees*, respectively (see [24, p. 51 and Definition 10.27]). Orlik and Solomon observed, using case-by-case checking, that an irreducible complex reflection group W of rank n is well-generated if and only if its degrees and codegrees satisfy

$$d_i + d_i^* = d_n$$

for all $i = 1, 2, \dots, n$. The reader is referred to [24, Appendix D.2] for a table of the degrees and codegrees of all irreducible complex reflection groups. Together with the classification of Shephard and Todd [33], this constitutes a classification of well-generated complex reflection groups: the irreducible well-generated complex reflection groups are

- The two infinite families $G(d,1,n)$ and $G(e,e,n)$, where d,e,n are positive integers,
- The exceptional groups $G_4, G_5, G_6, G_8, G_9, G_{10}, G_{14}, G_{16}, G_{17}, G_{18}, G_{20}, G_{21}$ of rank 2,
- The exceptional groups $G_{23} = H_3, G_{24}, G_{25}, G_{26}, G_{27}$ of rank 3,
- The exceptional groups $G_{28} = F_4, G_{29}, G_{30} = H_4, G_{32}$ of rank 4,
- The exceptional group G_{33} of rank 5,
- The exceptional groups $G_{34}, G_{35} = E_6$ of rank 6,
- The exceptional group $G_{36} = E_7$ of rank 7,
- And the exceptional group $G_{37} = E_8$ of rank 8.

In this list, we have made visible the groups $H_3, F_4, H_4, E_6, E_7, E_8$ which appear as exceptional groups in the classification of all irreducible *real* reflection groups (cf. [16]).

Let W be a well-generated complex reflection group of rank n, and let $T \subseteq W$ denote the set of *all* (complex) reflections in the group. Let $\ell_T : W \to \mathbb{Z}$ denote the word length in terms of the generators T. This word length is called *absolute length* or *reflection length*. Furthermore, we define a partial order $\le_T$ on W by

$$u \le_T w \quad \text{if and only if} \quad \ell_T(w) = \ell_T(u) + \ell_T(u^{-1}w). \tag{1}$$

This partial order is called *absolute order* or *reflection order*. As is well-known and easy to see, the equation in (1) is equivalent to the statement that every shortest representation of u by reflections occurs as an initial segment in some shortest product representation of w by reflections.

[1] We refer to [24, Definition 1.29] for the precise definition of "rank." Roughly speaking, the rank of a complex reflection group W is the minimal n such that W can be realized as reflection group on $\mathbb{C}^n$.

Now fix a (generalised) Coxeter element[2] $c \in W$ and a positive integer m. The *m-divisible non-crossing partitions* $NC^m(W)$ are defined as the set

$$NC^m(W) = \big\{(w_0; w_1, \dots, w_m) : w_0 w_1 \cdots w_m = c \text{ and } \ell_T(w_0) + \ell_T(w_1) + \cdots + \ell_T(w_m) = \ell_T(c)\big\}.$$

A partial order is defined on this set by

$$(w_0; w_1, \dots, w_m) \le (u_0; u_1, \dots, u_m) \quad \text{if and only if} \quad u_i \le_T w_i \text{ for } 1 \le i \le m.$$

We have suppressed the dependence on c, since we understand this definition up to isomorphism of posets. To be more precise, it can be shown that any two Coxeter elements are related to each other by conjugation and (possibly) an automorphism on the field of complex numbers (see [34, Theorem 4.2] or [24, Corollary 11.25]), and hence the resulting posets $NC^m(W)$ are isomorphic to each other. If $m = 1$, then $NC^1(W)$ can be identified with the set $NC(W)$ of non-crossing partitions for the (complex) reflection group W as defined by Bessis and Corran (cf. [9] and [8, Sect. 13]; their definition extends the earlier definition by Bessis [7] and Brady and Watt [11] for real reflection groups).

The following result has been proved by a collaborative effort of several authors (see [8, Proposition 13.1]).

Theorem 1. *Let W be an irreducible well-generated complex reflection group, and let $d_1 \le d_2 \le \cdots \le d_n$ be its degrees and $h := d_n$ its Coxeter number. Then*

$$|NC^m(W)| = \prod_{i=1}^{n} \frac{mh + d_i}{d_i}. \tag{2}$$

Remark 1. (1) The number in (2) is called the *Fuß–Catalan number* for the reflection group W.

(2) If c is a Coxeter element of a well-generated complex reflection group W of rank n, then $\ell_T(c) = n$. (This follows from [8, Sect. 7].)

[2]An element of an irreducible well-generated complex reflection group W of rank n is called a *Coxeter element* if it is *regular* in the sense of Springer [34] (see also [24, Definition 11.21]) and of order d_n. An element of W is called regular if it has an eigenvector which lies in no reflecting hyperplane of a reflection of W. It follows from an observation of Lehrer and Springer, proved uniformly by Lehrer and Michel [23] (see [24, Theorem 11.28]), that there is always a regular element of order d_n in an irreducible well-generated complex reflection group W of rank n. More generally, if a well-generated complex reflection group W decomposes as $W \cong W_1 \times W_2 \times \cdots \times W_k$, where the W_i's are irreducible, then a Coxeter element of W is an element of the form $c = c_1 c_2 \cdots c_k$, where c_i is a Coxeter element of W_i, $i = 1, 2, \dots, k$. If W is a *real* reflection group, that is, if all generators in T have order 2, then the notion of generalised Coxeter element given above reduces to that of a Coxeter element in the classical sense (cf. [16, Sect. 3.16]).

We conclude this section by recalling the definition of decomposition numbers from [17, 18, 20]. Although we need them here only for (very small) real reflection groups, and although, strictly speaking, they have been only defined for real reflection groups in [17, 18, 20], this definition can be extended to well-generated complex reflection groups without any extra effort, which we do now.

Given a well-generated complex reflection group W of rank n, types $T_1, T_2, \dots, T_d$ (in the sense of the classification of well-generated complex reflection groups) such that the sum of the ranks of the T_i's equals n, and a Coxeter element c, the *decomposition number* $N_W(T_1, T_2, \dots, T_d)$ is defined as the number of "minimal" factorisations $c = c_1 c_2 \cdots c_d$, "minimal" meaning that $\ell_T(c_1) + \ell_T(c_2) + \cdots + \ell_T(c_d) = \ell_T(c) = n$, such that, for $i = 1, 2, \dots, d$, the type of c_i as a parabolic Coxeter element is T_i. (Here, the term "parabolic Coxeter element" means a Coxeter element in some parabolic subgroup. It follows from [31, Proposition 6.3] that any element c_i is indeed a Coxeter element in a unique parabolic subgroup of W.[3] By definition, the type of c_i is the type of this parabolic subgroup.) Since any two Coxeter elements are related to each other by conjugation plus field automorphism, the decomposition numbers are independent of the choice of the Coxeter element c.

The decomposition numbers for real reflection groups have been computed in [17, 18, 20]. To compute the decomposition numbers for well-generated complex reflection groups is a task that remains to be done.

3 Cyclic Sieving I

In this section we present the first cyclic sieving conjecture due to Armstrong [3, Conjecture 5.4.7], and to Bessis and Reiner [10, Conjecture 6.4].

Let $\phi : NC^m(W) \to NC^m(W)$ be the map defined by

$$(w_0; w_1, \dots, w_m) \mapsto \big((cw_mc^{-1})w_0(cw_mc^{-1})^{-1}; cw_mc^{-1}, w_1, w_2, \dots, w_{m-1}\big). \tag{3}$$

It is indeed not difficult to see that, if the $(m+1)$-tuple on the left-hand side is an element of $NC^m(W)$, then so is the $(m+1)$-tuple on the right-hand side. For $m = 1$, this action reduces to conjugation by the Coxeter element c (applied to w_1). Cyclic sieving arising from conjugation by c has been the subject of [10].

[3] The uniqueness can be argued as follows: suppose that c_i were a Coxeter element in two parabolic subgroups of W, say U_1 and U_2. Then it must also be a Coxeter element in the intersection $U_1 \cap U_2$. On the other hand, the absolute length of a Coxeter element of a complex reflection group U is always equal to $\mathrm{rk}(U)$, the rank of U. (This follows from the fact that, for each element u of U, we have $\ell_T(u) = \mathrm{codim}\big(\ker(u - \mathrm{id})\big)$, with id denoting the identity element in U; see e.g. [31, Proposition 1.3]). We conclude that $\ell_T(c_i) = \mathrm{rk}(U_1) = \mathrm{rk}(U_2) = \mathrm{rk}(U_1 \cap U_2)$, This implies that $U_1 = U_2$.

It is easy to see that ϕ^{mh} acts as the identity, where h is the Coxeter number of W (see (10) and Lemma 6 below). By slight abuse of notation, let C_1 be the cyclic group of order mh generated by ϕ. (The slight abuse consists in the fact that we insist on C_1 to be a cyclic group of order mh, while it may happen that the order of the action of ϕ given in (3) is actually a proper divisor of mh.)

Given these definitions, we are now in the position to state the first cyclic sieving conjecture of Armstrong, respectively of Bessis and Reiner. By the results of [19] and of this paper, it becomes the following theorem.

Theorem 2. *For an irreducible well-generated complex reflection group W and any $m \geq 1$, the triple $(NC^m(W), \mathrm{Cat}^m(W;q), C_1)$, where $\mathrm{Cat}^m(W;q)$ is the q-analogue of the Fuß–Catalan number defined by*

$$\mathrm{Cat}^m(W;q) := \prod_{i=1}^{n} \frac{[mh + d_i]_q}{[d_i]_q}, \tag{4}$$

exhibits the cyclic sieving phenomenon in the sense of Reiner, Stanton and White [29]. Here, n is the rank of W, $d_1, d_2, \ldots, d_n$ are the degrees of W, h is the Coxeter number of W, and $[\alpha]_q := (1 - q^\alpha)/(1 - q)$.

Remark 2. We write $\mathrm{Cat}^m(W)$ for $\mathrm{Cat}^m(W;1)$.

By definition of the cyclic sieving phenomenon, we have to prove that $\mathrm{Cat}^m(W;q)$ is a polynomial in q with non-negative integer coefficients, and that

$$|\,\mathrm{Fix}_{NC^m(W)}(\phi^p)| = \mathrm{Cat}^m(W;q)\big|_{q=e^{2\pi i p/mh}}, \tag{5}$$

for all p in the range $0 \leq p < mh$. The first fact is established in the next section, while the proof of the second is achieved by making use of several auxiliary results, given in Sect. 5, to reduce the proof to a finite problem, and a subsequent case-by-case analysis. All details of this analysis can be found in [21, Sect. 6]. In the present paper, we content ourselves with discussing the cases where $W = G_{24}$ and where $W = G_{37} = E_8$, since these suffice to convey the flavour of the necessary computations.

4 The q-Fusz–Catalan Numbers $\mathrm{Cat}^m(W;q)$

The purpose of this section is to provide an elementary and (essentially) self-contained proof of the fact that, for all irreducible complex reflection groups W, the q-Fuß–Catalan number $\mathrm{Cat}^m(W;q)$ is a polynomial in q with non-negative integer coefficients. For most of the groups, this is a known property. However, aside from the fact that, for many of the known cases, the proof is very indirect and uses deep algebraic results on rational Cherednik algebras, there still remained some cases where this property had not been formally established. The reader is referred to the Theorem in Sect. 1.6 of [15], which says that, under the assumption of a certain rank condition [15, Hypothesis 2.4], the q-Fuß–Catalan number $\mathrm{Cat}^m(W;q)$ is a Hilbert series of a finite-dimensional quotient of the ring of invariants of W and also the graded character of a finite-dimensional irreducible representation of a spherical rational Cherednik algebra associated with W. At present, this rank condition has been proven for all irreducible well-generated complex reflection groups apart from $G_{17}, G_{18}, G_{29}, G_{33}, G_{34}$; see [25, Tables 8 and 9, column "rank"] and the recent paper [26], which establishes the result in the case of G_{32}.

In the sequel, aside from the standard notation $[\alpha]_q = (1-q^\alpha)/(1-q)$ for q-integers, we shall also use the q-binomial coefficient, which is defined by

$$\begin{bmatrix} n \\ k \end{bmatrix}_q := \begin{cases} 1, & \text{if } k=0, \\ \frac{[n]_q\,[n-1]_q\cdots[n-k+1]_q}{[k]_q\,[k-1]_q\cdots[1]_q}, & \text{if } k>0. \end{cases}$$

We begin with several auxiliary results. The first of these (Proposition 1) is well-known (and follows, for example, from [1, Eqs. (3.3.3) and (3.3.4)], or from [1, Theorem 3.1]). The second (Proposition 2) follows by replacing n by $mn+1$ and j by n in Theorem 2 of [2].

Proposition 1. *For all non-negative integers n and k, the q-binomial coefficient $\begin{bmatrix} n \\ k \end{bmatrix}_q$ is a polynomial in q with non-negative integer coefficients.*

Proposition 2. *For all non-negative integers m and n, the q-Fuß–Catalan number of type A_n,*

$$\frac{1}{[(m+1)n+1]_q}\begin{bmatrix} (m+1)n+1 \\ n \end{bmatrix}_q,$$

is a polynomial in q with non-negative integer coefficients.

The purpose of the next lemma is to lay the basis for the proof of the positivity of coefficients in the polynomial in Corollary 1.

Lemma 1. *If a and b are coprime positive integers, then*

$$\frac{[ab]_q}{[a]_q\,[b]_q} \tag{6}$$

is a polynomial in q of degree $(a-1)(b-1)$, all of whose coefficients are in $\{0,1,-1\}$. Moreover, if one disregards the coefficients which are 0, then $+1$'s and (-1)'s alternate, and the constant coefficient as well as the leading coefficient of the polynomial equal $+1$.

Proof. Let $\Phi_n(q)$ denote the n-th cyclotomic polynomial in q. Using the classical formula

$$1-q^n = \prod_{d\mid n}\Phi_d(q),$$

we see that

$$\frac{(1-q)(1-q^{ab})}{(1-q^a)(1-q^b)} = \prod_{\substack{d_1|a,\, d_1\neq 1\\ d_2|a,\, d_2\neq 1}} \Phi_{d_1 d_2}(q),$$

so that, manifestly, the expression in (6) is a polynomial in q. The claim concerning the degree of this polynomial is obvious.

In order to establish the claim on the coefficients, we start with a sub-expression of (6),

$$\frac{(1-q^{ab})}{(1-q^a)(1-q^b)} = \left(\sum_{i=0}^{b-1} q^{ia}\right)\left(\sum_{j=0}^{\infty} q^{jb}\right) = \sum_{k=0}^{\infty} C_k q^k, \tag{7}$$

say. The assumption that a and b are coprime implies that $0 \leq C_k \leq 1$ for $k \leq (a-1)(b-1)$. Multiplying both sides of (7) by $1-q$, we obtain the equation

$$\frac{[ab]_q}{[a]_q\,[b]_q} = (1-q)\sum_{k=0}^{(a-1)(b-1)} C_k q^k + (1-q)\sum_{k=(a-1)(b-1)+1}^{\infty} C_k q^k. \tag{8}$$

By our previous observation on the coefficients C_k with $k \leq (a-1)(b-1)$, it is obvious that the coefficients of the first expression on the right-hand side of (8) are alternately $+1$ and -1, when 0's are disregarded. Since we already know that the left-hand side is a polynomial in q of degree $(a-1)(b-1)$, we may ignore the second expression.

The proof is concluded by observing that the claims on the constant and leading coefficients are obvious. □

Corollary 1. *Let a and b be coprime positive integers, and let γ be an integer with $\gamma \geq (a-1)(b-1)$. Then the expression*

$$\frac{[\gamma]_q\,[ab]_q}{[a]_q\,[b]_q}$$

is a polynomial in q with non-negative integer coefficients.

Proof. Let

$$\frac{[ab]_q}{[a]_q\,[b]_q} = \sum_{k=0}^{(a-1)(b-1)} D_k q^k.$$

We then have

$$\frac{[\gamma]_q\,[ab]_q}{[a]_q\,[b]_q} = \sum_{N=0}^{(a-1)(b-1)+\gamma-1} q^N \sum_{k=\max\{0,N-\gamma+1\}}^{N} D_k. \tag{9}$$

If $N \le \gamma - 1$, then, by Lemma 1, the sum over k on the right-hand side of (9) equals $1 - 1 + 1 - 1 + \cdots$, which is manifestly non-negative. On the other hand, if $N > \gamma - 1$, then we may rewrite the sum over k on the right-hand side of (9) as

$$\sum_{k=\max\{0,N-\gamma+1\}}^{N} D_k = \sum_{k=N-\gamma+1}^{(a-1)(b-1)} D_k = \sum_{k=0}^{(a-1)(b-1)+\gamma-1-N} D_{(a-1)(b-1)-k}.$$

Again, by Lemma 1, this sum equals $1 - 1 + 1 - 1 + \cdots$, which is manifestly non-negative. □

The next lemma collects positivity results for coefficients in polynomials given by rational function expressions of special form.

Lemma 2. *Let α and β be positive integers. The following expressions are polynomials in q with non-negative integer coefficients:*

(a) $[\alpha]_{q^3}\,[\beta]_{q^4}\,\frac{[72]_q[3]_q[4]_q}{[8]_q[9]_q[12]_q}$ *for* $\alpha \ge 6$ *and* $\beta \ge 8$;
(b) $[\alpha]_q\,[\beta]_{q^4}\,\frac{[15]_q}{[3]_q[5]_q}\,\frac{[72]_q[3]_q[4]_q}{[8]_q[9]_q[12]_q}$ *for* $\alpha \ge 26$ *and* $\beta \ge 8$;
(c) $[\alpha]_{q^3}\,[\beta]_{q^4}\,\frac{[90]_q[3]_q[4]_q}{[5]_q[6]_q[9]_q}$ *for* $\alpha \ge 18$ *and* $\beta \ge 3$;
(d) $[\alpha]_q\,[\beta]_{q^3}\,\frac{[90]_q[3]_q}{[5]_q[6]_q[9]_q}$ *for* $\alpha \ge 20$ *and* $\beta \ge 18$;
(e) $[\alpha]_q\,\frac{[15]_q}{[3]_q[5]_q}\,\frac{[12]_{q^3}}{[3]_{q^3}[4]_{q^3}}$ *for* $\alpha \ge 26$;
(f) $[\alpha]_q\,\frac{[15]_q}{[3]_q[5]_q}\,\frac{[6]_{q^3}}{[2]_{q^3}[3]_{q^3}}$ *for* $\alpha \ge 14$;
(g) $[\alpha]_q\,[\beta]_{q^2}\,\frac{[84]_q[2]_q}{[4]_q[6]_q[7]_q}$ *for* $\alpha \ge 30$ *and* $\beta \ge 20$;
(h) $[\alpha]_q\,[\beta]_q\,\frac{[105]_q}{[3]_q[5]_q[7]_q}$ *for* $\alpha \ge 24$ *and* $\beta \ge 68$;
(i) $[\alpha]_q\,[\beta]_q\,\frac{[70]_q}{[2]_q[5]_q[7]_q}$ *for* $\alpha \ge 24$ *and* $\beta \ge 34$;
(j) $[\alpha]_{q^2}\,[\beta]_{q^5}\,\frac{[30]_q[2]_q[3]_q[5]_q}{[6]_q[10]_q[15]_q}$ *for* $\alpha \ge 4$ *and* $\beta \ge 2$;
(k) $[\alpha]_q\,[\beta]_{q^5}\,\frac{[14]_q}{[2]_q[7]_q}\,\frac{[30]_q[2]_q[3]_q[5]_q}{[6]_q[10]_q[15]_q}$ *for* $\alpha \ge 14$ *and* $\beta \ge 2$;
(l) $[\alpha]_q\,[\beta]_{q^2}\,\frac{[35]_q}{[5]_q[7]_q}\,\frac{[30]_q[2]_q[3]_q[5]_q}{[6]_q[10]_q[15]_q}$ *for* $\alpha \ge 32$ *and* $\beta \ge 12$;
(m) $[\alpha]_{q^2}\,[\beta]_{q^5}\,\frac{[60]_q[2]_q[3]_q[5]_q}{[10]_q[12]_q[15]_q}$ *for* $\alpha \ge 16$ *and* $\beta \ge 2$;
(n) $[\alpha]_q\,[\beta]_{q^2}\,\frac{[35]_q}{[5]_q[7]_q}\,\frac{[60]_q[2]_q[3]_q[5]_q}{[10]_q[12]_q[15]_q}$ *for* $\alpha \ge 56$ *and* $\beta \ge 4$;
(o) $[\alpha]_q\,[\beta]_{q^5}\,\frac{[14]_q}{[2]_q[7]_q}\,\frac{[60]_q[2]_q[3]_q[5]_q}{[10]_q[12]_q[15]_q}$ *for* $\alpha \ge 38$ *and* $\beta \ge 2$;
(p) $[\alpha]_q\,[\beta]_{q^3}\,\frac{[126]_q[3]_q}{[6]_q[7]_q[9]_q}$ *for* $\alpha \ge 30$ *and* $\beta \ge 26$;
(q) $[\alpha]_q\,[\beta]_{q^3}\,\frac{[252]_q[3]_q}{[7]_q[9]_q[12]_q}$ *for* $\alpha \ge 66$ *and* $\beta \ge 54$;
(r) $[\alpha]_q\,[\beta]_{q^2}\,\frac{[140]_q[2]_q}{[4]_q[7]_q[10]_q}$ *for* $\alpha \ge 54$ *and* $\beta \ge 34$.

Proof. All these assertions have a very similar flavour, and so do their proofs. In order to avoid repetition, proof details are only provided for items (a) and (j); the proofs of items (b)–(i) and (p)–(r) follow the pattern exhibited in the proof of item (a), while the proofs of items (k)–(o) follow that of the proof of item (j). Full details are found in [21, Sect. 4].

In order to establish item (a), we start with the factorisation

$$\frac{[72]_q\,[3]_q\,[4]_q}{[8]_q\,[9]_q\,[12]_q} = (1-q^3+q^9-q^{15}+q^{18})(1-q^4+q^8-q^{12}+q^{16}-q^{20}+q^{24}-q^{28}+q^{32}).$$

It should be observed that both factors on the right-hand side have the property that coefficients are in $\{0,1,-1\}$ and that $(+1)$'s and (-1)'s alternate, if one disregards the coefficients which are 0. If we now apply the same idea as in the proof of Corollary 1, then we see that $[\alpha]_{q^3}$ times the first factor is a polynomial in q with non-negative integer coefficients, as is $[\beta]_{q^4}$ times the second factor. Taken together, this establishes the claim.

Now we turn to item (j). We have

$$\frac{[30]_q\,[2]_q\,[3]_q\,[5]_q}{[6]_q\,[10]_q\,[15]_q} = 1+q-q^3-q^4-q^5+q^7+q^8.$$

If we multiply this expression by $[\alpha]_{q^2}$, then, for $\alpha=4$ we obtain

$$1+q+q^2-q^5-q^9+q^{12}+q^{13}+q^{14},$$

for $\alpha=5$ we obtain

$$1+q+q^2-q^5+q^8-q^{11}+q^{14}+q^{15}+q^{16},$$

and, for $\alpha\ge 6$, we obtain

$$1+q+q^2-q^5+q^8+q^{10}+p_1(q)+q^{2\alpha-4}+q^{2\alpha-2}-q^{2\alpha+1}+q^{2\alpha+4}+q^{2\alpha+5}+q^{2\alpha+6},$$

where $p_1(q)$ is a polynomial in q with non-negative coefficients of order at least 11 and degree at most $2\alpha-5$. In all cases it is obvious that the product of the result and $[\beta]_{q^5}$, with $\beta\ge 2$, is a polynomial in q with non-negative coefficients. ☐

We are now ready for the proof of the main result of this section.

Theorem 3. *For all irreducible well-generated complex reflection groups and positive integers m, the q-Fuß–Catalan number* $\mathrm{Cat}^m(W;q)$ *is a polynomial in q with non-negative integer coefficients.*

Proof. First, let $W = A_n$. In this case, the degrees are $2, 3, \dots, n+1$, and hence

$$\mathrm{Cat}^m(A_n;q) = \frac{1}{[(m+1)n+1]_q} \begin{bmatrix} (m+1)n+1 \\ n \end{bmatrix}_q,$$

which, by Proposition 2, is a polynomial in q with non-negative integer coefficients.

Next, let $W = G(d,1,n)$. In this case, the degrees are $d, 2d, \dots, nd$, and hence

$$\mathrm{Cat}^m(G(d,1,n);q) = \begin{bmatrix} (m+1)n \\ n \end{bmatrix}_{q^d},$$

which, by Proposition 1, is a polynomial in q with non-negative integer coefficients.

Now, let $W = G(e,e,n)$. In this case, the degrees are $e, 2e, \dots, (n-1)e, n$, and hence

$$\begin{aligned}\mathrm{Cat}^m(G(e,e,n);q) &= \frac{[m(n-1)e+n]_q}{[n]_q} \prod_{i=1}^{n-1} \frac{[m(n-1)e+ie]_q}{[ie]_q} \\ &= \begin{bmatrix} (m+1)(n-1) \\ n-1 \end{bmatrix}_{q^e} + q^n [e]_{q^n} \begin{bmatrix} (m+1)(n-1) \\ n \end{bmatrix}_{q^e},\end{aligned}$$

which, by Proposition 1, is a polynomial in q with non-negative integer coefficients.

It remains to verify the claim for the exceptional groups.

For the groups $W = G_6, G_9, G_{14}, G_{17}, G_{21}$, and partially for the groups $W = G_{20}, G_{23}, G_{28}, G_{30}, G_{33}, G_{35}, G_{36}, G_{37}$ (depending on congruence properties of the parameter m), polynomiality and non-negativity of coefficients of the corresponding q-Fuß–Catalan number can be directly read off by a proper rearrangement of the terms in the defining expression; for example, for $W = G_{21}$ (with degrees given by $12, 60$) we have

$$\mathrm{Cat}^m(G_{21};q) = \frac{[60m+12]_q\,[60m+60]_q}{[12]_q\,[60]_q} = [5m+1]_{q^{12}}\,[m+1]_{q^{60}},$$

which is manifestly a polynomial in q with non-negative integer coefficients.

For the groups $G_5, G_{10}, G_{18}, G_{26}, G_{27}, G_{29}, G_{34}$, the terms in the defining expression of the corresponding q-Fuß–Catalan number can be arranged in a manner so that a q-binomial coefficient appears; polynomiality and non-negativity of coefficients then follow from Proposition 1. For example, for $W = G_{34}$ (with degrees given by $6, 12, 18, 24, 30, 42$) we have

$$\begin{aligned}&\mathrm{Cat}^m(G_{34};q) \\ &\quad= \frac{[42m+6]_q\,[42m+12]_q\,[42m+18]_q\,[42m+24]_q\,[42m+30]_q\,[42m+42]_q}{[6]_q\,[12]_q\,[18]_q\,[24]_q\,[30]_q\,[42]_q} \\ &\quad= [m+1]_{q^{42}} \begin{bmatrix} 7m+5 \\ 5 \end{bmatrix}_{q^6},\end{aligned}$$

which, written in this form, is obviously a polynomial in q with non-negative integer coefficients.

On the other hand, for the groups $G_4, G_8, G_{16}, G_{25}, G_{32}$, the terms in the defining expression of the corresponding q-Fuß–Catalan number can be arranged in a manner so that a q-Fuß–Catalan number of type A appears and Proposition 2 applies; for example, for $W = G_{32}$ (with degrees given by $12, 18, 24, 30$) we have

$$\begin{aligned} \mathrm{Cat}^m(G_{32}; q) &= \frac{[30m+12]_q\,[30m+18]_q\,[30m+24]_q\,[30m+30]_q}{[12]_q\,[18]_q\,[24]_q\,[30]_q} \\ &= \frac{1}{[5m+6]_{q^6}} \begin{bmatrix} 5m+6 \\ 5 \end{bmatrix}_{q^6}, \end{aligned}$$

which indeed fits into the framework of Proposition 2 and, hence, is a polynomial in q with non-negative integer coefficients.

In the other cases, the more "specialised" auxiliary results given in Corollary 1 and Lemma 2 have to be applied. For the sake of illustration, and in order for the reader to get a feeling for the utility of Corollary 1 and the 18 assertions in Lemma 2, we exhibit one example of application for each of them below, with full details being provided in [21, Sect. 4]. In general, the idea is that, given a rational expression consisting of cyclotomic factors, as in the definition of the q-Fuß–Catalan numbers, one tries to place denominator factors below appropriate numerator factors so that one can divide out the denominator factor completely. For example, if we were to encounter the expression

$$\frac{[30m+12]_q \cdot (\text{other terms})}{[12]_q \cdot (\text{other terms})}$$

and know that m is even, then we would simplify this to

$$\left[\tfrac{5m+2}{2}\right]_{q^{12}} \cdot \frac{(\text{other terms})}{(\text{other terms})},$$

where $\left[\frac{5m+2}{2}\right]_{q^{12}}$ is manifestly a polynomial in q with non-negative integer coefficients. On the other hand, in a situation where *two* denominator factors "want" to divide a *single* numerator factor, we "extract" as much as we can from the numerator factor and compensate by additional "fudge" factors. To be more concrete, if we encounter the expression

$$\frac{[14m+14]_q \cdot (\text{other terms})}{[6]_q\,[14]_q \cdot (\text{other terms})}$$

and we know that $m \equiv 2 \pmod 3$, then we would try the rewriting

$$\left[\tfrac{m+1}{3}\right]_{q^{42}} \frac{[21]_{q^2}}{[3]_{q^2}\,[7]_{q^2}\,[2]_q} \cdot \frac{(\text{other terms})}{(\text{other terms})},$$

with the idea that we might find somewhere else a term $[2\alpha]_q$, which could be combined with the term $[2]_q$ in the denominator into $[2\alpha]_q/[2]_q = [\alpha]_{q^2}$, and then apply Corollary 1 to see that

$$[\alpha]_{q^2}\frac{[21]_{q^2}}{[3]_{q^2}\,[7]_{q^2}}$$

is a polynomial in q with non-negative integer coefficients (provided α is at least 12), with $\left[\frac{m+1}{3}\right]_{q^{42}}$ being such a polynomial in any case.

In situations where *three* denominator factors "want" to divide a *single* numerator factor, one has to perform more complicated rearrangements, in order to be able to apply one of the assertions from Lemma 2.

For example, for $W = G_{24}$, the degrees are $4, 6, 14$, and hence

$$\operatorname{Cat}^m(G_{24};q) = \frac{[14m+4]_q\,[14m+6]_q\,[14m+14]_q}{[4]_q\,[6]_q\,[14]_q}.$$

We have

$$\operatorname{Cat}^m(G_{24};q) = \begin{cases} \left[\frac{7m}{2}+1\right]_{q^4}\,\left[\frac{14m}{6}+1\right]_{q^6}\,[m+1]_{q^{14}}\,, & \text{if } m \equiv 0 \pmod 6,\\ \left[\frac{7m+2}{3}\right]_{q^6}\,\left[\frac{7m+3}{2}\right]_{q^4}\,[m+1]_{q^{14}}\,, & \text{if } m \equiv 1 \pmod 6,\\ \left[\frac{7m}{2}+1\right]_{q^4}\,[7m+3]_{q^2}\,\left[\frac{m+1}{3}\right]_{q^{42}}\,\frac{[21]_{q^2}}{[3]_{q^2}[7]_{q^2}}, & \text{if } m \equiv 2 \pmod 6,\\ [7m+2]_{q^2}\,\left[\frac{7m}{3}+1\right]_{q^6}\,\left[\frac{m+1}{2}\right]_{q^{28}}\,\frac{[14]_{q^2}}{[2]_{q^2}[7]_{q^2}}, & \text{if } m \equiv 3 \pmod 6,\\ \left[\frac{7m+2}{6}\right]_{q^{12}}\,\frac{[6]_{q^2}}{[2]_{q^2}[3]_{q^2}}\,[7m+3]_{q^2}\,[m+1]_{q^{14}}\,, & \text{if } m \equiv 4 \pmod 6,\\ [7m+2]_{q^2}\,\left[\frac{7m+3}{2}\right]_{q^4}\,\left[\frac{m+1}{3}\right]_{q^{42}}\,\frac{[21]_{q^2}}{[3]_{q^2}[7]_{q^2}}, & \text{if } m \equiv 5 \pmod 6, \end{cases}$$

which, by Corollary 1, are polynomials in q with non-negative integer coefficients in all cases.

For $W = G_{30} = H_4$, the degrees are $2, 12, 20, 30$, and hence

$$\operatorname{Cat}^m(H_4;q) = \frac{[30m+2]_q\,[30m+12]_q\,[30m+20]_q\,[30m+30]_q}{[2]_q\,[12]_q\,[20]_q\,[30]_q}.$$

If m is odd, then we may write

$$\operatorname{Cat}^m(H_4;q) = \left[\tfrac{15m+1}{2}\right]_{q^4}\,[5m+2]_{q^6}\,[3m+2]_{q^{10}}\,\left[\tfrac{m+1}{2}\right]_{q^{60}}\,\frac{[30]_{q^2}\,[2]_{q^2}\,[3]_{q^2}\,[5]_{q^2}}{[6]_{q^6}\,[10]_{q^2}\,[15]_{q^2}},$$

which, by Lemma 2.(j), is a polynomial in q with non-negative integer coefficients.

For $W = G_{35} = E_6$, the degrees are $2, 5, 6, 8, 9, 12$, and hence

$$\mathrm{Cat}^m(E_6;q) = \frac{[12m+2]_q\,[12m+5]_q\,[12m+6]_q\,[12m+8]_q\,[12m+9]_q\,[12m+12]_q}{[2]_q\,[5]_q\,[6]_q\,[8]_q\,[9]_q\,[12]_q}.$$

If $m \equiv 5 \pmod{30}$, then we have

$$\mathrm{Cat}^m(E_6;q) = [6m+1]_{q^2}\left[\tfrac{12m+5}{5}\right]_{q^5}[2m+1]_{q^6} \times [3m+2]_{q^4}[4m+3]_{q^3}\left[\tfrac{m+1}{6}\right]_{q^{72}}\frac{[72]_q\,[3]_q\,[4]_q}{[8]_q\,[9]_q\,[12]_q},$$

which, by Lemma 2.(a), is a polynomial in q with non-negative integer coefficients.

If $m \equiv 7 \pmod{30}$, then we have

$$\mathrm{Cat}^m(E_6;q) = \left[\tfrac{6m+1}{2}\right]_{q^4}[12m+5]_q\left[\tfrac{2m+1}{15}\right]_{q^{90}} \times \frac{[90]_q\,[3]_q\,[4]_q}{[5]_q\,[6]_q\,[9]_q}[3m+2]_{q^4}[4m+3]_{q^3}\left[\tfrac{m+1}{2}\right]_{q^{24}}\frac{[6]_{q^4}}{[2]_{q^4}\,[3]_{q^4}},$$

which, by Corollary 1 and Lemma 2.(c), is a polynomial in q with non-negative integer coefficients.

If $m \equiv 8 \pmod{30}$, then we have

$$\mathrm{Cat}^m(E_6;q) = [6m+1]_{q^2}[12m+5]_q[2m+1]_{q^6}\left[\tfrac{3m+2}{2}\right]_{q^8} \times \left[\tfrac{4m+3}{5}\right]_{q^{15}}\frac{[15]_q}{[3]_q\,[5]_q}\left[\tfrac{m+1}{3}\right]_{q^{36}}\frac{[12]_{q^3}}{[3]_{q^3}[4]_{q^3}},$$

which, by Lemma 2.(e), is a polynomial in q with non-negative integer coefficients.

If $m \equiv 13 \pmod{30}$, then we have

$$\mathrm{Cat}^m(E_6;q) = [6m+1]_{q^2}[12m+5]_q\left[\tfrac{2m+1}{3}\right]_{q^{18}}\frac{[6]_{q^3}}{[2]_{q^3}[3]_{q^3}} \times [3m+2]_{q^4}\left[\tfrac{4m+3}{5}\right]_{q^{15}}\frac{[15]_q}{[3]_q\,[5]_q}\left[\tfrac{m+1}{2}\right]_{q^{24}}\frac{[6]_{q^4}}{[2]_{q^4}[3]_{q^4}},$$

which, by Lemma 2.(f), is a polynomial in q with non-negative integer coefficients.

If $m \equiv 22 \pmod{30}$, then we have

$$\mathrm{Cat}^m(E_6;q) = [6m+1]_{q^2}[12m+5]_q\left[\tfrac{2m+1}{15}\right]_{q^{90}}\frac{[90]_q[3]_q}{[5]_q[6]_q[9]_q} \times \left[\tfrac{3m+2}{2}\right]_{q^8}[4m+3]_{q^3}[m+1]_{q^{12}},$$

which, by Lemma 2.(d), is a polynomial in q with non-negative integer coefficients.

If $m \equiv 23 \pmod{30}$, then we have

$$\operatorname{Cat}^m(E_6;q) = [6m+1]_{q^2}[12m+5]_q[2m+1]_{q^6} \times [3m+2]_{q^4}\left[\tfrac{4m+3}{5}\right]_{q^{15}}\frac{[15]_q}{[3]_q\,[5]_q}\left[\tfrac{m+1}{6}\right]_{q^{72}}\frac{[72]_q\,[3]_q\,[4]_q}{[8]_q\,[9]_q\,[12]_q},$$

which, by Lemma 2.(b), is a polynomial in q with non-negative integer coefficients.

For $W = G_{36} = E_7$, the degrees are $2, 6, 8, 10, 12, 14, 18$, and hence

$$\operatorname{Cat}^m(E_7;q) = \frac{[18m+2]_q\,[18m+6]_q\,[18m+8]_q\,[18m+10]_q}{[2]_q\,[6]_q\,[8]_q\,[10]_q} \times \frac{[18m+12]_q\,[18m+14]_q\,[18m+18]_q}{[12]_q\,[14]_q\,[18]_q}.$$

If $m \equiv 18 \pmod{140}$, then we have

$$\operatorname{Cat}^m(E_7;q) = [9m+1]_{q^2}\left[\tfrac{3m+1}{5}\right]_{q^{30}}\frac{[15]_{q^2}}{[3]_{q^2}\,[5]_{q^2}} \times \left[\tfrac{9m+4}{2}\right]_{q^4}[9m+5]_{q^2}\left[\tfrac{3m+2}{28}\right]_{q^{168}}\frac{[84]_{q^2}\,[2]_{q^2}}{[4]_{q^2}\,[6]_{q^2}\,[7]_{q^2}}[9m+7]_{q^2}[m+1]_{q^{18}},$$

which, by Corollary 1 and Lemma 2.(g), is a polynomial in q with non-negative integer coefficients.

If $m \equiv 23 \pmod{140}$, then we have

$$\operatorname{Cat}^m(E_7;q) = \left[\tfrac{9m+1}{4}\right]_{q^8}\left[\tfrac{3m+1}{35}\right]_{q^{210}}\frac{[105]_{q^2}}{[3]_{q^2}[5]_{q^2}[7]_{q^2}}[9m+4]_{q^2}[9m+5]_{q^2} \times [3m+2]_{q^6}[9m+7]_{q^2}\left[\tfrac{m+1}{2}\right]_{q^{36}}\frac{[6]_{q^6}}{[2]_{q^6}[3]_{q^6}},$$

which, by Corollary 1 and Lemma 2.(h), is a polynomial in q with non-negative integer coefficients.

If $m \equiv 54 \pmod{140}$, then we have

$$\operatorname{Cat}^m(E_7;q) = [9m+1]_{q^2}[3m+1]_{q^6}\left[\tfrac{9m+4}{70}\right]_{q^{140}}\frac{[70]_{q^2}}{[2]_{q^2}[5]_{q^2}[7]_{q^2}}[9m+5]_{q^2} \times \left[\tfrac{3m+2}{4}\right]_{q^{24}}\frac{[6]_{q^4}}{[2]_{q^4}[3]_{q^4}}[9m+7]_{q^2}[m+1]_{q^{18}}.$$

If one decomposes $[9m+7]_{q^2}$ as $[\frac{9m}{2}+4]_{q^4}+q^2[\frac{9m}{2}+3]_{q^4}$, then one sees that, by Corollary 1 and Lemma 2.(i), this is a polynomial in q with non-negative integer coefficients.

For $W = G_{37} = E_8$, the degrees are $2, 8, 12, 14, 18, 20, 24, 30$, and hence

$$\mathrm{Cat}^m(E_7;q) = \frac{[30m+2]_q\,[30m+8]_q\,[30m+12]_q\,[30m+14]_q}{[2]_q\,[8]_q\,[12]_q\,[14]_q} \times \frac{[30m+18]_q\,[30m+20]_q\,[30m+24]_q\,[30m+30]_q}{[18]_q\,[20]_q\,[24]_q\,[30]_q}.$$

If $m \equiv 3 \pmod{84}$, then we have

$$\mathrm{Cat}^m(E_8;q) = \left[\tfrac{15m+1}{2}\right]_{q^4}\left[\tfrac{15m+4}{7}\right]_{q^{14}}[5m+2]_{q^6}\left[\tfrac{15m+7}{4}\right]_{q^8}\left[\tfrac{5m+3}{6}\right]_{q^{36}}\frac{[6]_{q^6}}{[2]_{q^6}\,[3]_{q^6}} \times [3m+2]_{q^{10}}[5m+4]_{q^6}\left[\tfrac{m+1}{4}\right]_{q^{120}}\frac{[60]_{q^2}\,[2]_{q^2}\,[3]_{q^2}\,[5]_{q^2}}{[10]_{q^2}\,[12]_{q^2}\,[15]_{q^2}},$$

which, by Corollary 1 and Lemma 2.(m), is a polynomial in q with non-negative integer coefficients.

If $m \equiv 8 \pmod{84}$, then we have

$$\mathrm{Cat}^m(E_8;q) = [15m+1]_{q^2}\left[\tfrac{15m+4}{4}\right]_{q^8}\left[\tfrac{5m+2}{42}\right]_{q^{252}}\frac{[126]_{q^2}[3]_{q^2}}{[6]_{q^2}[7]_{q^2}[9]_{q^2}} \times [15m+7]_{q^2}[5m+3]_{q^6}\left[\tfrac{3m+2}{2}\right]_{q^{20}}\left[\tfrac{5m+4}{4}\right]_{q^{24}}[m+1]_{q^{30}},$$

which, by Lemma 2.(p), is a polynomial in q with non-negative integer coefficients.

If $m \equiv 11 \pmod{84}$, then we have

$$\mathrm{Cat}^m(E_8;q) = \left[\tfrac{15m+1}{2}\right]_{q^4}[15m+4]_{q^2}\left[\tfrac{5m+2}{3}\right]_{q^{18}}\left[\tfrac{15m+7}{4}\right]_{q^8}\left[\tfrac{5m+3}{2}\right]_{q^{12}} \times \left[\tfrac{3m+2}{7}\right]_{q^{70}}\frac{[35]_{q^2}}{[5]_{q^2}\,[7]_{q^2}}[5m+4]_{q^6}\left[\tfrac{m+1}{4}\right]_{q^{120}}\frac{[60]_{q^2}\,[2]_{q^2}\,[3]_{q^2}\,[5]_{q^2}}{[10]_{q^2}\,[12]_{q^2}\,[15]_{q^2}},$$

which, by Corollary 1 and Lemma 2.(n), is a polynomial in q with non-negative integer coefficients.

If $m \equiv 16 \pmod{84}$, then we have

$$\mathrm{Cat}^m(E_8;q) = [15m+1]_{q^2}\left[\tfrac{15m+4}{4}\right]_{q^8}\left[\tfrac{5m+2}{2}\right]_{q^{12}}[15m+7]_{q^2}[5m+3]_{q^6} \times \left[\tfrac{3m+2}{2}\right]_{q^{20}}\left[\tfrac{5m+4}{84}\right]_{q^{504}}\frac{[252]_{q^2}\,[3]_{q^2}}{[7]_{q^2}\,[9]_{q^2}\,[12]_{q^2}}[m+1]_{q^{30}},$$

which, by Lemma 2.(q), is a polynomial in q with non-negative integer coefficients.

If $m \equiv 18 \pmod{84}$, then we have

$$\mathrm{Cat}^m(E_8;q) = [15m+1]_{q^2}\left[\tfrac{15m+4}{2}\right]_{q^4}\left[\tfrac{5m+2}{4}\right]_{q^{24}}[15m+7]_{q^2}\left[\tfrac{5m+3}{3}\right]_{q^{18}} \left[\tfrac{3m+2}{28}\right]_{q^{280}}\frac{[140]_{q^2}[2]_{q^2}}{[4]_{q^2}[7]_{q^2}[10]_{q^2}}\left[\tfrac{5m+4}{2}\right]_{q^{12}}[m+1]_{q^{30}},$$

which, by Lemma 2.(r), is a polynomial in q with non-negative integer coefficients.

If $m \equiv 21 \pmod{84}$, then we have

$$\mathrm{Cat}^m(E_8;q) = \left[\tfrac{15m+1}{4}\right]_{q^8}[15m+4]_{q^2}[5m+2]_{q^6}\left[\tfrac{15m+7}{14}\right]_{q^{28}}\frac{[14]_{q^2}}{[2]_{q^2}\,[7]_{q^2}}\left[\tfrac{5m+3}{12}\right]_{q^{72}} \times \frac{[12]_{q^6}}{[3]_{q^6}\,[4]_{q^6}}[3m+2]_{q^{10}}[5m+4]_{q^6}\left[\tfrac{m+1}{2}\right]_{q^{60}}\frac{[30]_{q^2}[2]_{q^2}[3]_{q^2}[5]_{q^2}}{[6]_{q^2}[10]_{q^2}[15]_{q^2}},$$

which, by Corollary 1 and Lemma 2.(k), is a polynomial in q with non-negative integer coefficients.

If $m \equiv 25 \pmod{84}$, then we have

$$\mathrm{Cat}^m(E_8;q) = \left[\tfrac{15m+1}{4}\right]_{q^8}[15m+4]_{q^2}[5m+2]_{q^6}\left[\tfrac{15m+7}{2}\right]_{q^4}\left[\tfrac{5m+3}{4}\right]_{q^{24}} \times \left[\tfrac{3m+2}{7}\right]_{q^{70}}\frac{[35]_{q^2}}{[5]_{q^2}\,[7]_{q^2}}\left[\tfrac{5m+4}{3}\right]_{q^{18}}\left[\tfrac{m+1}{2}\right]_{q^{60}}\frac{[30]_{q^2}[2]_{q^2}[3]_{q^2}[5]_{q^2}}{[6]_{q^2}[10]_{q^2}[15]_{q^2}},$$

which, by Lemma 2.(l), is a polynomial in q with non-negative integer coefficients.

If $m \equiv 27 \pmod{84}$, then we have

$$\mathrm{Cat}^m(E_8;q) = \left[\tfrac{15m+1}{14}\right]_{q^{28}}\frac{[14]_{q^2}}{[2]_{q^2}\,[7]_{q^2}}[15m+4]_{q^2}[5m+2]_{q^6}\left[\tfrac{15m+7}{4}\right]_{q^8}\left[\tfrac{5m+3}{6}\right]_{q^{36}} \times \frac{[6]_{q^6}}{[2]_{q^6}\,[3]_{q^6}}[3m+2]_{q^{10}}[5m+4]_{q^6}\left[\tfrac{m+1}{4}\right]_{q^{120}}\frac{[60]_{q^2}\,[2]_{q^2}\,[3]_{q^2}\,[5]_{q^2}}{[10]_{q^2}\,[12]_{q^2}\,[15]_{q^2}},$$

which, by Corollary 1 and Lemma 2.(o), is a polynomial in q with non-negative integer coefficients.

All other cases are disposed of in a similar fashion. □

5 Auxiliary Results I

This section collects several auxiliary results which allow us to reduce the problem of proving Theorem 2, or the equivalent statement (5), for the 26 exceptional groups listed in Sect. 2 to a finite problem. While Lemmas 4 and 5 cover special choices of the parameters, Lemmas 3 and 7 afford an inductive procedure. More precisely, if we assume that we have already verified Theorem 2 for all groups of smaller rank, then Lemmas 3 and 7, together with Lemmas 4 and 8, reduce the verification of Theorem 2 for the group that we are currently considering to a finite problem; see Remark 3. The final lemma of this section, Lemma 9, disposes of complex reflection groups with a special property satisfied by their degrees.

Let $p = am + b$, $0 \le b < m$. We have

$$\begin{aligned} \phi^p\big((w_0; w_1, \dots, w_m)\big) \\ = (*; c^{a+1} w_{m-b+1} c^{-a-1}, c^{a+1} w_{m-b+2} c^{-a-1}, \dots, c^{a+1} w_m c^{-a-1}, \\ c^a w_1 c^{-a}, \dots, c^a w_{m-b} c^{-a}\big), \end{aligned} \tag{10}$$

where $*$ stands for the element of W which is needed to complete the product of the components to c.

Lemma 3. *It suffices to check (5) for p a divisor of mh. More precisely, let p be a divisor of mh, and let k be another positive integer with* $\gcd(k, mh/p) = 1$*, then we have*

$$\mathrm{Cat}^m(W; q)\big|_{q=e^{2\pi i p/mh}} = \mathrm{Cat}^m(W; q)\big|_{q=e^{2\pi i kp/mh}} \tag{11}$$

and

$$|\,\mathrm{Fix}_{NC^m(W)}(\phi^p)| = |\,\mathrm{Fix}_{NC^m(W)}(\phi^{kp})|. \tag{12}$$

Proof. For (11), this follows immediately from

$$\lim_{q \to \zeta} \frac{[\alpha]_q}{[\beta]_q} = \begin{cases} \frac{\alpha}{\beta} & \text{if } \alpha \equiv \beta \equiv 0 \pmod{d}, \\ 1 & \text{otherwise}, \end{cases} \tag{13}$$

where ζ is a primitive d-th root of unity and α, β are non-negative integers such that $\alpha \equiv \beta \pmod{d}$.

In order to establish (12), suppose that $x \in \mathrm{Fix}_{NC^m(W)}(\phi^p)$, that is, $x \in NC^m(W)$ and $\phi^p(x) = x$. It obviously follows that $\phi^{kp}(x) = x$, so that $x \in \mathrm{Fix}_{NC^m(W)}(\phi^{kp})$. To establish the converse, note that, if $\gcd(k, mh/p) = 1$, then there exists k' with $k'k \equiv 1 \pmod{\frac{mh}{p}}$. It follows that, if $x \in \mathrm{Fix}_{NC^m(W)}(\phi^{kp})$, that is, if $x \in NC^m(W)$ and $\phi^{kp}(x) = x$, then $x = \phi^{k'kp}(x) = \phi^p(x)$, whence $x \in \mathrm{Fix}_{NC^m(W)}(\phi^p)$. □

Lemma 4. *Let p be a divisor of mh. If p is divisible by m, then (5) is true.*

Proof. According to (10), the action of ϕ^p on $NC^m(W)$ is described by

$$\phi^p\big((w_0; w_1, \dots, w_m)\big) = (*; c^{p/m} w_1 c^{-p/m}, \dots, c^{p/m} w_m c^{-p/m}\big).$$

Hence, if $(w_0; w_1, \dots, w_m)$ is fixed by ϕ^p, then each individual w_i must be fixed under conjugation by $c^{p/m}$.

Using the notation $W' = \mathrm{Cent}_W(c^{p/m})$, the previous observation means that $w_i \in W'$, $i = 1, 2, \dots, m$. Springer [34, Theorem 4.2] (see also [24, Theorem 11.24(iii)]) proved that W' is a well-generated complex reflection group whose degrees coincide with those degrees of W that are divisible by mh/p. It was furthermore shown in [10, Lemma 3.3] that

$$NC(W) \cap W' = NC(W'). \tag{14}$$

Hence, the tuples $(w_0; w_1, \dots, w_m)$ fixed by ϕ^p are in fact identical with the elements of $NC^m(W')$, which implies that

$$|\,\mathrm{Fix}_{NC^m(W)}(\phi^p)| = |NC^m(W')|. \tag{15}$$

Application of Theorem 1 with W replaced by W' and of the "limit rule" (13) then yields that

$$|NC^m(W')| = \prod_{\substack{1 \le i \le n \\ \frac{mh}{p} | d_i}} \frac{mh + d_i}{d_i} = \mathrm{Cat}^m(W; q)\big|_{q=e^{2\pi i p/mh}}. \tag{16}$$

Combining (15) and (16), we obtain (5). This finishes the proof of the lemma. □

Lemma 5. *Equation* (5) *holds for all divisors* p *of* m.

Proof. Using (13) and the fact that the degrees of irreducible well-generated complex reflection groups satisfy $d_i < h$ for all $i < n$, we see that

$$\mathrm{Cat}^m(W; q)\big|_{q=e^{2\pi i p/mh}} = \begin{cases} m+1 & \text{if } m = p, \\ 1 & \text{if } m \neq p. \end{cases}$$

On the other hand, if $(w_0; w_1, \dots, w_m)$ is fixed by ϕ^p, then, because of the action (10), we must have $w_1 = w_{p+1} = \cdots = w_{m-p+1}$ and $w_1 = c w_{m-p+1} c^{-1}$. In particular, $w_1 \in \mathrm{Cent}_W(c)$. By the theorem of Springer cited in the proof of Lemma 4, the subgroup $\mathrm{Cent}_W(c)$ is itself a complex reflection group whose degrees are those degrees of W that are divisible by h. The only such degree is h itself, hence $\mathrm{Cent}_W(c)$ is the cyclic group generated by c. Moreover, by (14), we obtain that $w_1 = \varepsilon$, the identity element of W, or $w_1 = c$. Therefore, for $m = p$ the set $\mathrm{Fix}_{NC^m(W)}(\phi^p)$ consists of the $m+1$ elements $(w_0; w_1, \dots, w_m)$ obtained by choosing $w_i = c$ for a particular i between 0 and m, all other w_j's being equal to ε, while, for $m \neq p$, we have

$$\mathrm{Fix}_{NC^m(W)}(\phi^p) = \big\{(c; \varepsilon, \dots, \varepsilon)\big\},$$

whence the result. □

Lemma 6. *Let W be an irreducible well-generated complex reflection group all of whose degrees are divisible by d. Then each element of W is fixed under conjugation by $c^{h/d}$.*

Proof. By the theorem of Springer cited in the proof of Lemma 4, the subgroup $W' = \mathrm{Cent}_W(c^{h/d})$ is itself a complex reflection group whose degrees are those degrees of W that are divisible by d. Thus, by our assumption, the degrees of W' coincide with the degrees of W, and hence W' must be equal to W. Phrased differently, each element of W is fixed under conjugation by $c^{h/d}$, as claimed. □

Lemma 7. *Let W be an irreducible well-generated complex reflection group of rank n, and let $p = m_1h_1$ be a divisor of mh, where $m = m_1m_2$ and $h = h_1h_2$. Without loss of generality, we assume that* $\gcd(h_1, m_2) = 1$. *Suppose that Theorem 2 has already been verified for all irreducible well-generated complex reflection groups with rank $< n$. If h_2 does not divide all degrees d_i, then Eq. (5) is satisfied.*

Proof. Let us write $h_1 = am_2 + b$, with $0 \le b < m_2$. The condition $\gcd(h_1, m_2) = 1$ translates into $\gcd(b, m_2) = 1$. From (10), we infer that

$$\begin{aligned}\phi^p\big((w_0; w_1, \dots, w_m)\big)\\ = (*; c^{a+1}w_{m-m_1b+1}c^{-a-1}, c^{a+1}w_{m-m_1b+2}c^{-a-1}, \dots, c^{a+1}w_m c^{-a-1},\\ c^a w_1 c^{-a}, \dots, c^a w_{m-m_1b}c^{-a}\big).\end{aligned} \tag{17}$$

Supposing that $(w_0; w_1, \dots, w_m)$ is fixed by ϕ^p, we obtain the system of equations

$$\begin{aligned} w_i &= c^{a+1}w_{i+m-m_1b}c^{-a-1}, \quad i = 1, 2, \dots, m_1b,\\ w_i &= c^a w_{i-m_1b}c^{-a}, \quad i = m_1b+1, m_1b+2, \dots, m,\end{aligned}$$

which, after iteration, implies in particular that

$$w_i = c^{b(a+1)+(m_2-b)a}w_i c^{-b(a+1)-(m_2-b)a} = c^{h_1}w_i c^{-h_1}, \quad i = 1, 2, \dots, m.$$

It is at this point where we need $\gcd(b, m_2) = 1$. The last equation shows that each w_i, $i = 1, 2, \dots, m$, and thus also w_0, lies in $\mathrm{Cent}_W(c^{h_1})$. By the theorem of Springer cited in the proof of Lemma 4, this centraliser subgroup is itself a complex reflection group, W' say, whose degrees are those degrees of W that are divisible by $h/h_1 = h_2$. Since, by assumption, h_2 does not divide *all* degrees, W' has rank strictly less than n. Again by assumption, we know that Theorem 2 is true for W', so that in particular,

$$|\operatorname{Fix}_{NC^m(W')}(\phi^p)| = \operatorname{Cat}^m(W'; q)\big|_{q=e^{2\pi i p/mh}}.$$

The arguments above together with (14) show that

$$\operatorname{Fix}_{NC^m(W)}(\phi^p) = \operatorname{Fix}_{NC^m(W')}(\phi^p).$$

On the other hand, using (13) it is straightforward to see that

$$\mathrm{Cat}^m(W;q)\big|_{q=e^{2\pi ip/mh}} = \mathrm{Cat}^m(W';q)\big|_{q=e^{2\pi ip/mh}}.$$

This proves (5) for our particular p, as required. □

Lemma 8. *Let W be an irreducible well-generated complex reflection group of rank n, and let $p = m_1h_1$ be a divisor of mh, where $m = m_1m_2$ and $h = h_1h_2$. We assume that* $\gcd(h_1, m_2) = 1$. *If $m_2 > n$ then*

$$\mathrm{Fix}_{NC^m(W)}(\phi^p) = \big\{(c;\varepsilon,\dots,\varepsilon)\big\}.$$

Proof. Let us suppose that $(w_0; w_1,\dots,w_m) \in \mathrm{Fix}_{NC^m(W)}(\phi^p)$ and that there exists a $j \ge 1$ such that $w_j \ne \varepsilon$. By (17), it then follows for such a j that also $w_k \ne \varepsilon$ for all $k \equiv j - lm_1b \pmod m$, where, as before, b is defined as the unique integer with $h_1 = am_2 + b$ and $0 \le b < m_2$. Since, by assumption, $\gcd(b, m_2) = 1$, there are exactly m_2 such k's which are distinct mod m. However, this implies that the sum of the absolute lengths of the w_i's, $0 \le i \le m$, is at least $m_2 > n$, a contradiction to Remark 1.(2). □

Remark 3. (1) If we put ourselves in the situation of the assumptions of Lemma 7, then we may conclude that Eq. (5) only needs to be checked for pairs (m_2, h_2) subject to the following restrictions:

$$m_2 \ge 2, \quad \gcd(h_1, m_2) = 1, \quad \text{and } h_2 \text{ divides all degrees of } W. \tag{18}$$

Indeed, Lemmas 4 and 7 together imply that Eq. (5) is always satisfied in all other cases.

(2) Still putting ourselves in the situation of Lemma 7, if $m_2 > n$ and m_2h_2 does not divide any of the degrees of W, then Eq. (5) is satisfied. Indeed, Lemma 8 says that in this case the left-hand side of (5) equals 1, while a straightforward computation using (13) shows that in this case the right-hand side of (5) equals 1 as well.

(3) It should be observed that this leaves a finite number of choices for m_2 to consider, whence a finite number of choices for (m_1, m_2, h_1, h_2). Altogether, there remains a finite number of choices for $p = h_1m_1$ to be checked.

Lemma 9. *Let W be an irreducible well-generated complex reflection group of rank n with the property that $d_i \mid h$ for $i = 1, 2, \dots, n$. Then Theorem 2 is true for this group W.*

Proof. By Lemma 3, we may restrict ourselves to divisors p of mh.

Suppose that $e^{2\pi ip/mh}$ is a d_i-th root of unity for some i. In other words, mh/p divides d_i. Since d_i is a divisor of h by assumption, the integer mh/p also divides h. But this is equivalent to saying that m divides p, and Eq. (5) holds by Lemma 4.

Now assume that mh/p does not divide any of the d_i's. Then, by (13), the right-hand side of (5) equals 1. On the other hand, $(c;\varepsilon,\dots,\varepsilon)$ is always an element of

$\mathrm{Fix}_{NC^m(W)}(\phi^p)$. To see that there are no others, we make appeal to the classification of all irreducible well-generated complex reflection groups, which we recalled in Sect. 2. Inspection reveals that all groups satisfying the hypotheses of the lemma have rank $n \le 2$. Except for the groups contained in the infinite series $G(d,1,n)$ and $G(e,e,n)$ for which Theorem 2 has been established in [19], these are the groups $G_5, G_6, G_9, G_{10}, G_{14}, G_{17}, G_{18}, G_{21}$. We now discuss these groups case by case, keeping the notation of Lemma 7. In order to simplify the argument, we note that Lemma 8 implies that Eq. (5) holds if $m_2 > 2$, so that in the following arguments we always may assume that $m_2 = 2$.

CASE G_5. The degrees are 6, 12, and therefore Remark 3.(1) implies that Eq. (5) is always satisfied.

CASE G_6. The degrees are 4, 12, and therefore, according to Remark 3.(1), we need only consider the case where $h_2 = 4$ and $m_2 = 2$, that is, $p = 3m/2$. Then (17) becomes

$$\begin{aligned}&\phi^p\big((w_0; w_1, \dots, w_m)\big)\\&= \big(c^2 w_{\frac{m}{2}+1} c^{-2}, c^2 w_{\frac{m}{2}+2} c^{-2}, \dots, c^2 w_m c^{-2}, c w_1 c^{-1}, \dots, c w_{\frac{m}{2}} c^{-1}\big).\end{aligned} \tag{19}$$

If $(w_0; w_1, \dots, w_m)$ is fixed by ϕ^p and not equal to $(c; \varepsilon, \dots, \varepsilon)$, there must exist an i with $1 \le i \le \frac{m}{2}$ such that $\ell_T(w_i) = \ell_T(w_{\frac{m}{2}+i}) = 1$, $w_{\frac{m}{2}+i} = c w_i c^{-1}$, $w_i w_{\frac{m}{2}+i} = w_i c w_i c^{-1} = c$, and all w_j, with $j \ne i, \frac{m}{2}+i$, equal ε. However, with the help of the *GAP* package `CHEVIE` [14, 27], one verifies that there is no w_i in G_6 such that

$$\ell_T(w_i) = 1 \quad \text{and} \quad w_i c w_i c^{-1} = c$$

are simultaneously satisfied. Hence, the left-hand side of (5) is equal to 1, as required.

CASE G_9. The degrees are $8, 24$, and therefore, according to Remark 3.(1), we need only consider the case where $h_2 = 8$ and $m_2 = 2$, that is, $p = 3m/2$. This is the same p as for G_6. Again, `CHEVIE` finds no solution. Hence, the left-hand side of (5) is equal to 1, as required.

CASE G_{10}. The degrees are $12, 24$, and therefore Remark 3.(1) implies that Eq. (5) is always satisfied.

CASE G_{14}. The degrees are $6, 24$, and therefore Remark 3.(1) implies that Eq. (5) is always satisfied.

CASE G_{17}. The degrees are $20, 60$, and therefore, according to Remark 3.(1), we need only consider the cases where $h_2 = 20$ or $h_2 = 4$. In the first case, $p = 3m/2$, which is the same p as for G_6. Again, `CHEVIE` finds no solution. In the second case, $p = 15m/2$. Then (17) becomes

$$\begin{aligned}&\phi^p\big((w_0; w_1, \dots, w_m)\big)\\&\quad = \big(*; c^8 w_{\frac{m}{2}+1} c^{-8}, c^8 w_{\frac{m}{2}+2} c^{-8}, \dots, c^8 w_m c^{-8}, c^7 w_1 c^{-7}, \dots, c^7 w_{\frac{m}{2}} c^{-7}\big).\end{aligned} \tag{20}$$

By Lemma 6, every element of $NC(W)$ is fixed under conjugation by c^3, and, thus, on elements fixed by ϕ^p, the above action of ϕ^p reduces to the one in (19). This action was already discussed in the first case. Hence, in both cases, the left-hand side of (5) is equal to 1, as required.

CASE G_{18}. The degrees are 30, 60, and therefore Remark 3.(1) implies that Eq. (5) is always satisfied.

CASE G_{21}. The degrees are 12, 60, and therefore, according to Remark 3.(1), we need only consider the cases where $h_2 = 12$ or $h_2 = 4$. In the first case, $p = 5m/2$, so that (17) becomes

$$\phi^p\big((w_0; w_1, \dots, w_m)\big) = \big(*; c^3 w_{\frac{m}{2}+1} c^{-3}, c^3 w_{\frac{m}{2}+2} c^{-3}, \dots, c^3 w_m c^{-3}, c^2 w_1 c^{-2}, \dots, c^2 w_{\frac{m}{2}} c^{-2}\big). \tag{21}$$

If $(w_0; w_1, \dots, w_m)$ is fixed by ϕ^p and not equal to $(c; \varepsilon, \dots, \varepsilon)$, there must exist an i with $1 \le i \le \frac{m}{2}$ such that $\ell_T(w_i) = 1$ and $w_i c^2 w_i c^{-2} = c$. However, with the help of the *GAP* package CHEVIE [14, 27], one verifies that there is no such solution to this equation. In the second case, $p = 15m/2$. Then (17) becomes the action in (20). By Lemma 6, every element of $NC(W)$ is fixed under conjugation by c^5, and, thus, on elements fixed by ϕ^p, the action of ϕ^p in (20) reduces to the one in the first case. Hence, in both cases, the left-hand side of (5) is equal to 1, as required.

This completes the proof of the lemma. □

6 Exemplification of Case-by-Case Verification of Theorem 2

It remains to verify Theorem 2 for the groups G_4,G_8,G_{16},G_{20}, $G_{23} = H_3$,G_{24},G_{25},G_{26},G_{27}, $G_{28} = F_4$,G_{29},$G_{30} = H_4$,G_{32}, G_{33},G_{34},$G_{35} = E_6$,$G_{36} = E_7$,$G_{37} = E_8$. All details can be found in [21, Sect. 6]. We content ourselves with illustrating the type of computation that is needed here by going through the case of the group G_{24}, and by discussing some of the arguments needed for the group $G_{37} = E_8$.

In the sequel we write ζ_d for a primitive d-th root of unity.

6.1 CASE G_{24}

The degrees are 4, 6, 14, and hence we have

$$\mathrm{Cat}^m(G_{24}; q) = \frac{[14m + 14]_q\, [14m + 6]_q\, [14m + 4]_q}{[14]_q\, [6]_q\, [4]_q}.$$

Let ζ be a $14m$-th root of unity. In what follows, we abbreviate the assertion that "ζ is a primitive d-th root of unity" as "$\zeta = \zeta_d$." The following cases on the right-hand side of (5) occur:

$$\lim_{q\to\zeta} \mathrm{Cat}^m(G_{24};q) = m+1, \quad \text{if } \zeta = \zeta_{14}, \zeta_7, \tag{22}$$

$$\lim_{q\to\zeta} \mathrm{Cat}^m(G_{24};q) = \tfrac{7m+3}{3}, \quad \text{if } \zeta = \zeta_6, \zeta_3,\ 3 \mid m, \tag{23}$$

$$\lim_{q\to\zeta} \mathrm{Cat}^m(G_{24};q) = \tfrac{7m+2}{2}, \quad \text{if } \zeta = \zeta_4,\ 2 \mid m, \tag{24}$$

$$\lim_{q\to\zeta} \mathrm{Cat}^m(G_{24};q) = \mathrm{Cat}^m(G_{24}), \quad \text{if } \zeta = -1 \text{ or } \zeta = 1, \tag{25}$$

$$\lim_{q\to\zeta} \mathrm{Cat}^m(G_{24};q) = 1, \quad \text{otherwise.} \tag{26}$$

We must now prove that the left-hand side of (5) in each case agrees with the values exhibited in (22)–(26). The only cases not covered by Lemma 4 are the ones in (23), (24), and (26). (In both (22) and (25) we have $d \mid h$.)

We first consider (23). By Lemma 3, we are free to choose $p = 7m/3$ if $\zeta = \zeta_6$, respectively $p = 14m/3$ if $\zeta = \zeta_3$. In both cases, m must be divisible by 3.

We start with the case that $p = 7m/3$. From (10), we infer

$$\phi^p\big((w_0; w_1, \dots, w_m)\big)$$
$$= \big(*; c^3 w_{\frac{2m}{3}+1} c^{-3}, c^3 w_{\frac{2m}{3}+2} c^{-3}, \dots, c^3 w_m c^{-3}, c^2 w_1 c^{-2}, \dots, c^2 w_{\frac{2m}{3}} c^{-2}\big).$$

Supposing that $(w_0; w_1, \dots, w_m)$ is fixed by ϕ^p, we obtain the system of equations

$$w_i = c^3 w_{\frac{2m}{3}+i} c^{-3}, \quad i = 1, 2, \dots, \tfrac{m}{3}, \tag{27}$$

$$w_i = c^2 w_{i-\frac{m}{3}} c^{-2}, \quad i = \tfrac{m}{3}+1, \tfrac{m}{3}+2, \dots, m. \tag{28}$$

There are two distinct possibilities for choosing the w_i's, $1 \le i \le m$: either all the w_i's are equal to ε, or there is an i with $1 \le i \le \frac{m}{3}$ such that

$$\ell_T(w_i) = \ell_T(w_{i+\frac{m}{3}}) = \ell_T(w_{i+\frac{2m}{3}}) = 1.$$

Writing t_1, t_2, t_3 for $w_i, w_{i+\frac{m}{3}}, w_{i+\frac{2m}{3}}$, respectively, the Eqs. (27) and (28) reduce to

$$t_1 = c^3 t_3 c^{-3}, \tag{29}$$

$$t_2 = c^2 t_1 c^{-2}, \tag{30}$$

$$t_3 = c^2 t_2 c^{-2}. \tag{31}$$

One of these equations is in fact superfluous: if we substitute (30) and (31) in (29), then we obtain $t_1 = c^7 t_1 c^{-7}$ which is automatically satisfied due to Lemma 6 with $d = 2$.

Since $(w_0; w_1, \ldots, w_m) \in NC^m(G_{24})$, we must have $t_1 t_2 t_3 = c$. Combining this with (29)–(31), we infer that

$$t_1(c^2 t_1 c^{-2})(c^4 t_1 c^{-4}) = c. \tag{32}$$

With the help of CHEVIE, one obtains seven solutions for t_1 in this equation, each of them giving rise to $m/3$ elements of $\mathrm{Fix}_{NC^m(G_{24})}(\phi^p)$ since i (in w_i) ranges from 1 to $m/3$.

In total, we obtain $1 + 7\frac{m}{3} = \frac{7m+3}{3}$ elements in $\mathrm{Fix}_{NC^m(G_{24})}(\phi^p)$, which agrees with the limit in (23).

The case where $p = 14m/3$ can be treated in a similar fashion. In the end, it turns out that we have to solve the same enumeration problem as for $p = 7m/3$, and, consequently, the number of elements of $\mathrm{Fix}_{NC^m(G_{24})}(\phi^p)$ is the same, namely $\frac{7m+3}{3}$, as required.

Our next case is (24). Proceeding in a similar manner as before, we see that there is again the trivial possibility $(c; \varepsilon, \ldots, \varepsilon)$, and otherwise we have to find t_1 with $\ell_T(t_1) = 1$ satisfying the inequality

$$t_1(c^3 t_1 c^{-3}) \le_T c. \tag{33}$$

With the help of CHEVIE, one obtains 7 solutions for t_1 in this relation, each of them giving rise to $m/2$ elements of $\mathrm{Fix}_{NC^m(G_{24})}(\phi^p)$ since i (in w_i) ranges from 1 to $m/2$.

In total, we obtain $1 + 7\frac{m}{2} = \frac{7m+2}{2}$ elements in $\mathrm{Fix}_{NC^m(G_{24})}(\phi^p)$, which agrees with the limit in (24).

Finally, we turn to (26). By Remark 3, the only choices for h_2 and m_2 to be considered are $h_2 = 1$ and $m_2 = 3$, $h_2 = m_2 = 2$, and $h_2 = 2$ and $m_2 = 3$. These correspond to the choices $p = 14m/3$, $p = 7m/2$, respectively $p = 7m/3$, all of which have already been discussed as they do not belong to (26). Hence, (5) must necessarily hold, as required.

6.2 Case $G_{37} = E_8$

The degrees are $2, 8, 12, 14, 18, 20, 24, 30$, and hence we have

$$\mathrm{Cat}^m(E_8; q) = \frac{[30m+30]_q\,[30m+24]_q\,[30m+20]_q\,[30m+18]_q}{[30]_q\,[24]_q\,[20]_q\,[18]_q} \times \frac{[30m+14]_q\,[30m+12]_q\,[30m+8]_q\,[30m+2]_q}{[14]_q\,[12]_q\,[8]_q\,[2]_q}.$$

Let ζ be a $30m$-th root of unity. The cases occurring on the right-hand side of (5) not covered by Lemma 4 are:

$$\lim_{q\to\zeta} \mathrm{Cat}^m(E_8;q) = \tfrac{5m+4}{4}, \quad \text{if } \zeta=\zeta_{24},\ 4\mid m, \tag{34}$$

$$\lim_{q\to\zeta} \mathrm{Cat}^m(E_8;q) = \tfrac{3m+2}{2}, \quad \text{if } \zeta=\zeta_{20},\ 2\mid m, \tag{35}$$

$$\lim_{q\to\zeta} \mathrm{Cat}^m(E_8;q) = \tfrac{5m+3}{3}, \quad \text{if } \zeta=\zeta_{18},\zeta_9,\ 3\mid m, \tag{36}$$

$$\lim_{q\to\zeta} \mathrm{Cat}^m(E_8;q) = \tfrac{15m+7}{7}, \quad \text{if } \zeta=\zeta_{14},\zeta_7,\ 7\mid m, \tag{37}$$

$$\lim_{q\to\zeta} \mathrm{Cat}^m(E_8;q) = \tfrac{(5m+4)(5m+2)}{8}, \quad \text{if } \zeta=\zeta_{12},\ 2\mid m, \tag{38}$$

$$\lim_{q\to\zeta} \mathrm{Cat}^m(E_8;q) = \tfrac{(5m+4)(15m+4)}{16}, \quad \text{if } \zeta=\zeta_{8},\ 4\mid m, \tag{39}$$

$$\lim_{q\to\zeta} \mathrm{Cat}^m(E_8;q) = \tfrac{(5m+4)(3m+2)(5m+2)(15m+4)}{64}, \quad \text{if } \zeta=\zeta_{4},\ 2\mid m, \tag{40}$$

$$\lim_{q\to\zeta} \mathrm{Cat}^m(E_8;q) = \mathrm{Cat}^m(E_8), \quad \text{if } \zeta=-1 \text{ or } \zeta=1, \tag{41}$$

$$\lim_{q\to\zeta} \mathrm{Cat}^m(E_8;q) = 1, \quad \text{otherwise.} \tag{42}$$

We now have to prove that the left-hand side of (5) in each case agrees with the values exhibited in (34)–(42). Since the corresponding computations in the various cases are very similar, we concentrate here only on the cases (39) and (40), these two being representative of the types of arguments arising. As before, we refer the reader to [21, Sect. 6] for full details.

Let us consider the case in (39) first. By Lemma 3, we are free to choose $p = 15m/4$. In particular, m must be divisible by 4. From (10), we infer

$$\phi^p\big((w_0;w_1,\dots,w_m)\big) = \big(*;c^4w_{\frac{m}{4}+1}c^{-4},c^4w_{\frac{m}{4}+2}c^{-4},\dots,c^4w_mc^{-4},c^3w_1c^{-3},\dots,c^3w_{\frac{m}{4}}c^{-3}\big).$$

Supposing that $(w_0;w_1,\dots,w_m)$ is fixed by ϕ^p, we obtain the system of equations

$$w_i = c^4w_{\frac{m}{4}+i}c^{-4}, \quad i=1,2,\dots,\tfrac{3m}{4}, \tag{43}$$

$$w_i = c^3w_{i-\frac{3m}{4}}c^{-3}, \quad i=\tfrac{3m}{4}+1,\tfrac{3m}{4}+2,\dots,m. \tag{44}$$

There are several distinct possibilities for choosing the w_i's, $1\le i\le m$, which we summarize as follows:

(i) All the w_i's are equal to ε (and $w_0 = c$),
(ii) There is an i with $1 \le i \le \frac{m}{4}$ such that

$$1 \le \ell_T(w_i) = \ell_T(w_{i+\frac{m}{4}}) = \ell_T(w_{i+\frac{2m}{4}}) = \ell_T(w_{i+\frac{3m}{4}}) \le 2, \tag{45}$$

and the other w_j's, $1 \le j \le m$, are equal to ε,

(iii) There are i_1 and i_2 with $1 \le i_1 < i_2 \le \frac{m}{4}$ such that

$$\begin{aligned}\ell_T(w_{i_1}) &= \ell_T(w_{i_2}) = \ell_T(w_{i_1+\frac{m}{4}}) = \ell_T(w_{i_2+\frac{m}{4}})\\ &= \ell_T(w_{i_1+\frac{2m}{4}}) = \ell_T(w_{i_2+\frac{2m}{4}}) = \ell_T(w_{i_1+\frac{3m}{4}}) = \ell_T(w_{i_2+\frac{3m}{4}}) = 1,\end{aligned} \tag{46}$$

and all other w_j are equal to ε.

Moreover, since $(w_0; w_1, \dots, w_m) \in NC^m(E_8)$, we must have

$$w_i w_{i+\frac{m}{4}} w_{i+\frac{2m}{4}} w_{i+\frac{3m}{4}} \le_T c,$$

or

$$w_{i_1} w_{i_2} w_{i_1+\frac{m}{4}} w_{i_2+\frac{m}{4}} w_{i_1+\frac{2m}{4}} w_{i_2+\frac{2m}{4}} w_{i_1+\frac{3m}{4}} w_{i_2+\frac{3m}{4}} = c.$$

Together with Eqs. (43), (44), (45), and (46), this implies that

$$w_i = c^{15} w_i c^{-15} \quad \text{and} \quad w_i (c^{11} w_i c^{-11})(c^7 w_i c^{-7})(c^3 w_i c^{-3}) \le_T c, \tag{47}$$

or that

$$\begin{aligned}&w_{i_1} = c^{15} w_{i_1} c^{-15}, \quad w_{i_1} = c^{15} w_{i_2} c^{-15}, \quad \text{and}\\ &w_{i_1} w_{i_2} (c^{11} w_{i_1} c^{-11})(c^{11} w_{i_2} c^{-11})(c^7 w_{i_1} c^{-7})(c^7 w_{i_2} c^{-7})(c^3 w_{i_1} c^{-3})(c^3 w_{i_2} c^{-3}) = c.\end{aligned} \tag{48}$$

Here, the first equation in (47) and the first two equations in (48) are automatically satisfied due to Lemma 6 with $d = 2$.

With the help of Stembridge's *Maple* package `coxeter` [37], one obtains 30 solutions for w_i in (47) with $\ell_T(w_i) = 1$, 45 solutions for w_i with $\ell_T(w_i) = 2$ and w_i of type A_1^2 (as a parabolic Coxeter element; see the end of Sect. 2), and 20 solutions for w_i with $\ell_T(w_i) = 2$ and w_i of type A_2. Each of them gives rise to $m/4$ elements of $\mathrm{Fix}_{NC^m(E_8)}(\phi^p)$ since i ranges from 1 to $m/4$.

The number of solutions in Case (iii) can be computed from our knowledge of the solutions in Case (ii) according to type, using some elementary counting arguments. Namely, the number of solutions of (48) is equal to

$$45 \cdot 2 + 20 \cdot 3 = 150,$$

since an element of type A_1^2 can be decomposed in two ways into a product of two elements of absolute length 1, while for an element of type A_2 this can be done in 3 ways.

In total, we obtain $1 + (30 + 45 + 20)\frac{m}{4} + 150\binom{m/4}{2} = \frac{(5m+4)(15m+4)}{16}$ elements in $\mathrm{Fix}_{NC^m(E_8)}(\phi^p)$, which agrees with the limit in (39).

Next, we discuss the case in (40). By Lemma 3, we are free to choose $p = 15m/2$. In particular, m must be divisible by 2. From (10), we infer

$$\phi^p\big((w_0; w_1, \dots, w_m)\big)$$
$$= (*; c^8 w_{\frac{m}{2}+1} c^{-8}, c^8 w_{\frac{m}{2}+2} c^{-8}, \dots, c^8 w_m c^{-8}, c^7 w_1 c^{-7}, \dots, c^7 w_{\frac{m}{2}} c^{-7}\big).$$

Supposing that $(w_0; w_1, \dots, w_m)$ is fixed by ϕ^p, we obtain the system of equations

$$w_i \quad = c^8 w_{\frac{m}{2}+i} c^{-8}, \quad i = 1, 2, \dots, \tfrac{m}{2}, \tag{49}$$

$$w_i = c^7 w_{i-\frac{m}{2}} c^{-7}, \quad i = \tfrac{m}{2} + 1, \tfrac{m}{2} + 2, \dots, m. \tag{50}$$

There are several distinct possibilities for choosing the w_i's, $1 \le i \le m$:

(i) All the w_i's are equal to ε (and $w_0 = c$),
(ii) There is an i with $1 \le i \le \frac{m}{2}$ such that

$$1 \le \ell_T(w_i) = \ell_T(w_{i+\frac{m}{2}}) \le 4, \tag{51}$$

and the other w_j's, $1 \le j \le m$, are equal to ε,
(iii) There are i_1 and i_2 with $1 \le i_1 < i_2 \le \frac{m}{2}$ such that

$$\ell_1 := \ell_T(w_{i_1}) = \ell_T(w_{i_1+\frac{m}{2}}) \ge 1, \quad \ell_2 := \ell_T(w_{i_2}) = \ell_T(w_{i_2+\frac{m}{2}}) \ge 1,$$
$$\text{and} \quad \ell_1 + \ell_2 \le 4, \tag{52}$$

and the other w_j's, $1 \le j \le m$, are equal to ε,
(iv) There are i_1, i_2, i_3 with $1 \le i_1 < i_2 < i_3 \le \frac{m}{2}$ such that

$$\ell_1 := \ell_T(w_{i_1}) = \ell_T(w_{i_1+\frac{m}{2}}) \ge 1, \quad \ell_2 := \ell_T(w_{i_2}) = \ell_T(w_{i_2+\frac{m}{2}}) \ge 1,$$
$$\ell_3 := \ell_T(w_{i_3}) = \ell_T(w_{i_3+\frac{m}{2}}) \ge 1, \quad \text{and} \quad \ell_1 + \ell_2 + \ell_3 \le 4, \tag{53}$$

and the other w_j's, $1 \le j \le m$, are equal to ε,
(v) There are i_1, i_2, i_3, i_4 with $1 \le i_1 < i_2 < i_3 < i_4 \le \frac{m}{2}$ such that

$$\ell_T(w_{i_1}) = \ell_T(w_{i_2}) = \ell_T(w_{i_3}) = \ell_T(w_{i_4})$$
$$= \ell_T(w_{i_1+\frac{m}{2}}) = \ell_T(w_{i_2+\frac{m}{2}}) = \ell_T(w_{i_3+\frac{m}{2}}) = \ell_T(w_{i_4+\frac{m}{2}}) = 1, \tag{54}$$

and all other w_j's are equal to ε.

Moreover, since $(w_0; w_1, \dots, w_m) \in NC^m(E_8)$, we must have $w_i w_{i+\frac{m}{2}} \le_T c$, respectively $w_{i_1} w_{i_2} w_{i_1+\frac{m}{2}} w_{i_2+\frac{m}{2}} \le_T c$, respectively

$$w_{i_1}w_{i_2}w_{i_3}w_{i_1+\frac{m}{2}}w_{i_2+\frac{m}{2}}w_{i_3+\frac{m}{2}} \le_T c,$$

respectively

$$w_{i_1}w_{i_2}w_{i_3}w_{i_4}w_{i_1+\frac{m}{2}}w_{i_2+\frac{m}{2}}w_{i_3+\frac{m}{2}}w_{i_4+\frac{m}{2}} = c.$$

Together with Eqs. (49), (50), and (51)–(54), this implies that

$$w_i = c^{15}w_ic^{-15} \quad \text{and} \quad w_i(c^7w_ic^{-7}) \le_T c, \tag{55}$$

respectively that

$$w_{i_1} = c^{15}w_{i_1}c^{-15}, \quad w_{i_2} = c^{15}w_{i_2}c^{-15}, \quad \text{and} \quad w_{i_1}w_{i_2}(c^7w_{i_1}c^{-7})(c^7w_{i_2}c^{-7}) \le_T c, \tag{56}$$

respectively that

$$w_{i_1} = c^{15}w_{i_1}c^{-15}, \quad w_{i_2} = c^{15}w_{i_2}c^{-15}, \quad w_{i_3} = c^{15}w_{i_3}c^{-15},$$
$$\text{and} \quad w_{i_1}w_{i_2}w_{i_3}(c^7w_{i_1}c^{-7})(c^7w_{i_2}c^{-7})(c^7w_{i_3}c^{-7}) \le_T c, \tag{57}$$

respectively that

$$w_{i_1} = c^{15}w_{i_1}c^{-15}, \quad w_{i_2} = c^{15}w_{i_2}c^{-15}, \quad w_{i_3} = c^{15}w_{i_3}c^{-15}, \quad w_{i_4} = c^{15}w_{i_4}c^{-15},$$
$$\text{and} \quad w_{i_1}w_{i_2}w_{i_3}w_{i_4}(c^7w_{i_1}c^{-7})(c^7w_{i_2}c^{-7})(c^7w_{i_3}c^{-7})(c^7w_{i_4}c^{-7}) = c. \tag{58}$$

Here, the first equation in (55), the first two in (56), the first three in (57), and the first four in (58), are all automatically satisfied due to Lemma 6 with $d = 2$.

With the help of Stembridge's *Maple* package `coxeter` [37], one obtains

– 45 solutions for w_i in (55) with $\ell_T(w_i) = 1$,
– 150 solutions for w_i in (55) with $\ell_T(w_i) = 2$ and w_i of type A_1^2,
– 100 solutions for w_i in (55) with $\ell_T(w_i) = 2$ and w_i of type A_2,
– 75 solutions for w_i in (55) with $\ell_T(w_i) = 3$ and w_i of type A_1^3,
– 165 solutions for w_i in (55) with $\ell_T(w_i) = 3$ and w_i of type $A_1 * A_2$,
– 90 solutions for w_i in (55) with $\ell_T(w_i) = 3$ and w_i of type A_3,
– 15 solutions for w_i in (55) with $\ell_T(w_i) = 4$ and w_i of type $A_1^2 * A_2$,
– 45 solutions for w_i in (55) with $\ell_T(w_i) = 4$ and w_i of type $A_1 * A_3$;
– 5 solutions for w_i in (55) with $\ell_T(w_i) = 4$ and w_i of type A_2^2,
– 18 solutions for w_i in (55) with $\ell_T(w_i) = 4$ and w_i of type A_4,
– 5 solutions for w_i in (55) with $\ell_T(w_i) = 4$ and w_i of type D_4.

Each of them gives rise to $m/2$ elements of $\mathrm{Fix}_{NC^m(E_8)}(\phi^p)$ since i ranges from 1 to $m/2$. There are no solutions for w_i in (55) with w_i of type A_1^4.

Letting the computer find all solutions in cases (iii)–(v) would take years. However, the number of these solutions can be computed from our knowledge of the solutions in Case (ii) according to type, if this information is combined with the decomposition numbers in the sense of [17, 18, 20] (see the end of Sect. 2) and some elementary (multiset) permutation counting. The decomposition numbers for A_2, A_3, A_4, and D_4 of which we make use can be found in the appendix of [18].

To begin with, the number of solutions of (56) with $\ell_1 = \ell_2 = 1$ is equal to

$$n_{1,1} := 150 \cdot 2 + 100 \cdot N_{A_2}(A_1, A_1) = 600,$$

since an element of type A_1^2 can be decomposed in two ways into a product of two elements of absolute length 1, while for an element of type A_2 this can be done in $N_{A_2}(A_1, A_1) = 3$ ways. Similarly, the number of solutions of (56) with $\ell_1 = 2$ and $\ell_2 = 1$ is equal to

$$n_{2,1} := 75 \cdot 3 + 165 \cdot (1 + N_{A_2}(A_1, A_1)) + 90 \cdot N_{A_3}(A_2, A_1) = 1{,}425,$$

the number of solutions of (56) with $\ell_1 = 3$ and $\ell_2 = 1$ is equal to

$$n_{3,1} := 15 \cdot (2 + N_{A_2}(A_1, A_1)) + 45 \cdot (1 + N_{A_3}(A_2, A_1)) + 5 \cdot (2N_{A_2}(A_1, A_1))$$
$$+18 \cdot (N_{A_4}(A_3, A_1) + N_{A_4}(A_1 * A_2, A_1)) + 5 \cdot (N_{D_4}(A_3, A_1) + N_{D_4}(A_1^3, A_1)) = 660,$$

the number of solutions of (56) with $\ell_1 = \ell_2 = 2$ is equal to

$$n_{2,2} := 15 \cdot (2 + 2N_{A_2}(A_1, A_1)) + 45 \cdot (2N_{A_3}(A_2, A_1)) + 5 \cdot (2 + N_{A_2}(A_1, A_1)^2)$$
$$+ 18 \cdot (N_{A_4}(A_2, A_2) + N_{A_4}(A_1^2, A_1^2) + 2N_{A_4}(A_2, A_1^2))$$
$$+ 5 \cdot (N_{D_4}(A_2, A_2) + 2N_{D_4}(A_2, A_1^2)) = 1{,}195,$$

the number of solutions of (57) with $\ell_1 = \ell_2 = \ell_3 = 1$ is equal to

$$n_{1,1,1} := 75 \cdot 3! + 165 \cdot (3N_{A_2}(A_1, A_1)) + 90 N_{A_3}(A_1, A_1, A_1) = 3{,}375,$$

the number of solutions of (57) with $\ell_1 = 2$ and $\ell_2 = \ell_3 = 1$ is equal to

$$n_{2,1,1} := 15 \cdot (2 + N_{A_2}(A_1, A_1) + 2 \cdot 2 \cdot N_{A_2}(A_1, A_1))$$
$$+ 45 \cdot (2N_{A_3}(A_2, A_1) + N_{A_3}(A_1, A_1, A_1)) + 5 \cdot (2N_{A_2}(A_1, A_1) + 2N_{A_2}(A_1, A_1)^2)$$
$$+ 18 \cdot (N_{A_4}(A_2, A_1, A_1) + N_{A_4}(A_1^2, A_1, A_1))$$
$$+ 5 \cdot (N_{D_4}(A_2, A_1, A_1) + N_{D_4}(A_1^2, A_1, A_1)) = 2{,}850,$$

and the number of solutions of (58) is equal to

$$n_{1,1,1,1} := 15 \cdot (12N_{A_2}(A_1, A_1)) + 45 \cdot (4N_{A_3}(A_1, A_1, A_1)) + 5 \cdot (6N_{A_2}(A_1, A_1)^2)$$
$$+ 18 \cdot N_{A_4}(A_1, A_1, A_1, A_1) + 5 \cdot N_{D_4}(A_1, A_1, A_1, A_1) = 6{,}750.$$

In total, we obtain

$$
\begin{aligned}
1 &+ (45+150+100+75+165+90+15+45+5+18+5)\frac{m}{2} \\
&+ (n_{1,1}+2n_{2,1}+2n_{3,1}+n_{2,2})\binom{m/2}{2} + (n_{1,1,1}+3n_{2,1,1})\binom{m/2}{3} \\
&+ n_{1,1,1,1}\binom{m/2}{4} = \frac{(5m+4)(3m+2)(5m+2)(15m+4)}{64}
\end{aligned}
$$

elements in $\mathrm{Fix}_{NC^m(E_8)}(\phi^p)$, which agrees with the limit in (40).

7 Cyclic Sieving II

In this section we present the second cyclic sieving conjecture due to Bessis and Reiner [10, Conjecture 6.5].

Let $\psi : NC^m(W) \to NC^m(W)$ be the map defined by

$$(w_0; w_1, \dots, w_m) \mapsto \big(cw_m c^{-1}; w_0, w_1, \dots, w_{m-1}\big). \tag{59}$$

For $m = 1$, we have $w_0 = cw_1^{-1}$, so that this action reduces to the inverse of the *Kreweras complement* K_{id}^c as defined by Armstrong [3, Definition 2.5.3].

It is easy to see that $\psi^{(m+1)h}$ acts as the identity, where h is the Coxeter number of W (see (61) below). By slight abuse of notation as before, let C_2 be the cyclic group of order $(m+1)h$ generated by ψ.

Given these definitions, we are now in the position to state the second cyclic sieving conjecture of Bessis and Reiner. By the results of [19] and of this paper, it becomes the following theorem.

Theorem 4. *For an irreducible well-generated complex reflection group W and any $m \ge 1$, the triple $(NC^m(W), \mathrm{Cat}^m(W;q), C_2)$, where $\mathrm{Cat}^m(W;q)$ is the q-analogue of the Fuß–Catalan number defined in (4), exhibits the cyclic sieving phenomenon.*

By definition of the cyclic sieving phenomenon, we have to prove that

$$|\,\mathrm{Fix}_{NC^m(W)}(\psi^p)| = \mathrm{Cat}^m(W;q)\big|_{q=e^{2\pi i p/(m+1)h}}, \tag{60}$$

for all p in the range $0 \le p < (m+1)h$.

8 Auxiliary Results II

This section collects several auxiliary results which allow us to reduce the problem of proving Theorem 4, respectively the equivalent statement (60), for the 26 exceptional groups listed in Sect. 2 to a finite problem. The corresponding lemmas, Lemmas 10–15, are analogues of Lemmas 3–5 and 7–9 in Sect. 5.

Let $p = a(m+1) + b$, $0 \le b < m+1$. We have

$$\begin{aligned}\psi^p\big((w_0; w_1, \dots, w_m)\big) &= (c^{a+1} w_{m-b+1} c^{-a-1}; c^{a+1} w_{m-b+2} c^{-a-1}, \dots, c^{a+1} w_m c^{-a-1},\\ &\qquad c^a w_0 c^{-a}, \dots, c^a w_{m-b} c^{-a}\big). \end{aligned} \tag{61}$$

Lemma 10. *It suffices to check* (60) *for p a divisor of $(m+1)h$. More precisely, let p be a divisor of $(m+1)h$, and let k be another positive integer with* $\gcd(k, (m+1)h/p) = 1$, *then we have*

$$\operatorname{Cat}^m(W; q)\Big|_{q=e^{2\pi i p/(m+1)h}} = \operatorname{Cat}^m(W; q)\Big|_{q=e^{2\pi i k p/(m+1)h}} \tag{62}$$

and

$$|\operatorname{Fix}_{NC^m(W)}(\psi^p)| = |\operatorname{Fix}_{NC^m(W)}(\psi^{kp})|. \tag{63}$$

Proof. For (63), this follows in the same way as (12) in Lemma 3.

For (62), we must argue differently than in Lemma 3. Let us write $\zeta = e^{2\pi i p/(m+1)h}$. For a given group W, we write $S_1(W)$ for the set of all indices i such that $\zeta^{d_i - h} = 1$, and we write $S_2(W)$ for the set of all indices i such that $\zeta^{d_i} = 1$. By the rule of de l'Hospital, we have

$$\operatorname{Cat}^m(W; q)\Big|_{q=e^{2\pi i p/(m+1)h}} = \begin{cases} 0 & \text{if } |S_1(W)| > |S_2(W)|, \\ \frac{\prod_{i \in S_1(W)}(mh + d_i)}{\prod_{i \in S_2(W)} d_i} \frac{\prod_{i \notin S_1(W)}(1 - \zeta^{d_i - h})}{\prod_{i \notin S_2(W)}(1 - \zeta^{d_i})}, & \text{if } |S_1(W)| = |S_2(W)|. \end{cases} \tag{64}$$

Since, by Theorem 3, $\operatorname{Cat}^m(W; q)$ is a polynomial in q, the case $|S_1(W)| < |S_2(W)|$ cannot occur.

We claim that, for the case where $|S_1(W)| = |S_2(W)|$, the factors in the quotient of products

$$\frac{\prod_{i \notin S_1(W)}(1 - \zeta^{d_i - h})}{\prod_{i \notin S_2(W)}(1 - \zeta^{d_i})}$$

cancel pairwise. If we assume the correctness of the claim, it is obvious that we get the same result if we replace ζ by ζ^k, where $\gcd(k, (m+1)h/p) = 1$, hence establishing (62).

In order to see that our claim is indeed valid, we proceed in a case-by-case fashion, making appeal to the classification of irreducible well-generated complex reflection groups, which we recalled in Sect. 2. First of all, since $d_n = h$, the set $S_1(W)$ is always non-empty as it contains the element n. Hence, if we want to have $|S_1(W)| = |S_2(W)|$, the set $S_2(W)$ must be non-empty as well. In other words, the integer $(m+1)h/p$ must divide at least one of the degrees $d_1, d_2, \dots, d_n$. In particular, this implies that, for each fixed reflection group W of exceptional type, only a finite number of values of $(m+1)h/p$ has to be checked. Writing M for $(m+1)h/p$, what needs to be checked is whether the *multi*sets (that is, multiplicities of elements must be taken into account)

$$\{(d_i - h) \bmod M : i \notin S_1(W)\} \quad \text{and} \quad \{d_i \bmod M : i \notin S_2(W)\}$$

are the same. Since, for a fixed irreducible well-generated complex reflection group, there is only a finite number of possibilities for M, this amounts to a routine verification. □

Lemma 11. *Let p be a divisor of $(m+1)h$. If p is divisible by $m+1$, then (60) is true.*

We leave the proof to the reader as it is completely analogous to the proof of Lemma 4.

Lemma 12. *Equation (60) holds for all divisors p of $m+1$.*

Proof. We have

$$\operatorname{Cat}^m(W;q)\big|_{q=e^{2\pi i p/(m+1)h}} = \begin{cases} 0 & \text{if } p < m+1, \\ m+1 & \text{if } p = m+1. \end{cases}$$

Here, the first case follows from (64) and the fact that we have $S_1(W) \supseteq \{n\}$ and $S_2(W) = \emptyset$ if $p \mid (m+1)$ and $p < m+1$.

On the other hand, if $(w_0; w_1, \dots, w_m)$ is fixed by ψ^p, then one can apply an argument similar to that in Lemma 5 with any w_i taking the role of w_1, $0 \le i \le m$. It follows that if $p = m+1$, the set $\operatorname{Fix}_{NC^m(W)}(\psi^p)$ consists of the $m+1$ elements $(w_0; w_1, \dots, w_m)$ obtained by choosing $w_i = c$ for a particular i between 0 and m, all other w_j's being equal to ε. If $p < m+1$, then there is no element in $\operatorname{Fix}_{NC^m(W)}(\psi^p)$. □

Lemma 13. *Let W be an irreducible well-generated complex reflection group of rank n, and let $p = m_1 h_1$ be a divisor of $(m+1)h$, where $m+1 = m_1 m_2$ and $h = h_1 h_2$. We assume that $\gcd(h_1, m_2) = 1$. Suppose that Theorem 4 has already been verified for all irreducible well-generated complex reflection groups with rank $< n$. If h_2 does not divide all degrees d_i, then Eq. (60) is satisfied.*

We leave the proof to the reader as it is completely analogous to the proof of Lemma 7.

Lemma 14. *Let W be an irreducible well-generated complex reflection group of rank n, and let $p = m_1h_1$ be a divisor of $(m+1)h$, where $m+1 = m_1m_2$ and $h = h_1h_2$. We assume that* $\gcd(h_1, m_2) = 1$. *If $m_2 > n$ then*

$$\mathrm{Fix}_{NC^m(W)}(\psi^p) = \emptyset.$$

We leave the proof to the reader as it is analogous to the proof of Lemma 8.

Remark 4. By applying the same reasoning as in Remark 3 with Lemmas 7 and 8 replaced by Lemmas 13 and 14, respectively, it follows that we only need to check (60) for pairs (m_2, h_2) satisfying (18) and $m_2 \le n$. This reduces the problem to a finite number of choices.

Lemma 15. *Let W be an irreducible well-generated complex reflection group of rank n with the property that $d_i \mid h$ for $i = 1, 2, \dots, n$. Then Theorem 4 is true for this group W.*

Proof. Proceeding in a fashion analogous to the beginning of the proof of Lemma 9, we may restrict to the case where $p \mid (m+1)h$ and $(m+1)h/p$ does not divide any of the d_i's. In this case, it follows from (64) and the fact that we have $S_1(W) \supseteq \{n\}$ and $S_2(W) = \emptyset$ that the right-hand side of (60) equals 0. Inspection of the classification of all irreducible well-generated complex reflection groups, which we recalled in Sect. 2, reveals that all groups satisfying the hypotheses of the lemma have rank $n \le 2$. Except for the groups contained in the infinite series $G(d, 1, n)$ and $G(e, e, n)$ for which Theorem 2 has been established in [19], these are the groups $G_5, G_6, G_9, G_{10}, G_{14}, G_{17}, G_{18}, G_{21}$. The verification of (60) can be done in a similar fashion as in the proof of Lemma 9. We illustrate this by going through the case of the group G_6. In analogy with the earlier situation, we note that Lemma 14 implies that Eq. (60) holds if $m_2 > 2$, so that in the following arguments we may assume that $m_2 = 2$.

CASE G_6. The degrees are 4, 12, and therefore, according to Remark 4, we need only consider the case where $h_2 = 4$ and $m_2 = 2$, that is, $p = 3(m+1)/2$. Then the action of ψ^p is given by

$$\psi^p\big((w_0; w_1, \dots, w_m)\big) = \big(c^2 w_{\frac{m+1}{2}} c^{-2}; c^2 w_{\frac{m+3}{2}} c^{-2}, \dots, c^2 w_m c^{-2}, c w_0 c^{-1}, \dots, c w_{\frac{m-1}{2}} c^{-1}\big). \qquad (65)$$

If $(w_0; w_1, \dots, w_m)$ is fixed by ψ^p, there must exist an i with $0 \le i \le \frac{m-1}{2}$ such that $\ell_T(w_i) = 1$, $w_i c w_i c^{-1} = c$, and all w_j, $j \ne i, \frac{m+1}{2} + i$, equal ε. However, with the help of CHEVIE, one verifies that there is no such solution to this equation. Hence, the left-hand side of (60) is equal to 0, as required.

This completes the proof of the lemma. □

9 Exemplification of Case-by-Case Verification of Theorem 4

It remains to verify Theorem 4 for the groups $G_4, G_8, G_{16}, G_{20}, G_{23} = H_3, G_{24}, G_{25}, G_{26}, G_{27}, G_{28} = F_4, G_{29}, G_{30} = H_4, G_{32}, G_{33}, G_{34}, G_{35} = E_6, G_{36} = E_7, G_{37} = E_8$. All details can be found in [21, Sect. 9]. We content ourselves with discussing the case of the group G_{24}, as this suffices to convey the flavour of the necessary computations.

In order to simplify our considerations, it should be observed that the action of ψ (given in (59)) is exactly the same as the action of ϕ (given in (3)) with m replaced by $m+1$ *on the components* $w_1, w_2, \dots, w_{m+1}$, that is, if we disregard the 0-th component of the elements of the generalised non-crossing partitions involved. The only difference which arises is that, while the $(m+1)$-tuples $(w_0; w_1, \dots, w_m)$ in (59) must satisfy $w_0 w_1 \cdots w_m = c$, for $w_1, w_2, \dots, w_{m+1}$ in (3) we only must have $w_1 w_2 \cdots w_{m+1} \le_T c$. Consequently, we may use the counting results from Sect. 6, except that we have to restrict our attention to those elements $(w_0; w_1, \dots, w_m, w_{m+1}) \in NC^{m+1}(W)$ for which $w_1 w_2 \cdots w_{m+1} = c$, or, equivalently, $w_0 = \varepsilon$.

9.1 Case G_{24}

The degrees are $4, 6, 14$, and hence we have

$$\mathrm{Cat}^m(G_{24}; q) = \frac{[14m+14]_q\,[14m+6]_q\,[14m+4]_q}{[14]_q\,[6]_q\,[4]_q}.$$

Let ζ be a $14(m+1)$-th root of unity. The following cases on the right-hand side of (60) occur:

$$\lim_{q\to\zeta} \mathrm{Cat}^m(G_{24}; q) = m+1, \quad \text{if } \zeta = \zeta_{14}, \zeta_7, \tag{66}$$

$$\lim_{q\to\zeta} \mathrm{Cat}^m(G_{24}; q) = \tfrac{7m+7}{3}, \quad \text{if } \zeta = \zeta_6, \zeta_3,\ 3 \mid (m+1), \tag{67}$$

$$\lim_{q\to\zeta} \mathrm{Cat}^m(G_{24}; q) = \mathrm{Cat}^m(G_{24}), \quad \text{if } \zeta = -1 \text{ or } \zeta = 1, \tag{68}$$

$$\lim_{q\to\zeta} \mathrm{Cat}^m(G_{24}; q) = 0, \quad \text{otherwise.} \tag{69}$$

We must now prove that the left-hand side of (60) in each case agrees with the values exhibited in (66)–(69). The only cases not covered by Lemma 11 are the ones in (67) and (69). On the other hand, the only cases left to consider according to Remark 4 are the cases where $h_2 = 1$ and $m_2 = 3$, $h_2 = 2$ and $m_2 = 3$, and $h_2 = m_2 = 2$. These correspond to the choices $p = 14(m+1)/3$,

$p = 7(m+1)/3$, respectively $p = 7(m+1)/2$. The first two cases belong to (67), while $p = 7(m+1)/2$ belongs to (69).

In the case that $p = 7(m+1)/3$, the action of ψ^p is given by

$$\psi^p\big((w_0; w_1, \dots, w_m)\big)$$
$$= (c^3 w_{\frac{2m+2}{3}} c^{-3}; c^3 w_{\frac{2m+5}{3}} c^{-3}, \dots, c^3 w_m c^{-3}, c^2 w_0 c^{-2}, \dots, c^2 w_{\frac{2m-1}{3}} c^{-2}\big).$$

Hence, for an i with $0 \le i \le \frac{m-2}{3}$, we must find an element $w_i = t_1$, where t_1 satisfies (32), so that we can set $w_{i+\frac{m+1}{3}} = c^2 t_1 c^{-2}$, $w_{i+\frac{2m+2}{3}} = c^4 t_1 c^{-4}$, and all other w_j's equal to ε. We have found seven solutions to the counting problem (32), and each of them gives rise to $(m+1)/3$ elements in $\mathrm{Fix}_{NC^m(G_{24})}(\psi^p)$ since the index i ranges from 0 to $(m-2)/3$.

On the other hand, if $p = 14(m+1)/3$, then the action of ψ^p is given by

$$\psi^p\big((w_0; w_1, \dots, w_m)\big)$$
$$= (c^5 w_{\frac{m+1}{3}} c^{-5}; c^5 w_{\frac{m+4}{3}} c^{-5}, \dots, c^5 w_m c^{-5}, c^4 w_0 c^{-4}, \dots, c^4 w_{\frac{m-2}{3}} c^{-4}\big).$$

By Lemma 6, every element of $NC(W)$ is fixed under conjugation by c^7, and, thus, the equations for t_1 in this case are the same as in the previous one where $p = 7(m+1)/3$.

Hence, in either case, we obtain $7\frac{m+1}{3} = \frac{7m+7}{3}$ elements in $\mathrm{Fix}_{NC^m(G_{24})}(\psi^p)$, which agrees with the limit in (67).

If $p = 7(m+1)/2$, the relevant counting problem is (33). However, no element $(w_0; w_1, \dots, w_m) \in \mathrm{Fix}_{NC^m(G_{24})}(\psi^p)$ can be produced in this way since the counting problem imposes the restriction that $\ell_T(w_0) + \ell_T(w_1) + \dots + \ell_T(w_m)$ be even, which contradicts the fact that $\ell_T(c) = n = 3$. This is in agreement with the limit in (69).

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Set Partitions with No m-Nesting

Marni Mishna and Lily Yen

Abstract A partition of $\{1, \dots, n\}$ has an m-nesting if it contains at least m disjoint blocks, and a subset of $2m$ points $i_1 < i_2 < \cdots < i_m < j_m < j_{m-1} < \cdots < j_1$, such that i_l and j_l are in the same block for all $1 \leq l \leq m$, but no other pairs are in the same block. In this note, we use generating trees to construct the class of partitions with no m-nesting, determine functional equations satisfied by the associated generating functions, and generate enumerative data for $m \geq 4$.

Keywords Set partition • Nesting • Pattern avoidance • Generating tree • Algebraic kernel method • Coefficient extraction • Enumeration

1 Introduction

Graphic representations of set partitions can contain various patterns and shapes. One particular pattern, known as an m-nesting, resembles a rainbow, for example. In this work we address the enumeration of set partitions that avoid m-nestings. These results are in the context of recent studies of other combinatorial objects that avoid similar or related patterns. We are particularly motivated by the study of protein folding [7] where such patterns arise in the molecular bonds and their presence has strong consequences on the geometry of the protein.

Our strategy parallels a recent generating tree approach used by Bousquet-Mélou to enumerate a family of pattern avoiding permutation classes [3]. A novel feature

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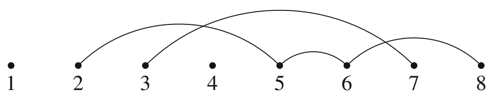
of this approach is that the length of the label in the generating tree is related to the length of the pattern avoided. Thus, the resulting expressions for generating functions are generic, and expressed in terms of m. The generating tree permits direct access to new enumerative data for set partitions avoiding m-nestings for some $m > 4$, and we present the equations as a starting point for further analysis.

1.1 Notation and Definitions

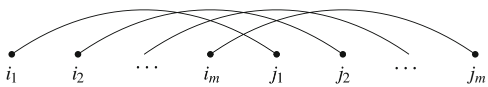
A set partition π of $[n] := \{1, 2, 3, \ldots, n\}$, denoted by $\pi \in \Pi_n$, is a collection of nonempty and mutually disjoint subsets of $[n]$, called *blocks*, whose union is $[n]$. The number of set partitions of $[n]$ into k blocks is denoted $S(n, k)$, and is known as a Stirling number of the second kind. The total number of partitions of $[n]$ is the *Bell* number $B_n = \sum_k S(n, k)$. We represent π by a graph on the vertex set $[n]$ whose edge set consists of arcs connecting elements of each block in numerical order. Such an edge set is called the *standard representation* of the partition π, as seen in [6]. For example, the standard representation of

$$1|2\,5\,6\,8|3\,7|4$$

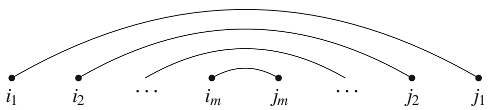
is given by the following graph with edge set $\{(2, 5), (5, 6), (6, 8), (3, 7)\}$:



With this representation, we can define two classes of patterns: crossings and nestings. An *m-crossing* of π is a collection of m edges $(i_1, j_1), (i_2, j_2), \ldots, (i_m, j_m)$ such that $i_1 < i_2 < \cdots < i_m < j_1 < j_2 < \cdots < j_m$. Using the standard representation, an m-crossing is drawn as follows:



Similarly, we define an *m-nesting* of π to be a collection of m edges (i_1, j_1), $(i_2, j_2), \ldots, (i_m, j_m)$ such that $i_1 < i_2 < \cdots < i_m < j_m < j_{m-1} < \cdots < j_1$. This is drawn:



A partition is m-noncrossing if it contains no m-crossing, and it is said to be m-nonnesting if it contains no m-nesting.

1.2 Context and Plan

Chen, Deng, Du, Stanley and Yan in [6], and independently Krattenthaler in [8], gave a non-trivial bijective proof that m-noncrossing partitions of $[n]$ are equinumerous with m-nonnesting partitions of $[n]$, for all values of m and n. A straightforward bijection with Dyck paths illustrates that 2-noncrossing partitions (or simply, noncrossing partitions) are counted by Catalan numbers. Bousquet-Mélou and Xin in [4] showed that the sequence counting 3-noncrossing partitions is P-recursive, that is, satisfies a linear recurrence relation with polynomial coefficients. Indeed, they determined an explicit recursion, complete with solution and asymptotic analysis. They further conjectured that m-noncrossing partitions are not P-recursive for all $m \geq 4$. Certainly, the limit as m goes to infinity is not D-finite, since Bell numbers are well known not to be P-recursive because of the composed exponentials in the generating function $B(x) = e^{e^x-1}$ (see Example 19 of [2]). If it turns out that m-noncrossing partitions do have a D-finite generating function, then we have a very interesting refinement of a non-D-finite class.

Since m-noncrossing partitions of $[n]$ and m-nonnesting partitions of $[n]$ are equinumerous, we study m-nonnesting partitions in this paper and show how to generate the class using generating trees, and how to determine a recursion satisfied by the counting sequence for m-nonnesting partitions.

Our approach is an adaptation of Bousquet-Mélou's recent work on the enumeration of permutations with no long monotone subsequence in [3]. She combined the ideas of recursive construction for permutations via generating trees and the algebraic kernel method to determine and solve functional equations with multiple catalytic variables.

In Sect. 2, we employ Bousquet-Mélou's generating tree construction to find functional equations satisfied by the generating functions for set partitions with no m-nesting. The resulting equations, though similar to the equations arising in [3], have a key structural difference which resists a similar treatment of the algebraic kernel method followed by a constant term extraction as used by Bousquet-Mélou in [3]. However, the process does yield the result for nonnesting set partitions counted by the Catalan numbers. We refer interested readers to [9] for the processing of functional equations in the spirit of [3].

Using our constructions we generate new enumerative data for $m > 4$, discuss the limiting factors in data generation, and assess the current state of recurrences and explicit forms.

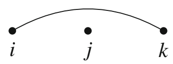
2 Generating Trees and Functional Equations

The generating tree construction for the class of m-nonnesting partitions is based on a standard generating tree description of partitions, and the constraint is incorporated using a vector labelling system. The generating tree construction has an immediate translation to a functional equation with m-variate series.

2.1 A Generating Tree for Set Partitions

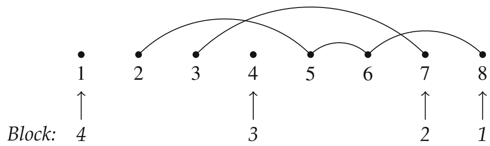
Let π be a set partition. Define $\mathrm{ne}(\pi)$ to be the maximal i such that π has an i-nesting, also called the *maximal nesting number* of π, and let $\Pi_n^{(m)}$ be the set of partitions of $[n]$ for $n \geq 0$ (where $n = 0$ means the empty partition) with $\mathrm{ne}(\pi) \leq m$, thus $(m+1)$-nonnesting. We define the union $\Pi^{(m)} = \cup_n \Pi_n^{(m)}$.

Note that an arc over a fixed point is not a 2-nesting, but a 1-nesting:



We next describe how to generate all set partitions via generating trees in the fashion of [2]. First, order the blocks of a given partition, π, by the maximal element of each block in descending order.

Example 1. The first block of 1|2 5 6 8|3 7|4 is 2 5 6 8; the second block is 3 7; the third block is singleton 4; and 1 is the last block. Using the standard representation,



we number the blocks in descending order (from the right to the left) according to the maximal element in each block (that is, the rightmost vertex of each block).

With the order of blocks thus defined, we warm up by generating all set partitions without nesting restriction first. Figure 1 contains the generating tree for all set partitions, in addition to the generating tree for the number of children of each node from the tree of set partitions to indicate how enumeration can be facilitated.

1. Begin with Ø as the top node of the tree. It has only one child, so the corresponding node in the tree for the number of children is labelled 1.
2. To produce the $n+1$st level of nodes, take each set partition at the nth level, and either add $n+1$ as a singleton, or join $n+1$ to block j for each $1 \leq j \leq k$ if the set partition has k blocks.

Summarizing the description above in the notation of [2], we recall that the rewriting rule of a generating tree is denoted by:

$$[(s_0), \{(k) \to (e_{1,k})(e_{2,k}) \dots (e_{k,k})\}],$$

where s_0 denotes the degree of the root, and for any node labelled k, that is, with k descendants, the label of each descendent is given by $(e_{j,k})$ for $1 \leq j \leq k$. Thus,

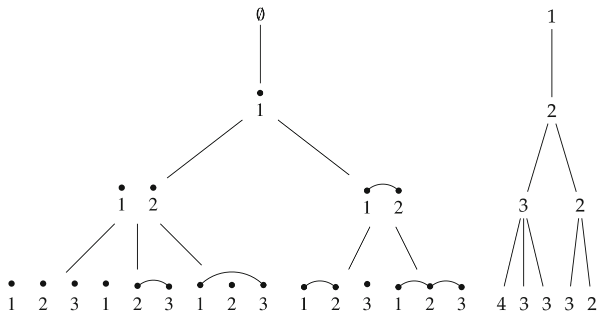


Fig. 1 Generating tree for set partitions and its corresponding generating tree of the number of children

the class of set partitions has a generating tree of labels given by $[(1) : (k) \to (k+1)(k)^{k-1}]$.

2.2 A Vector Label to Track Nestings

The generating tree of set partitions generates all set partitions π graded by n, the size of π, but it does not keep track of nesting numbers. Also note that the number of children of π is one more than the number of blocks of π. Let us now address nestings.

Fix m. In order to keep track of nesting numbers, we need to define the *label* of $\pi \in \Pi^{(m)}$. To identify the position of a nesting, we consider the relative position of the smallest vertex incident to the nesting. Thus, the *rightmost* j-nesting is the set of j edges forming a j-nesting pattern such that its minimal incident vertex is greater than, or equal to the minimal vertex incident to all the other j-nestings. If one vertex is common to two j-nestings, we consider the second smallest incident vertex, and so on. Roughly, our labels keep track of the number of blocks to the right of a j-nesting that might potentially become a j-nesting based on how the next edge is added. Any edge added that affect nestings to the *left* of the right most j-nesting, will necessarily create a $j+1$ nesting because it will create an arc overtop of the rightmost j-nesting.

Definition 1. Define the label of a partition, $L(\pi) = (a_1(\pi), a_2(\pi), \ldots, a_m(\pi))$, or in short, $L(\pi) = (a_1, a_2, \ldots, a_m)$ as follows. For $1 \le j \le m$,

$$a_j(\pi) = \begin{cases} 1+ \text{ number of blocks in } \pi, & \text{if } \pi \text{ is } j\text{-nonnesting,} \\ \begin{array}{l} 1+ \text{ number of blocks ending to the right of} \\ \text{the smallest vertex in the rightmost } j\text{-nesting} \end{array} & \text{otherwise.} \end{cases}$$

Example 2. To continue the example, let $\pi = 1|2\,5\,6\,8|3\,7|4$ and suppose $m = 3$. Then $L(1|2\,5\,6\,8|3\,7|4) = (3, 4, 5)$ for the following reasons. The rightmost

1-nesting is the edge with largest vertex endpoint: $(6,8)$. Hence, $a_1(\pi) = 3$ because blocks 1 and 2 end to the right of vertex 6. The rightmost 2-nesting is the set of edges $\{(5,6),(3,7)\}$ hence $a_2(\pi) = 4$ because 3 blocks end to the right of vertex 3. Finally, $a_3(\pi) = 5$ because the diagram has no 3-nesting, and is comprised of 4 blocks. Note that in this convention, the empty set partition has label $(1,1,\ldots,1)$, since it has no nestings and no blocks.

A set partition in $\Pi^{(m)}$ always has a_m children. This is one more than the number of blocks, if there is no m-nesting (and hence there is no risk that adding an edge will create an $m+1$-nesting). Otherwise, it indicates more than the number of blocks to which you can add an edge without creating an $m+1$-nesting. The label of a set partition is sufficient to derive the label of each of its children, and this process is described in the next proposition. Also, remark that the label is a non-decreasing sequence, since the rightmost j-nesting either contains the rightmost $j-1$ nesting or is to the left of it.

Proposition 1 (Labels of children). *Let π be in $\Pi_n^{(m)}$, the set of set partitions on $[n]$ avoiding $m+1$-nestings, and suppose the label of π is $L(\pi) = (a_1, a_2, \ldots, a_m)$. Then, the labels of the a_m set partitions of $\Pi_{n+1}^{(m)}$ obtained by recursive construction via the generating tree are*

$$(a_1+1, a_2+1, \ldots, a_m+1) \qquad \text{(Add } n+1 \text{ as a singleton to } \pi\text{)}$$

and

$$\begin{array}{lr}
(2, a_2, a_3, \ldots, a_{m-1}, a_m) & \text{(Add } n+1 \text{ to block 1)} \\
(3, a_2, a_3, \ldots, a_{m-1}, a_m) & \text{(Add } n+1 \text{ to block 2)} \\
 & \vdots \\
(a_1, a_2, a_3, \ldots, a_{m-1}, a_m) & \text{(Add } n+1 \text{ to block } a_1-1) \\
(a_1+1, a_1+1, a_3, \ldots, a_{m-1}, a_m) & \text{(Add } n+1 \text{ to block } a_1) \\
(a_1+1, a_1+2, a_3, \ldots, a_{m-1}, a_m) & \text{(Add } n+1 \text{ to block } a_1+1) \\
 & \vdots \\
(a_1+1, a_2+1, a_2+1, \ldots, a_{m-1}, a_m) & \text{(Add } n+1 \text{ to block } a_2) \\
 & \vdots \\
(a_1+1, a_2+1, a_3+1, \ldots, a_{m-1}+1, a_{m-1}+1) & \text{(Add } n+1 \text{ to block } a_{m-1}) \\
 & \vdots \\
(a_1+1, a_2+1, a_3+1, \ldots, a_{m-1}+1, a_m) & \text{(Add } n+1 \text{ to block } a_m-1)
\end{array}$$

Proof. By careful inspection. □

Example 3. Consider the following partition from $\Pi_8^{(3)}$. The reader can refer to its arc diagram in Example 1 which shows that it is 3-nonnesting, thus also

4-nonnesting. The partition 1|2 5 6 8|3 7|4 with label $(3, 4, 5)$ has five children and their respective labels are:

π	$L(\pi)$
1|2 5 6 8|3 7|4|9	$(4, 5, 6)$
1|2 5 6 8 9|3 7|4	$(2, 4, 5)$
1|2 5 6 8|3 7 9|4	$(3, 4, 5)$
1|2 5 6 8|3 7|4 9	$(4, 4, 5)$
1 9|2 5 6 8|3 7|4	$(4, 5, 5)$

Example 4. As we mentioned before, 2-nonnesting set partitions are counted by Catalan numbers. The generating tree construction given in Proposition 1 restricted to this case is given by

$$[(1) : (k) \to (k+1)(2)(3)\dots(k)],$$

which is the same construction for Catalan numbers given in [2]. The generating tree for 3-noncrossing partitions is given by

$$[(1,1) : (i,j) \to (i+1,j+1)(2,j)(3,j)\cdots(i,j)(i+1,i+1)(i+1,i+2)\dots(i+1,j)].$$

2.3 A Functional Equation for the Generating Function

The simple structure of the labels in Proposition 1 permits a direct translation from the generating tree to a functional equation.

Let us define $\tilde{F}(u_1, u_2, \dots, u_m; t)$ to be the ordinary generating function of partitions in $\Pi^{(m)}$ counted by the statistics a_1, a_2, …, a_m and by size,

$$\begin{aligned} \tilde{F}(u_1, u_2, \dots, u_m; t) &:= \sum_{\pi \in \Pi^{(m)}} u_1^{a_1(\pi)} u_2^{a_2(\pi)} \dots u_m^{a_m(\pi)} t^{|\pi|} \\ &= \sum_{a_1, a_2, \dots, a_m} \tilde{F}_{\mathbf{a}}(t) u_1^{a_1} u_2^{a_2} \dots u_m^{a_m}, \end{aligned}$$

where $\tilde{F}_{\mathbf{a}}(t)$ is the size generating function for the set partitions of $\Pi^{(m)}$ with the label $\mathbf{a} = (a_1, a_2, \dots, a_m)$. For example, when $m = 2$,

$$\tilde{F}(\mathbf{u}; t) = u_1 u_2 + {u_1}^2 {u_2}^2 t + \left({u_1}^3 {u_2}^3 + {u_1}^2 {u_2}^2\right) t^2 + \left({u_1}^4 {u_2}^4 + 2\,{u_1}^3 {u_2}^3 + {u_1}^2 {u_2}^2 + {u_1}^2 {u_2}^3\right) t^3 + \dots.$$

Proposition 1 implies

$$\tilde{F}(u_1,\ldots,u_m;t) = u_1u_2\ldots u_m + tu_1u_2\ldots u_m\tilde{F}(u_1,u_2,\ldots,u_m;t)$$
$$+\,t\sum_{a_1,a_2,\ldots,a_m}\tilde{F}_{\mathbf{a}}(t)u_2^{a_2}u_3^{a_3}\ldots u_m^{a_m}\sum_{\alpha=2}^{a_1}u_1^{\alpha}$$
$$+\,t\sum_{a_1,a_2,\ldots,a_m}\tilde{F}_{\mathbf{a}}(t)\sum_{j=2}^{m}\sum_{\alpha=a_{j-1}+1}^{a_j}u_1^{a_1+1}u_2^{a_2+1}\ldots u_{j-1}^{a_{j-1}+1}u_j^{\alpha}u_{j+1}^{a_{j+1}}\ldots u_m^{a_m}.$$

We can simplify the expression using the finite geometric series sum formula to rewrite this as the following expression.

Proposition 2. *The ordinary generating function of partitions in $\Pi^{(m)}$ counted by the statistics a_1, a_2, …, a_m and by size, denoted $\tilde{F}(u_1,u_2,\ldots,u_m;t)$, or simply $\tilde{F}(\mathbf{u};t)$ satisfies the following functional equation:*

$$\tilde{F}(\mathbf{u};t) = u_1\ldots u_m + tu_1u_2\ldots u_m\tilde{F}(\mathbf{u};t) + tu_1\left(\frac{\tilde{F}(\mathbf{u};t)-u_1\tilde{F}(1,u_2,\ldots,u_m;t)}{u_1-1}\right)$$
$$+\,t\sum_{j=2}^{m}u_1u_2\ldots u_j\left(\frac{\tilde{F}(\mathbf{u};t)-\tilde{F}(u_1,\ldots,u_{j-2},u_{j-1}u_j,1,u_{j+1},\ldots,u_m;t)}{u_j-1}\right). \tag{1}$$

3 Computing Series Expansions

Notice that in Eq. (1), if one has a series expansion of $\bar{F}(\mathbf{u};t)$ correct up to t^k, then substituting this series into RHS of Eq. (1) yields the series expansion of $\bar{F}$ correct to t^{k+1} because the RHS of Eq. (1) contains a term free of t; otherwise, the degree of t is increased by 1. We have iterated Eq. (1) to get enumerative data for up to $m = 9$.

For 3-nonnesting set partitions, an average laptop running Maple 15 can produce 70 terms in a reasonable time (less than 24 h). For $m = 4$, only 38 terms; $m = 5$, 27 terms; $m = 6$, 20 terms; $m = 7$, 16 terms, $m = 8$, 12 terms; and finally $m = 9$, 12 terms. The limitation seems memory space due to the growing complication in the functional equation when m gets larger (Table 1).

4 Conclusion

The generating tree approach permits a direct translation to a functional equation involving an arbitrary number of catalytic variables satisfied by set partitions avoiding $m+1$-nestings for any positive integer m. We avoid passing through

Table 1 Numbers of set partitions of n avoiding an $m + 1$-nesting. The OEIS numbers refer to entries in the Online Encyclopedia of Integer Sequences [1]. The entries in light grey emphasize that the restriction has no effect on set partitions of that size

		n														
m	OEIS #	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	A000108	1	2	5	14	42	132	429	1,430	4,862	16,796	58,786	208,012	742,900	2,674,440	9,694,845
2	A108304	1	2	5	15	52	202	859	3,930	19,095	97,566	520,257	2,877,834	16,434,105	96,505,490	580,864,901
3	A108305	1	2	5	15	52	203	877	4,139	21,119	115,495	671,969	4,132,936	26,723,063	180,775,027	1,274,056,792
4	A192126	1	2	5	15	52	203	877	4,140	21,147	115,974	678,530	4,212,654	27,627,153	190,624,976	1,378,972,826
5	A192127	1	2	5	15	52	203	877	4,140	21,147	115,975	678,570	4,213,596	27,644,383	190,897,649	1,382,919,174
6	A192128	1	2	5	15	52	203	877	4,140	21,147	115,975	678,570	4,213,597	27,644,437	190,899,321	1,382,958,475

vacillating lattice walks or tableaux. The functional equation can be iterated to generate series data for $m + 1$-nonnesting set partitions, but ideally we would like to solve the equations, or find some other format from which more information can be obtained. For example, perhaps under further scrutiny one can decide if the generating functions are D-finite or not.

One possible route to a proof of non-D-finiteness is to use our expressions to determine bounds on the order and the coefficient degrees of the minimal differential equation satisfied by the generating function. Though a tantalizingly simple idea, the limitation is the lack of series data for large m.

The generating tree studied is for $m + 1$-nonnesting set partitions. The authors have tried to study a generating tree for $m + 1$-noncrossing set partitions in the hope of reproving the result of Chen et al. in [6] by tree isomorphism. However, the authors were unable to generate $m + 1$-noncrossing set partitions.

Finally, our generating tree approach is limited only to the non-enhanced case. For a more general treatment of the subject involving enhanced set partitions and permutations, both enhanced and non-enhanced, we refer the reader to [5] by Burrill, Elizalde, Mishna, and Yen.

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The Distribution of Zeros of the Derivative of a Random Polynomial

Robin Pemantle and Igor Rivin

Abstract In this note we initiate the probabilistic study of the critical points of polynomials of large degree with a given distribution of roots. Namely, let f be a polynomial of degree n whose zeros are chosen IID from a probability measure μ on $\mathbb{C}$. We conjecture that the zero set of f' always converges in distribution to μ as $n \to \infty$. We prove this for measures with finite one-dimensional energy. When μ is uniform on the unit circle this condition fails. In this special case the zero set of f' converges in distribution to that of the IID Gaussian random power series, a well known determinantal point process.

Keywords Gauss-Lucas theorem • Gaussian series • Critical points • Random polynomials

1 Introduction

Since Gauss, there has been considerable interest in the location of the *critical points* (zeros of the derivative) of polynomials whose zeros were known – Gauss noted that these critical points were points of equilibrium of the electrical field whose charges were placed at the zeros of the polynomial, and this immediately leads to the proof of the well-known Gauss-Lucas Theorem, which states that the critical points of a polynomial f lie in the convex hull of the zeros of f (see, e.g. [18, Theorem 6.1]).

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There are too many refinements of this result to state. A partial list (of which several have precisely the same title!) is as follows: [1, 3, 5–9, 12, 14, 16, 17, 19, 20, 22–26]). Among these, we mention two extensions that are easy to state.

- Jensen's theorem: if $p(z)$ has real coefficients, then the non-real critical points of p lie in the union of the "Jensen Disks", where a Jensen disk J is a disk one of whose diameters is the segment joining a pair of conjugate (non-real) roots of p.
- Marden's theorem: Suppose the zeroes z_1, z_2, and z_3 of a third-degree polynomial $p(z)$ are non-collinear. There is a unique ellipse inscribed in the triangle with vertices z_1, z_2, z_3 and tangent to the sides at their midpoints: the Steiner inellipse. The foci of that ellipse are the zeroes of the derivative $p'(z)$.

There has not been any *probabilistic* study of critical points (despite the obvious statistical physics connection) from this viewpoint. There has been a very extensive study of random polynomials (some of it quoted further down in this paper), but generally this has meant some distribution on the coefficients of the polynomial, and not its roots [4]. Let us now define our problem:

Let μ be a probability measure on the complex numbers. Let $\{X_n : n \geq 0\}$ be random variables on a probability space $(\Omega, \mathcal{F}, \mathbb{P})$ that are IID with common distribution μ. Let

$$f_n(z) := \prod_{j=1}^{n} (z - X_j)$$

be the random polynomial whose roots are $X_1, \ldots, X_n$. For any polynomial f we let $\mathcal{Z}(f)$ denote the empirical distribution of the roots of f, for example, $\mathcal{Z}(f_n) = \frac{1}{n} \sum_{j=1}^{n} \delta_{X_j}$.

The question we address in this paper is:

Question 1.1. When are the zeros of f_n' stochastically similar to the zeros of f_n?

Some examples show why we expect this.

Example 1.1. Suppose μ concentrates on real numbers. Then f_n has all real zeros and the zeros of f_n' interlace the zeros of f_n. It is immediate from this that the empirical distribution of the zeros of f_n' converges to μ as $n \to \infty$. The same is true when μ is concentrated on any affine line in the complex plane: interlacing holds and implies convergence of the zeros of f_n' to μ.[1] Once the support of μ is not contained in an affine subspace, however, the best we can say geometrically about the roots of f_n' is that they are contained in the convex hull of the roots of f_n; this is the Gauss-Lucas Theorem.

[1] Even in this case there are interesting probabilistic questions concerning the distribution of critical points of f_n close to the edge of the support of μ, see [15]

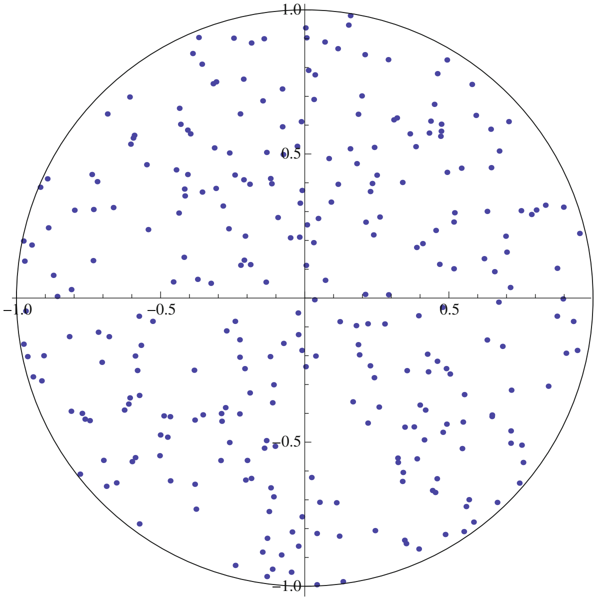

Fig. 1 Critical points of a polynomial whose roots are uniformly sampled inside the unit disk

Example 1.2. Suppose the measure μ is atomic. If $\mu(a) = p > 0$ then the multiplicity of a as a zero of f_n is $n(p + o(1))$. The mulitplicity of a as a zero of f_n' is one less than the multplicity as a zero of f_n, hence also $n(p + o(1))$. This is true for each of the countably many atoms, whence it follows again that the empirical distribution of the zeros of f_n' converges to μ.

Atomic measures are weakly dense in the space of all measures. Sufficient continuity of the roots of f' with respect to the roots of f would therefore imply that the zeros of f_n' always converge in distribution to μ as $n \to \infty$. In fact we conjecture this to be true.

Example 1.3. Our first experimental example has the roots of f uniformly distributed in the unit disk. In the figure, we sample 300 points from the uniform distribution in the disk, and plot the critical points (see Fig. 1). The reader may or may not be convinced that the critical points are uniformly distributed.

Example 1.4. Our second example takes polynomials with roots uniformly distributed on the unit *circle*, and computes the critical points. In Fig. 2 we do this with a sample of size 300. One sees that the convergence is rather quick.

Remark 1. The figures were produced with Mathematica. However, the reader wishing to try this at home should increase precision because Mathematica (and Maple, Matlab and R) do not use the best method of computing zeros of polynomials.

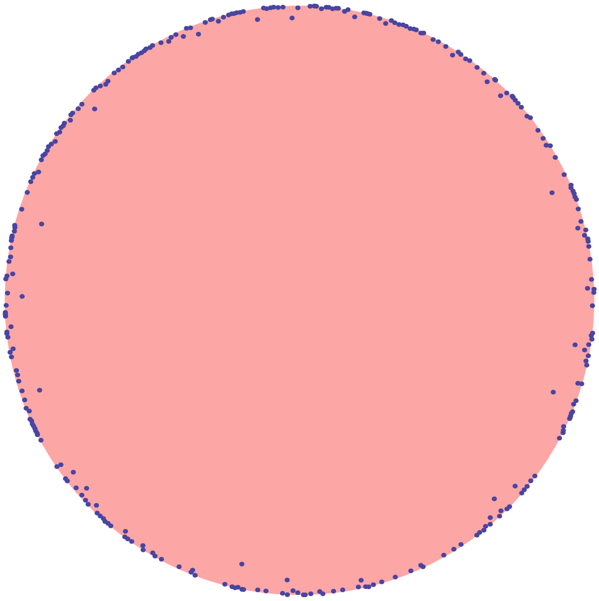

Fig. 2 Critical points of polynomial whose roots are uniformly sampled on the unit circle

Conjecture 1. For any μ, as $n \to \infty$, $\mathcal{Z}(f')$ converges weakly to μ.

There may indeed be such a continuity argument, though the following counterexample shows that one would at least need to rule out some exceptional sets of low probability. Suppose that $f(z) = z^n - 1$. As $n \to \infty$, the distribution of the roots of f converge weakly to the uniform distribution on the unit circle. The roots of f_n' however are all concentrated at the origin. If one moves one of the n roots of f_n along the unit circle, until it meets the next root, a distance of order $1/n$, then one root of f_n' zooms from the origin out to the unit circle. This shows that small perturbations in the roots of f can lead to large perturbations in the roots of f'. It seems possible, though, that this is only true for a "small" set of "bad" functions f.

1.1 A Little History

This circle of questions was first raised in discussions between one of us (IR) and the late Oded Schramm, when IR was visiting at Microsoft Research for the auspicious week of 9/11/2001. Schramm and IR had some ideas on how to approach the questions, but were somewhat stuck. There was always an intent to return to these questions, but Schramm's passing in September 2008 threw the plans into chaos. We (RP and IR) hope we can do justice to Oded's memory.

These questions are reminscent of questions of the kind often raised by Herb Wilf, that sound simple but are not. This work was first presented at a conference in Herb's honor and we hope it serves as a fitting tribute to Herb as well.

2 Results and Notations

Our goal in this paper is to prove cases of Conjecture 1.

Definition 2. We definite the p-energy of μ to be

$$\mathcal{E}_p(\mu) := \left(\int \int \frac{1}{|z-w|^p} \, d\mu(z) \, d\mu(w) \right)^{1/p} .$$

Since in the sequel we will only be using the 1-energy, we will write $\mathcal{E}$ for $\mathcal{E}_1$.

By Fubini's Theorem, when μ has finite 1-energy, the function V_μ defined by

$$V_\mu(z) := \int \frac{1}{z-w} \, d\mu(w)$$

is well defined and in $L^1(\mu)$.

Remark 2. The potential function V_μ is sometimes called the *Cauchy transform* of the measure μ. Commonly it is implied that μ is supported on $\mathbb{R}$ or on the boundary of a region over which z varies, but this need not be the case and is not the case for us (except in Theorem 2).

Theorem 1. *Suppose μ has finite 1-energy and that*

$$\mu \left\{ z : V_\mu(z) = 0 \right\} = 0 . \tag{1}$$

Then $\mathcal{Z}(f_n')$ converges in distribution to μ as $n \to \infty$.

A natural set of examples of μ with finite 1-energy is provided by the following observation:

Observation 1. *Suppose $\Omega \subset \mathbb{C}$ has Hausdorff dimension greater than one, and μ is in the measure class of the Hausdorff measure on Ω. Then μ has finite* 1*-energy.*

Proof. This is essentially the content of [11][Theorem 4.13(b)]. □

In particular, if μ is uniform in an open subset (with compact closure) of $\mathbb{C}$, its 1-energy is finite.

A natural special case to which Theorem 1 does not apply is when μ is uniform on the unit circle; here the 1-energy is just barely infinite.

Theorem 2. *If μ is uniform on the unit circle then $\mathcal{Z}(f_n)$ converges to the unit circle in probability.*

This result is somewhat weak because we do not prove $\mathcal{Z}(f_n)$ has a limit in distribution, only that all subsequential limits are supported on the unit circle. By the Gauss-Lucas Theorem, all roots of f_n have modulus less than 1, so the convergence to μ is from the inside. Weak convergence to μ implies that only $o(n)$ points can be at distance $\Theta(1)$ inside the cirle; the number of such points turns out to be $\Theta(1)$. Indeed quite a bit can be said about the small outliers. For $0 < \rho < 1$, define $B_\rho := \{z : |z| \le \rho\}$. The following result, which implies Theorem 2, is based on a very pretty result of Peres and Virag [21, Theorems 1 and 2] which we will quote in due course.

Theorem 3. *For any $\rho \in (0,1)$, as $n \to \infty$, the set $\mathcal{Z}(g_n) \cap B_\rho$ of zeros of g_n on B_ρ converges in distribution to a determinantal point process on B_ρ with the so-called Bergmann kernel $\pi^{-1}(1 - z_i \overline{z_j})^2$. The number $N(\rho)$ of zeros is distributed as the sum of independent Bernoullis with means ρ^{2k}, $1 \le k < \infty$.*

2.1 Distance Functions on the Space of Probability Measures

If μ and ν are probability measures on a separable metric space S, then the **Prohorov**[2] distance $|\mu - \nu|_P$ is defined to be the least ϵ such that for every set A, $\mu(A) \le \nu(A^\epsilon) + \epsilon$ and $\nu(A) \le \mu(A^\epsilon) + \epsilon$. Here, A^ϵ is the set of all points within distance ϵ of some point of A. The Prohorov metric metrizes convergence in distribution. We view collections of points in $\mathbb{C}$ (e.g., the zeros of f_n) as probability measures on $\mathbb{C}$, therefore the Prohorov metric serves to metrize convergence of zero sets. The space of probability measures on S, denoted $\mathcal{P}(S)$, is itself a separable metric space, therefore one can define the Prohorov metric on $\mathcal{P}(S)$, and this metrizes convergence of laws of random zero sets.

The Ky Fan metric on random variables on a fixed probability space will be of some use as well. Defined by $K(X,Y) = \inf\{\epsilon : \mathbb{P}(d(X,Y) > \epsilon) < \epsilon\}$, this metrizes convergence in probability. The two metrics are related (this is Strassen's Theorem):

$$|\mu - \nu|_P = \inf\{K(X,Y) : X \sim \mu,\ Y \sim \nu\}\,. \tag{2}$$

A good reference for the facts mentioned above is available on line [13]. We will make use of Rouché's Theorem. There are a number of formulations, of which the most elementary is probably the following statement proved as Theorem 10.10 in [2].

Theorem 4 (Rouché). *If f and g are analytic on a topological disk, B, and $|g| < |f|$ on ∂B, then f and $f + g$ have the same number of zeros on B.*

[2] Also known as the Prokhorov and the Lévy-Pro(k)horov distance

3 Proof of Theorem 1

We begin by stating some lemmas. The first is nearly a triviality.

Lemma 1. *Suppose μ has finite 1-energy. Then*

(i)

$$t \cdot \mathbb{P}\left(|X_0 - X_1| \le \frac{1}{t}\right) \to 0\,.$$

(ii) for any $C > 0$,

$$\mathbb{P}\left(\min_{1\le j\le n} |X_j - X_{n+1}| \le \frac{C}{n}\right) \to 0\,;$$

Proof. For part (i) observe that $\limsup t \cdot \mathbb{P}(|X_0 - X_1| \le 1/t) \le 2 \limsup 2^j \cdot \mathbb{P}\left(|X_0 - X_1| \le 2^{-j}\right)$ as t goes over reals and j goes over integers. We then have

$$\begin{aligned}
\infty &> \mathcal{E}(\mu)\\
&= \mathbb{E}\,\frac{1}{|X_0 - X_1|}\\
&\ge \frac{1}{2}\mathbb{E} \sum_{j\in\mathbb{Z}} 2^j \mathbf{1}_{|X_0 - X_1| \le 2^{-j}}\\
&= \frac{1}{2}\sum_j 2^j \mathbb{P}\left(|X_0 - X_1| \le 2^{-j}\right)
\end{aligned}$$

and from the finiteness of the last sum it follows that the summand goes to zero. Part (ii) follows from part (i) upon observing, by symmetry, that

$$\mathbb{P}\left(\min_{1\le j\le n} |X_j - X_{n+1}| \le \frac{C}{n}\right) \le n\,\mathbb{P}\left(|X_0 - X_1| \le \frac{C}{n}\right)\,. \qquad \square$$

Define the nth empirical potential function $V_{\mu,n}$ by

$$V_{\mu,n}(z) := \frac{1}{n}\sum_{j=1}^{n} \frac{1}{z - X_j}$$

which is also the integral in w of $1/(z-w)$ against the measure $\mathcal{Z}(f_n)$. Our next lemma bounds $V'_{\mu,n}(z)$ on the disk $B := B_{C/n}(X_{n+1})$.

Lemma 2. *For all* $\epsilon > 0$,

$$\mathbb{P}\left(\sup_{z \in B} |V'_{\mu,n}(z)| \geq \epsilon n\right) \to 0$$

as $n \to \infty$.

Proof. Let G_n denote the event that $\min_{1 \leq j \leq n} |X_j - X_{n+1}| > 2C/n$. Let $S_n := \sup_{z \in B} |V'_{\mu,n}(z)|$. We will show that

$$\mathbb{E} S_n \mathbf{1}_{G_n} = o(n) \tag{3}$$

as $n \to \infty$. By Markov's inequality, this implies that $\mathbb{P}(S_n \mathbf{1}_{G_n} \geq \epsilon n) \to 0$ for all $\epsilon > 0$ as $n \to \infty$. By part (ii) of Lemma 1 we know that $\mathbb{P}(G_n) \to 1$, which then establishes that $\mathbb{P}(S_n \geq \epsilon n) \to 0$, proving the lemma.

In order to show (3) we begin with

$$|V'_{\mu,n}(z)| = \left| \frac{1}{n} \sum_{j=1}^{n} \frac{-1}{(z - X_j)^2} \right| \leq \frac{1}{n} \sum_{j=1}^{n} \frac{1}{|z - X_j|^2} .$$

Therefore,

$$S_n \mathbf{1}_{G_n} \leq \frac{1}{n} \sum_{j=1}^{n} \frac{1}{(|X_{n+1} - X_j| - C/n)^2} \mathbf{1}_{G_n} \leq \frac{1}{n} \sum_{j=1}^{n} \frac{4}{|X_{n+1} - X_j|^2} \mathbf{1}_{G_n} , \tag{4}$$

where we have used the triangle inequality, thus:

$$|z - X_j| = |(z - X_{n+1}) + (x_{n+1} - X_j)| \geq |X_{n+1} - X_j| - |z - X_{n+1}| .$$

Since we are in B, we know that $|z - X_{n+1}| \leq C/n$, and since we are in G_n, we know that $C/n < |X_{n+1} - X_j|/2$.

Because S_n is the supremum of an average of n summands and the summands are exchangeable, the expectation of $S_n \mathbf{1}_{G_n}$ is bounded from above by the expectation of one summand. Referring to (4), and using the fact that G_n is contained in the event that $|X_{n+1} - X_1| > 2C/n$, this gives

$$\mathbb{E} S_n \mathbf{1}_{G_n} \leq \mathbb{E} \frac{4}{|X_{n+1} - X_1|^2} \mathbf{1}_{|X_{n+1} - X_1| \geq 2C/n} .$$

A standard inequality for nonnegative variables (integrate by parts) is

$$\mathbb{E} W^2 \mathbf{1}_{W \leq t} \leq \int_0^t 2s \mathbb{P}(W \geq s)\, ds .$$

When applied to $W = |X_{n+1} - X_1|^{-1}$ and $t = n/(2C)$, this yields

$$\mathbb{E} S_n \mathbf{1}_{G_n} \leq \int_0^{n/(2C)} 2s\, \mathbb{P}\left(\frac{1}{|X_0 - X_1|} > s \right) ds\,.$$

The integrand goes to zero as $n \to \infty$ by part (i) of Lemma 1. It follows that the integral is $o(n)$, proving the lemma. □

Define the lower modulus of V to distance C/n by

$$\underline{V}_n^C(z) := \inf_{w:|w-z|\leq C/n} \left| V_{\mu,n}(w) \right| \,.$$

This depends on the argument μ as well as C and n but we omit this from the notation.

Lemma 3. *Assume μ has finite 1-energy. Then as $n \to \infty$, the random variable $\underline{V}_n^C(X_{n+1})$ converges in probability, and hence in distribution, to $|V_\mu(X_{n+1})|$.*

In the sequel we will need the Glivenko-Cantelli Theorem [10, Theorem 1.7.4]. Let $X_1, \ldots, X_n, \ldots$ be independent, identically distributed random variables in $\mathbb{R}$ with common cumulative distribution function F. The *empirical distribution function* F_n for $X_1, \ldots, X_n$ is defined by

$$F_n(x) = \frac{1}{n} \sum_{i=1}^{n} I_{(-\infty,x]}(X_i),$$

where I_C is the indicator function of the set C. For every fixed x, $F_n(x)$ is a sequence of random variables, which converges to $F(x)$ almost surely by the strong law of large numbers. Glivenko-Cantelli Theorem strengthen this by proving *uniform convergence* of F_n to F.

Theorem 5 (Glivenko-Cantelli).

$$\|F_n - F\|_\infty = \sup_{x\in\mathbb{R}} |F_n(x) - F(x)| \longrightarrow 0 \quad \textit{almost surely.}$$

The following Corollary is immediate:

Corollary 1. *Let f be a bounded continuous function on $\mathbb{R}$. Then*

$$\lim_{n\to\infty} \int_{\mathbb{R}} f dF_n = \int_{\mathbb{R}} f dF, \quad \textit{almost surely.}$$

Another immediate Corollary is:

Corollary 2. *With notation as in the statement of Theorem 5, the Prohorov distance between F_n and F converges to zero almost surely.*

Proof of Lemma 3. It is equivalent to show that $\underline{V}_n^C - |V_\mu(X_{n+1})| \to 0$ in probability, for which it sufficient to show

$$\sup_{u \in B} \left| V_{\mu,n}(u) - V_\mu(X_{n+1}) \right| \to 0 \tag{5}$$

in probability. This will be shown by proving the following two statements:

$$\sup_{u \in B} \left| V_{\mu,n}(u) - V_{\mu,n}(X_{n+1}) \right| \to 0 \text{ in probability ;} \tag{6}$$

$$\left| V_{\mu,n}(X_{n+1}) - V_\mu(X_{n+1}) \right| \to 0 \text{ in probability .} \tag{7}$$

The left-hand side of (6) is bounded above by $(C/n)\sup_{u \in B} |V'_{\mu,n}(u)|$. By Lemma 2, for any $\epsilon > 0$, the probability of this exceeding $C\epsilon$ goes to zero as $n \to \infty$. This establishes (6).

For (7) we observe, using Dominated Convergence, that under the finite 1-energy condition,

$$\mathcal{E}^K(\mu) := \int\int \frac{1}{|z-w|} \mathbf{1}_{|z-w|^{-1} \geq K} \, d\mu(z)\, d\mu(w) \to 0$$

as $K \to \infty$. Define $\phi^{K,z}$ by

$$\phi^{K,z}(w) = \frac{1}{z-w} \frac{|z-w|}{\max\{|z-w|, 1/K\}}$$

in other words, it agrees with $1/(z-w)$ except that we multiply by a nonegative real so as to truncate the magnitude at K. We observe for later use that

$$\left| \phi^{K,z}(w) - \frac{1}{|z-w|} \right| \leq \frac{1}{|z-w|} \mathbf{1}_{|z-w|^{-1} \geq K}$$

so that

$$\int\int \left| \phi^{K,z}(w) - \frac{1}{|z-w|} \right| d\mu(z)\, d\mu(w) \leq \mathcal{E}^K(\mu) \to 0\,. \tag{8}$$

We now introduce the truncated potential and truncated empirical potential with respect to $\phi^{K,z}$:

$$V_\mu^K(z) := \int \phi^{K,z}(w)\, d\mu(w)$$

$$V_{\mu,n}^K(z) := \int \phi^{K,z}(w)\, d\mathcal{Z}(f_n)(w)\,.$$

We claim that

$$\mathbb{E}\left|V_\mu^K(X_{n+1}) - V_\mu(X_{n+1})\right| \le \mathcal{E}^K(\mu)\,. \tag{9}$$

Indeed,

$$V_\mu(X_{n+1}) - V_\mu^K(X_{n+1}) = \int \left(\frac{1}{z - X_{n+1}} - \phi^{K,z}(X_{n+1})\right) d\mu(z)$$

so taking an absolute value inside the integral, then integrating against the law of X_{n+1} and using (8) proves (9). The empirical distribution $V_{\mu,n}$ has mean μ and is independent of X_{n+1}, therefore the same argument proves

$$\mathbb{E}\left|V_{\mu,n}^K(X_{n+1}) - V_{\mu,n}(X_{n+1})\right| \le \mathcal{E}^K(\mu) \tag{10}$$

independent of the value of n.

We now have two thirds of what we need for the triangle inequality. That is, to show (7) we will show that the following three expressions may all be made smaller than ϵ with probability $1-\epsilon$.

$$V_{\mu,n}(X_{n+1}) - V_{\mu,n}^K(X_{n+1})$$

$$V_{\mu,n}^K(X_{n+1}) - V_\mu^K(X_{n+1})$$

$$V_\mu^K(X_{n+1}) - V_\mu(X_{n+1})$$

Choosing K large enough so that $\mathcal{E}^K(\mu) < \epsilon^2$, this follows for the third of these follows by (9) and for the first of these by (10). Fixing this value of K, we turn to the middle expression. The function $\phi^{K,z}$ is bounded and continuous. By the Corollary 1 to the Glivenko-Cantelli Theorem 5, the empirical law $\mathcal{Z}(f_n)$ converges weakly to μ, meaning that the integral of any bounded continuous function ϕ against $\mathcal{Z}(f_n)$ converges in probability to the integral of ϕ against μ. Setting $\phi := \phi^{K,z}$ and $z := X_{n+1}$ proves that $V_{\mu,n}^K(X_{n+1}) - V_\mu^K(X_{n+1})$ goes to zero in probability, establishing the middle statement (it is in fact true conditionally on X_{n+1}) and concluding the proof. □

Proof of Theorem 1. Suppose that $\underline{V}_n^C(X_{n+1}) > 1/C$. Then for all w with $|w - X_{n+1}| \le C/n$, we have

$$f_n'(w) = \sum_{j=1}^n \frac{1}{w - X_j} = nV_{\mu,n}(w) \ge \frac{n}{C}$$

and hence

$$\left|f_n'(w)\right| = n\left|V_{\mu,n}(w)\right| \geq n\underline{V}_n^C(X_{n+1}) \geq \frac{n}{C}\,.$$

To apply Rouché's Theorem to the functions $1/f_n'$ and $z - X_{n+1}$ on the disk $B := B_{C/n}(X_{n+1})$ we note that $|1/f_n'| < C/n = |z - X_{n+1}|$ on ∂B and hence that the sum has precisely one zero in B, call it a_{n+1}. Taking reciprocals we see that a_{n+1} is also the unique value in $z \in B$ for which $f_n'(z) = -1/(z - X_{n+1})$. But $f_n'(z) + 1/(z - X_{n+1}) = f_{n+1}'(z)$, whence f_{n+1}' has the unique zero a_{n+1} on B.

Now fix any $\delta > 0$. Using the hypothesis that $\mu\{z : V_\mu(z) = 0\} = 0$, we pick a $C > 0$ such that $\mathbb{P}(|V_\mu(X_{n+1})| \leq 2/C) \leq \delta/2$. By Lemma 3, there is an n_0 such that for all $n \geq n_0$,

$$\mathbb{P}\left(\underline{V}^C(X_{n+1}) \leq \frac{1}{C}\right) \leq \delta\,.$$

It follows that the probability that f_{n+1}' has a unique zero a_{n+1} in B is at least $1-\delta$ for $n \geq n_0$. By symmetry, we see that for each j, the probability is also at least $1-\delta$ that f_{n+1}' has a unique zero, call it a_j, in the ball of radius C/n centered at X_j; equivalently, the expected number of $j \leq n+1$ for which there is not a unique zero of f_{n+1}' in $B_{C/n}(X_j)$ is at most δn for $n \geq n_0$.

Define x_j to equal a_j if f_{n+1}' has a unique root in $B_{C/n}(X_j)$ and the minimum distance from X_j to any X_i with $i \leq n+1$ and $i \neq j$ is at least $2C/n$. By convention, we define x_j to be the symbol Δ if either of these conditions fails. The values x_j other than Δ are distinct roots of f_{n+1}' and each such value is within distance C/n of a different root of f_{n+1}. Using part (*ii*) of Lemma 1 we see that the expected number of j for which $x_j = \Delta$ is $o(n)$. It follows that $\mathbb{P}(|\mathcal{Z}(f_{n+1}) - \mathcal{Z}(f_{n+1}')|_P \geq 2\delta) \to 0$ as $n \to \infty$. But also the Prohorov distance between $\mathcal{Z}(f_{n+1})$ and μ converges to zero by Corollary 2. The Prohorov distance metrizes convergence in distribution and $\delta > 0$ was arbitrary, so the theorem is proved. □

4 Proof of Remaining Theorems

Let $\mathcal{G} := \sum_{j=0}^{\infty} Y_j z^j$ denote the standard complex Gaussian power series where $\{Y_j(\omega)\}$ are IID standard complex normals. The results we require from [21] are as follows.

Proposition 1 ([21]). *The set of zeros of $\mathcal{G}$ in the unit disk is a determinantal point process with joint intensities*

$$p(z_1, \ldots, z_n) = \pi^{-n} \det\left[\frac{1}{(1 - z_i\overline{z}_j)^2}\right]\,.$$

The number $N(\rho)$ of zeros of $\mathcal{G}$ on B_ρ is distributed as the sum of independent Bernoullis with means ρ^{2k}, $1 \le k < \infty$.

To use these results we broaden them to random series whose coefficients are nearly IID Gaussian.

Lemma 4. *Let $\{g_n := \sum_{r=0}^{\infty} a_{nr} z^r\}$ be a sequence of power series. Suppose*

(i) For each k, the k-tuple $(a_{n,1}, \ldots, a_{n,k})$ converges weakly as $n \to \infty$ to a k-tuple of IID standard complex normals;
(ii) $\mathbb{E}|a_{nr}| \le 1$ for all n and r.

Then on each disk B_ρ, the set $\mathcal{Z}(g_i) \cap B_\rho$ converges weakly to $\mathcal{Z}(\mathcal{G}) \cap \rho$.

Proof. Throughout the proof we fix $\rho \in (0,1)$ and denote $B := B_\rho$. Suppose an analytic function h has no zeros on ∂B. Denote by $||g - h||_B$ the sup norm on functions restricted to B. Note that if $h_n \to h$ uniformly on B then $\mathcal{Z}(h_n) \cap B \to \mathcal{Z}(h) \cap B$ in the weak topology on probability measures on B, provided that h has no zero on ∂B. We apply this with $h = \mathcal{G} := \sum_{j=0}^{\infty} Y_j z^j$ where $\{Y_j(\omega)\}$ are IID standard complex normals. For almost every ω, $h(\omega)$ has no zeros on ∂B. Hence given $\epsilon > 0$ there is almost surely a $\delta(\omega) > 0$ such that $||g - \mathcal{G}||_B < \delta$ implies $|\mathcal{Z}(g) - \mathcal{Z}(\mathcal{G})|_P < \epsilon$. Pick $\delta_0(\epsilon)$ small enough so that $\mathbb{P}(\delta(\omega) \le \delta_0) < \epsilon/3$; thus $||g - \mathcal{G}||_B < \delta_0$ implies $|\mathcal{Z}(g) - \mathcal{Z}(\mathcal{G})| < \epsilon$ for all $\mathcal{G}$ outside a set of measure at most $\epsilon/3$.

By hypothesis (ii),

$$\mathbb{E}\left|\sum_{r=k+1}^{\infty} a_{nr} z^r\right| \le \frac{\rho^{k+1}}{1-\rho} .$$

Thus, given $\epsilon > 0$, once k is large enough so that $\rho^{k+1}/(1-\rho) < \epsilon\delta_0(\epsilon)/6$, we see that

$$\mathbb{P}\left(\left|\sum_{r=k+1}^{\infty} a_{nr} z^r\right| \ge \frac{\delta_0(\epsilon)}{2}\right) \le \frac{\epsilon}{3} .$$

For such a $k(\epsilon)$ also $|\sum_{r=k+1}^{\infty} Y_r z^r| \le \epsilon/3$. By hypothesis (i), given $\epsilon > 0$ and the corresponding $\delta(\epsilon)$ and $k(\epsilon)$, we may choose n_0 such that $n \ge n_0$ implies that the law of $(a_{n1}, \ldots, a_{nk})$ is within $\min\{\epsilon/3, \delta_0(\epsilon)/(2k)\}$ of the product of k IID standard complex normals in the Prohorov metric. By the equivalence of the Prohorov metric to the minimal Ky Fan metric, there is a pair of random variables $\tilde{g}$ and $\tilde{h}$ such that $\tilde{g} \sim g_n$ and $\tilde{h} \sim \mathcal{G}$ and, except on a set of of measure $\epsilon/3$, each of the first k coefficients of $\tilde{g}$ is within $\delta_0/(2k)$ of the corresponding coefficient of $\mathcal{G}$. By the choice of $k(\epsilon)$, we then have

$$\mathbb{P}(||\tilde{g} - \tilde{h}||_B \ge \delta_0) \le \frac{2\epsilon}{3} .$$

By the choice of δ_0, this implies that

$$\mathbb{P}(|\mathcal{Z}(\tilde{g}) - \mathcal{Z}(\tilde{h})|_P \geq \epsilon) < \epsilon \,.$$

Because $\tilde{g} \sim g_n$ and $\tilde{h} \sim \mathcal{G}$, we see that the law of $\mathcal{Z}(g_n) \cap B$ and the law of $\mathcal{Z}(\mathcal{G}) \cap B$ are within ϵ in the Prohorov metric on laws on measures. Because $\epsilon > 0$ was arbitrary, we see that the law of $\mathcal{Z}(g_n) \cap B$ converges to the law of $\mathcal{Z}(\mathcal{G}) \cap B$. □

Proof of Theorem 3. Let $\rho < 1$ be fixed for the duration of this argument and denote $B := B_\rho$. Let

$$g_n(z) := \frac{f_n'(z)}{f(z)} = \sum_{j=1}^{n} \frac{1}{z - X_j} \,.$$

Because $|X_j| = 1$, the rational function $1/(z - X_j) = -X_j^{-1}/(1 - X_j^{-1} z)$ is analytic on the open unit disk and represented there by the power series $-\sum_{r=0}^{\infty} X_j^{-r-1} z^r$. It follows that $-g_n/\sqrt{n}$ is analytic on the open unit disk and represented there by the power series $-g_n(z)/\sqrt{n} = \sum_{r=0}^{\infty} a_{nr} z^r$ where

$$a_{nr} = n^{-1/2} \sum_{j=1}^{n} X_j^{-r-1} \,.$$

The function $-g_n/\sqrt{n}$ has the same zeros on B as does f_n', the normalization by $-1/\sqrt{n}$ being inserted as a convenience for what is about to come.

We will apply Lemma 4 to the sequence $\{g_n\}$. The coefficients a_{nj} are normalized power sums of the variables $\{X_j\}$. For each $r \geq 0$ and each j, the variable X_j^{-r-1} is uniformly distributed on the unit circle. It follows that $\mathbb{E} a_{nr} = 0$ and that $\mathbb{E} a_{nr} \overline{a_{nr}} = n^{-1} \sum_{ij} X_i^{-r-1} \overline{X_j}^{-r-1} = n^{-1} \sum_{ij} \delta_{ij} = 1$. In particular, $\mathbb{E}|a_{nr}| \leq (\mathbb{E}|a_{nr}|^2)^{1/2} = 1$, satisfying the second hypothesis of Lemma 4. For the first hypothesis, fix k, let $\theta_j = \text{Arg}(X_j)$, and let $\mathbf{v}^{(j)}$ denote the $(2k)$-vector $(\cos(\theta_j)$, $-\sin(\theta_j)$, $\cos(2\theta_j)$, $-\sin(2\theta_j)$, ..., $\cos(k\theta_j)$, $-\sin(k\theta_j))$; in other words, $\mathbf{v}^{(j)}$ is the complex k-vector $(X_j^{-1}, X_j^{-2}, \ldots, X_j^{-k})$ viewed as a real $(2k)$-vector. For each $1 \leq s, t \leq 2k$ we have $\mathbb{E}\mathbf{v}_s^{(j)} \mathbf{v}_t^{(j)} = (1/2)\delta_{ij}$. Also the vectors $\{\mathbf{v}^{(j)}\}$ are independent as j varies. It follows from the multivariate central limit theorem (see, e.g., [10, Theorem 2.9.6]) that $\mathbf{u}^{(n)} := n^{-1/2} \sum_{j=1}^{n} \mathbf{v}^{(j)}$ converges to $1/\sqrt{2}$ times a standard $(2k)$-variate normal. For $1 \leq r \leq k$, the coefficient a_{nr} is equal to $\mathbf{u}_{2r-1}^{(n)} + i\,\mathbf{u}_{2r}^{(n)}$. Thus $\{a_{nr} : 1 \leq r \leq k\}$ converges in distribution as $n \to \infty$ to a k-tuple of IID standard complex normals. The hypotheses of Lemma 4 being verified, the theorem now follows from Proposition 1. □

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On the Distribution of Small Denominators in the Farey Series of Order N

C.L. Stewart*

In memory of Professor Herb Wilf

1 Introduction

Let N be a positive integer. The Farey series of order N is the sequence of rationals h/k with h and k coprime and $1 \leq h \leq k \leq N$ arranged in increasing order between 0 and 1, see [1]. There are $\varphi(k)$ rationals with denominator k in F_N and thus the number of terms in F_N is R where

$$R = R(N) = \varphi(1) + \varphi(2) + \cdots + \varphi(N) = \frac{3}{\pi^2}N^2 + O(N \log N) \qquad (1)$$

(see Theorem 330 of [3]). Let

$$S(N) = \sum_{i=1}^{N} q_i$$

where q_i denotes the smallest denominator possessed by a rational from F_N which lies in the interval $\left(\frac{i-1}{N}, \frac{i}{N}\right]$. In [4] Kruyswijk and Meijer proved that

$$N^{3/2} \ll S(N) \ll N^{3/2} \qquad (2)$$

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and they remarked that the function $S(N)$ is connected with a problem in combinatorial group theory. In particular, C. Schaap proved that for any prime p, $S(p) = p^2 - p + 1 - L(p)$ where $L = L(p)$ is the largest integer for which there is a sequence of integers $a_1, \ldots, a_L$ with $1 \leq a_1 \leq a_2 \leq \cdots \leq a_L \leq p - 1$ for which $a_1 + \cdots + a_j \not\equiv 0(\bmod\ p)$ for $1 \leq j \leq L$. An examination of Kruyswijk and Meijer's proof shows that the implied constants in (2) may be made explicit and that $\frac{1}{\pi^2}N^{3/2} < S(N) < 96N^{3/2}$ for N sufficiently large. They conjectured that $\lim_{N\to\infty} S(N)/N^{3/2}$ exists and is equal to $(\frac{4}{\pi})^2 = 1.62\ldots$. Numerical work seems to be in agreement with this conjecture. In the report [5] we gave an alternative proof of (2) and in fact showed that

$$1.20N^{3/2} < S(N) < 2.33N^{3/2}$$

for N sufficiently large. We are now able to refine this estimate.

Theorem 1. *For N sufficiently large*

$$1.35N^{3/2} < S(N) < 2.04N^{3/2}.$$

Our proof of Theorem 1 depends on two results of R.R. Hall [2] on the distribution and the second moments of gaps in the Farey series.

2 Preliminary Lemmas

Let N be a positive integer and let $F_N = \{x_1, \ldots, x_R\}$ where $0 < x_1 < \cdots < x_R = 1$. Put $\ell_1 = x_1$ and $\ell_r = x_r - x_{r-1}$ for $r = 2, \ldots, R$ so that the ℓ_i's correspond to gaps in the Farey series with the points 0 and 1 identified.

Lemma 1. *There is a positive number C_0 such that for $N \geq 2$,*

$$\sum_{r=1}^{R} \ell_r^2 < (C_0 \log N)/N^2.$$

Proof. This follows from Theorem 1 of [2]. □

For each positive real number t and each positive integer N we define $\sigma_N(t)$ to be the number of gaps ℓ_r for which $\ell_r > t/N^2$. Thus

$$\sigma_N(t) = \sum_{\substack{r=1 \\ t<N^2\ell_r}}^{R} 1.$$

We also define $\delta_N(t)$ by

$$\delta_N(t) = \sigma_N(t)/R(N).$$

Then $\delta_N(t)$ is a distribution function and Hall [2] proves that $\delta_N(t)$ tends to a limit as N tends to infinity.

Lemma 2. *If* $4 \le t \le N$ *and* $w = w(t)$ *is the smaller root of the equation* $w^2 = t(w-1)$ *then*

$$\delta_N(t) = 2t^{-1}(1 - w + 2\log w) + O(t^{-1}N^{-1}\log N + N^{-3/2}).$$

If $1 \le t \le 4$ *then*

$$\delta_N(t) = 2t^{-1}\left(1 + \log t - \frac{t}{2}\right) + O(N^{-1}\log N).$$

Proof. The first assertion follows from Theorem 4 of [2] together with (1). The second assertion follows from (1.2) of [2]. ☐

Let us define $f(t)$ for $1 \le t$ by

$$f(t) = \begin{cases} 2\left(1 + \log t - \frac{t}{2}\right) & \text{for } 1 \le t \le 4 \\ 2(1 - w + 2\log w) & \text{for } 4 < t \end{cases} \tag{3}$$

where

$$w = \frac{t}{2}\left(1 - \left(1 - \frac{4}{t}\right)^{1/2}\right) \quad \text{for } 4 < t.$$

Observe that

$$\lim_{t\to\infty} f(t)/(2/t) = 1. \tag{4}$$

Lemma 3. *For* $4 \le t \le N$ *we have*

$$\sigma_N(t) \le \frac{24(2\log 2 - 1)}{\pi^2}\left(\frac{N}{t}\right)^2 + O\left(\frac{N}{t}\log N + N^{1/2}\right).$$

Proof. Since $\sigma_N(t) = R(N)\delta_N(t)$ it suffices, by (1) and Lemma 2 to show that for $t \ge 4$, $g(t)$ is a decreasing function of t where

$$g(t) = t(2\log w(t) - (w(t) - 1)).$$

Since

$$w(t) = \left(t - t\,(1 - 4/t)^{1/2}\right)/2$$

we find that

$$g'(t) = 2\log w - (w-1) + ((2/w) - 1)tw'(t)$$

so

$$g'(t) = 2\log w - 2w + 2.$$

On observing that $\log(1+x) \le x$ for $x \ge 0$ and putting $x = w - 1$ we conclude that

$$g'(t) \le 2(w-1) - 2w + 2 = 0$$

whenever $w \ge 1$. Since, for $t > 4$,

$$w(t) = 1 + \frac{1}{t} + \frac{2}{t^2} + \cdots + \frac{c_n}{t^n} + \cdots$$

where the c_n are positive numbers we see that $w > 1$ for $t > 4$ hence for $t \ge 4$. Thus $g(t)$ is a decreasing function of t as required. □

3 Further Preliminaries

For each positive integer M we define $\theta(M)$ to be the number of q_i's in the sum giving $S(N)$ which are larger than M. Thus

$$\theta(M) = \sum_{\substack{i=1 \\ q_i > M}}^{N} 1.$$

For positive integers j and M let $\psi(j)$ $(= \psi_M(j))$ denote the number of gaps ℓ_r in F_M of size larger than $\frac{j}{N}$. Accordingly we have

$$\psi(j) = \sum_{\substack{r=1 \\ \ell_r > \frac{j}{N}}}^{R(M)} 1.$$

A gap ℓ_r in F_M with $\ell_r \le \frac{j+1}{N}$ properly contains at most j intervals $\left(\frac{h-1}{N}, \frac{h}{N}\right]$ with $1 \le h \le N$. $\theta(M)$ is the total number of intervals $\left(\frac{h-1}{N}, \frac{h}{N}\right]$ which are properly contained in gaps of F_M. Thus

$$\theta(M) \le \psi(1) + \psi(2) + \cdots.$$

Similarly a gap ℓ_r in F_M with $\ell_r > \frac{j+1}{N}$ properly contains at least j intervals of the form $\left(\frac{h-1}{N}, \frac{h}{N}\right]$. Therefore

$$\psi(2) + \psi(3) + \cdots \leq \theta(M).$$

Since $\psi(j) = \sigma_M\left(\frac{jM^2}{N}\right)$, it follows that

$$\sum_{j=2}^{v} \sigma_M\left(\frac{jM^2}{N}\right) \leq \theta(M) \leq \sum_{j=1}^{v} \sigma_M\left(\frac{jM^2}{N}\right), \tag{5}$$

where v $(= v(M))$ satisfies

$$v < \frac{N}{M} \leq v + 1. \tag{6}$$

Let u_1 be the number of rationals $\frac{h}{k}$ with $(h, k) = 1$ and $1 \leq h \leq k \leq \sqrt{N}$. Then by (1)

$$u_1 = \frac{3}{\pi^2}N + O(N^{1/2}\log N) \tag{7}$$

and the sum S_1 of the denominators of these rationals is

$$S_1 = \sum_{k \leq \sqrt{N}} k\varphi(k).$$

By Abel summation and (1) we find that

$$S_1 = \frac{2}{\pi^2}N^{3/2} + O(N \log N). \tag{8}$$

Observe that if q is an integer with $1 \leq q \leq \sqrt{N}$ then each rational p/q with p positive and coprime with q contributes a term q to $S(N)$. Thus S_1 is the sum of the u_1 smallest terms in the sum giving $S(N)$. Put

$$u_2 = N - u_1 \tag{9}$$

and let S_2 be the sum of the u_2 largest q's which appear in the sum for $S(N)$. Then

$$S(N) = S_1 + S_2. \tag{10}$$

4 The Upper Bound in Theorem 1

In order to establish an upper bound for $S(N)$ we shall establish an upper bound for S_2 and then appeal to (8) and (10).

For any positive integer M with $M \le N$ we have

$$S_2 \le Mu_2 + \theta(M) + \theta(M+1) + \cdots + \theta(N). \tag{11}$$

Put $\lambda = 1.38$ and $M_1 = [\lambda N^{1/2}]$. Since $\lambda(1 - 3/\pi^2) < 0.96054$ and $\theta(M_1) \le N$, it follows from (7), (9) and (11) that

$$S_2 < 0.96054 N^{3/2} + \theta(M_1+1) + \theta(M_1+2) + \cdots + \theta(N) \tag{12}$$

for N sufficiently large. Next, put

$$S_3 = \sum_{M_1 < M < N^{3/5}} \theta(M) \quad \text{and} \quad S_4 = \sum_{N^{3/5} \le M \le N} \theta(M).$$

Thus, by (12),

$$S_2 < 0.96054\, N^{3/2} + S_3 + S_4. \tag{13}$$

Let us first estimate S_4. To that end recall that $\theta(M)$ is the number of q_i's in the sum $S(N)$ which are larger than M. Thus there are $\theta(M)$ intervals $\left(\frac{j-1}{N}, \frac{j}{N}\right]$ which contain no element of F_M. In particular there must exist differences $\ell_{r_1}, \ldots, \ell_{r_s}$ in F_M for which we can find positive integers $k_1, \ldots, k_s$ with $\ell_{r_i} \ge k_i/N$ for $i = 1, \ldots, s$ and such that $k_1 + \cdots + k_s \ge \theta(M)$. Thus we certainly have

$$\sum_{i=1}^{s} \ell_{r_i}^2 \ge \frac{\theta(M)}{N^2}. \tag{14}$$

On the other hand, by Lemma 1,

$$\sum_{r=1}^{R(M)} \ell_r^2 < C_0 M^{-2} \log M. \tag{15}$$

A comparison of (14) and (15) reveals that

$$\theta(M) < C_0 \frac{N^2}{M^2} \log M.$$

For $N^{3/5} \le M \le N$ we have $\log M \le \log N$ hence

$$\sum_{N^{3/5} \le M \le N} \theta(M) < C_0 N^2 \log N \int_{N^{3/5}-1}^{N} \frac{dM}{M^2}$$

so

$$S_4 < 2C_0 N^{7/5} \log N. \tag{16}$$

Next we estimate S_3. By (5)

$$S_3 = \sum_{M_1 < M < N^{3/5}} \theta(M) \le \sum_{M_1 < M < N^{3/5}} \sum_{j=1}^{v} \sigma_M\left(\frac{jM^2}{N}\right). \tag{17}$$

For $M < N^{3/5}$ we see from (6) that $v + 1$ is at least $N^{2/5}$, which in turn exceeds 10^4 for N sufficiently large. Then, by Lemma 3,

$$\begin{aligned}\sum_{M_1 < M < N^{3/5}} \sum_{10^4 < j \le v} \sigma_M\left(\frac{jM^2}{N}\right) &< \sum_{M_1 < M < N^{3/5}} \frac{N^2}{M^2} \sum_{10^4 < j < \infty} \left(\frac{1}{j}\right)^2 \\ &< 10^{-4} N^2 \sum_{M_1 < M < N^{3/5}} \frac{1}{M^2} \\ &< 10^{-4} N^{3/2},\end{aligned} \tag{18}$$

for N sufficiently large. Accordingly by (17) and (18)

$$S_3 < 10^{-4} N^{3/2} + \sum_{M_1 < M < N^{3/5}} \sum_{j=1}^{10^4} \sigma_M\left(\frac{jM^2}{N}\right). \tag{19}$$

Let $\varepsilon > 0$. For N sufficiently large in terms of ε

$$R(M) < \left(\frac{3}{\pi^2} + \varepsilon\right) M^2$$

hence

$$\sigma_M\left(\frac{jM^2}{N}\right) = R(M)\delta_M\left(\frac{jM^2}{N}\right) < \left(\frac{3}{\pi^2} + \varepsilon\right) M^2 \delta_M\left(\frac{jM^2}{N}\right)$$

and so

$$\sigma_M\left(\frac{jM^2}{N}\right) < \left(\frac{3}{\pi^2} + \varepsilon\right) \frac{N}{j} \left(\frac{jM^2}{N} \delta_M\left(\frac{jM^2}{N}\right)\right). \tag{20}$$

It follows from Lemma 2 and (3) that for $j \le 10^4$ and $M \le N^{3/5}$

$$\frac{jM^2}{N} \delta_M\left(\frac{jM^2}{N}\right) = f\left(\frac{jM^2}{N}\right) + O\left(\frac{\log N}{N}\right).$$

Thus, by (4), for N sufficiently large in terms of ε

$$\frac{jM^2}{N}\delta_M\left(\frac{jM^2}{N}\right) < (1+\varepsilon)f\left(\frac{jM^2}{N}\right). \tag{21}$$

For each integer j with $1 \le j \le 10^4$ we find from (20) and (21) that

$$\sum_{M_1<M<N^{3/5}} \sigma_M\left(\frac{jM^2}{N}\right) < \left(\frac{3}{\pi^2}+\varepsilon\right)(1+\varepsilon)\frac{N}{j}\sum_{M_1<M<N^{3/5}} f\left(\frac{jM^2}{N}\right). \tag{22}$$

The function f is continuous and it is increasing on $(1,4)$ and decreasing on $(4,\infty)$. Accordingly, with $\Delta = 1/\log N$, we have

$$\sum_{M_1<M<N^{3/5}} f\left(\frac{jM^2}{N}\right)$$
$$< \left(\sum_{1\le k<(N^{3/5}-M_1)/[\Delta\sqrt{N}]} f\left(\frac{j(M_1+k[\Delta\sqrt{N}])^2}{N}\right)[\Delta\sqrt{N}]\right) + O\left(\frac{\sqrt{N}}{\log N}\right)$$

which is, for N sufficiently large,

$$< \left(\sum_{1\le k<N^{1/5}} f\left(\frac{j(\lambda\sqrt{N}+O(1)+k(\Delta\sqrt{N}+O(1)))^2}{N}\right)(\Delta\sqrt{N}+O(1))\right) + O\left(\frac{\sqrt{N}}{\log N}\right).$$

Therefore, for N sufficiently large in terms of ε,

$$\sum_{M_1<M<N^{3/5}} f\left(\frac{jM^2}{N}\right) < (1+\varepsilon)N^{1/2}\sum_{1\le k<N^{1/5}} f\left(j(\lambda+k\Delta)^2 + O\left(k^2N^{-1/2}\right)\right)\cdot\Delta$$
$$< (1+\varepsilon)^2N^{1/2}\int_\lambda^\infty f(jt^2)dt. \tag{23}$$

Thus, by (22) and (23),

$$\sum_{j=1}^{10^4}\sum_{M_1<M<N^{3/5}} \sigma_M\left(\frac{jM^2}{N}\right)$$
$$< \left(\frac{3}{\pi^2}+\varepsilon\right)(1+\varepsilon)^3N^{3/2}\sum_{j=1}^{10^4}\frac{1}{j}\int_\lambda^\infty f(jt^2)dt. \tag{24}$$

Evaluating with MAPLE we find that

$$\sum_{j=1}^{10^4} \frac{1}{j} \int_{\lambda}^{\infty} f(jt^2)dt < 2.8640. \tag{25}$$

Therefore, by (24) and (25), for N sufficiently large,

$$\sum_{j=1}^{10^4} \sum_{M_1 < M < N^{3/5}} \sigma_M \left(\frac{jM^2}{N}\right) < 0.8706\, N^{3/2}. \tag{26}$$

By (19) and (26)

$$S_3 < 0.8707\, N^{3/2} \tag{27}$$

for N sufficiently large. Further, by (13), (16) and (27),

$$S_2 < 1.8313\, N^{3/2}$$

for N sufficiently large. Our result now follows from (8) and (10).

5 The Lower Bound in Theorem 1

The value of the smallest q_i in S_2 exceeds $\sqrt{N}$ and so

$$S_2 \geq [\sqrt{N}]u_2 + \theta([\sqrt{N}]) + \theta([\sqrt{N}] + 1) + \cdots + \theta(N)$$

hence, by (7) and (9),

$$S_2 \geq \left(1 - \frac{3}{\pi^2}\right) N^{3/2} + O(N \log N) + \theta([\sqrt{N}]) + \cdots + \theta(N). \tag{28}$$

Certainly

$$\theta([\sqrt{N}]) + \cdots + \theta(N) \geq \sum_{N^{1/2} < M < N^{3/5}} \theta(M)$$

and for M with $M < N^{3/5}$ we see from (6) that $v + 1$ is at least $N^{2/5}$. Therefore, by (5), for N sufficiently large

$$\sum_{N^{1/2} < M < N^{3/5}} \theta(M) > \sum_{N^{1/2} < M < N^{3/5}} \sum_{j=2}^{10^4} \sigma_M \left(\frac{jM^2}{N}\right)$$

and so, by (28),

$$S_2 > \left(1 - \frac{3}{\pi^2}\right) N^{3/2} + O(N \log N) + \sum_{j=2}^{10^4} \sum_{N^{1/2} < M < N^{3/5}} \sigma_M \left(\frac{jM^2}{N}\right). \tag{29}$$

We shall now estimate the double sum in (29). Let $\varepsilon > 0$. For N sufficiently large in terms of ε

$$R(M) > \left(\frac{3}{\pi^2} - \varepsilon\right) M^2$$

hence

$$\sigma_M \left(\frac{jM^2}{N}\right) = R(M)\delta_M \left(\frac{jM^2}{N}\right) > \left(\frac{3}{\pi^2} - \varepsilon\right) M^2 \delta_M \left(\frac{jM^2}{N}\right)$$

and so

$$\sigma_M \left(\frac{jM^2}{N}\right) > \left(\frac{3}{\pi^2} - \varepsilon\right) \frac{N}{j} \left(\frac{jM^2}{N} \delta_M \left(\frac{jM^2}{N}\right)\right). \tag{30}$$

It follows from Lemma 2 and (3) that for $j \leq 10^4$ and $M \leq N^{3/5}$

$$\frac{jM^2}{N} \delta_M \left(\frac{jM^2}{N}\right) = f\left(\frac{jM^2}{N}\right) + O\left(\frac{\log N}{N}\right).$$

Thus, by (4), for N sufficiently large in terms of ε

$$\frac{jM^2}{N} \delta_M \left(\frac{jM^2}{N}\right) > (1 - \varepsilon) f\left(\frac{jM^2}{N}\right). \tag{31}$$

For each integer j with $2 \leq j \leq 10^4$ we find from (30) and (31) that

$$\begin{aligned} &\sum_{N^{1/2} < M < N^{3/5}} \sigma_M \left(\frac{jM^2}{N}\right) \\ &\qquad > \left(\frac{3}{\pi^2} - \varepsilon\right) (1 - \varepsilon) \frac{N}{j} \sum_{N^{1/2} < M < N^{3/5}} f\left(\frac{jM^2}{N}\right). \end{aligned} \tag{32}$$

The function f is continuous and it is increasing on $(1, 4)$ and decreasing on $(4, \infty)$. Accordingly, with $\Delta = 1/\log N$, we have

$$\sum_{N^{1/2}<M<N^{3/5}} f\left(\frac{jM^2}{N}\right)$$
$$\geq \left(\sum_{1\leq k<(N^{3/5}-N^{1/2})/[\Delta\sqrt{N}]} f\left(\frac{j([\sqrt{N}]+k[\Delta\sqrt{N}])^2}{N}\right)[\Delta\sqrt{N}]\right) + O\left(\frac{\sqrt{N}}{\log N}\right)$$

which is, for N sufficiently large,

$$\geq \left(\sum_{1\leq k<N^{1/10}} f\left(\frac{j(\sqrt{N}+O(1)+k(\Delta\sqrt{N}+O(1)))^2}{N}\right)(\Delta\sqrt{N}+O(1))\right) + O\left(\frac{\sqrt{N}}{\log N}\right).$$

Therefore, for N sufficiently large in terms of ε,

$$\begin{aligned}\sum_{N^{1/2}<M<N^{3/5}} f\left(\frac{jM^2}{N}\right) &> (1-\varepsilon)N^{1/2} \sum_{1\leq k\,<\,N^{1/10}} f(j(1+k\Delta)^2+O(k^2N^{-1/2}))\cdot\Delta \\ &> (1-\varepsilon)^2 N^{1/2}\int_1^\infty f(jt^2)dt. \end{aligned} \tag{33}$$

Thus, by (32) and (33),

$$\begin{aligned}&\sum_{j=2}^{10^4}\cdot \sum_{N^{1/2}<M<N^{3/5}} \sigma_m\left(\frac{jM^2}{N}\right) \\ &\quad > \left(\frac{3}{\pi^2}-\varepsilon\right)(1-\varepsilon)^3 N^{3/2}\sum_{j=2}^{10^4}\frac{1}{j}\int_1^\infty f(jt^2)dt. \end{aligned} \tag{34}$$

Evaluating with MAPLE we find that

$$\sum_{j=2}^{10^4}\frac{1}{j}\int_1^\infty f(jt^2)dt > 1.5098. \tag{35}$$

Therefore by (34) and (35), for N sufficiently large

$$\sum_{j=2}^{10^4}\sum_{N^{1/2}<M<N^{3/5}} \sigma_M\left(\frac{jM^2}{N}\right) > 0.4589\,N^{3/2}. \tag{36}$$

By (8), (10), (29) and (36) we see that

$$S(N) > \left(1 - \frac{1}{\pi^2} + 0.458\right) N^{3/2} > 1.35\, N^{3/2}$$

for N sufficiently large and the result now follows.

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Lost in Translation

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In memory of Herb Wilf

Abstract We explain the use and set grounds about applicability of algebraic transformations of arithmetic hypergeometric series for proving Ramanujan's formulae for $1/\pi$ and their generalisations.

Keywords π • Ramanujan • Arithmetic hypergeometric series • Algebraic transformation • Modular function

The principal goal of this note is to set some grounds about applicability of algebraic transformations of (arithmetic) hypergeometric series for proving Ramanujan's formulae for $1/\pi$ and their numerous generalisations. The technique was successfully used in quite different situations [7, 16, 18–20] and was dubbed as 'translation method' by J. Guillera, although the name does not give any clue about the method itself. In theory, one could think of the method as a way to reduce (rather than translate) the identity in question to a simpler one, but the simpler identity may be much more involved than the original in many perspectives. (Also, "Lost in reduction" sounds menacingly.)

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Consider the following problem: *Show that*

$$\sum_{n=0}^{\infty} \frac{(4n)!}{n!^4}(3+40n) \cdot \frac{1}{28^{4n}} = \frac{49}{3\sqrt{3}\pi}\,. \tag{1}$$

Step 0. It comes as a useful rule: prior to any attempts to prove an identity verify it numerically. The convergence of the series on the left-hand side of (1) is reasonably fast (more than three decimal places per term), so you shortly convince yourself that the both sides are

3.00167954174086782511722204637061140316354861532948799857432 6 . . . .

Step 1. Series of the type given in (1) should be quite special. With a little search you identify

$$\sum_{n=0}^{\infty} \frac{(4n)!}{n!^4}\left(\frac{x}{256}\right)^n = {}_3F_2\left(\begin{matrix}\frac14,\ \frac12,\ \frac34\\ 1,\ 1\end{matrix}\,\middle|\, x\right) = \sum_{n=0}^{\infty} \frac{\left(\frac14\right)_n\left(\frac12\right)_n\left(\frac34\right)_n}{(1)_n(1)_n}\frac{x^n}{n!}\,, \tag{2}$$

a hypergeometric series, where the notation $(a)_n$ (*Pochhammer's symbol* or *shifted factorial*) stands for $\Gamma(a+n)/\Gamma(a) = a(a+1)\cdots(a+n-1)$. A generalised hypergeometric series

$${}_mF_{m-1}\left(\begin{matrix}a_1,\ a_2,\ \dots,\ a_m\\ b_2,\ \dots,\ b_m\end{matrix}\,\middle|\, x\right) := \sum_{n=0}^{\infty} \frac{(a_1)_n(a_2)_n\cdots(a_m)_n}{(b_2)_n\cdots(b_m)_n}\frac{x^n}{n!}$$

is an object of intensive study since Euler [2, 17]; one of its important properties is the linear differential equation

$$\left(\left(x\frac{\mathrm{d}}{\mathrm{d}x}\right)\prod_{j=2}^{m}\left(x\frac{\mathrm{d}}{\mathrm{d}x}+b_j-1\right) - x\prod_{j=1}^{m}\left(x\frac{\mathrm{d}}{\mathrm{d}x}+a_j\right)\right)F = 0 \tag{3}$$

satisfied by the series. The required identity (1) can be therefore transformed to the more conceptual form

$$\sum_{n=0}^{\infty} \frac{\left(\frac14\right)_n\left(\frac12\right)_n\left(\frac34\right)_n}{n!^3}\,\frac{3+40n}{7^{4n}} = \left(3+40x\frac{\mathrm{d}}{\mathrm{d}x}\right){}_3F_2\left(\begin{matrix}\frac14,\ \frac12,\ \frac34\\ 1,\ 1\end{matrix}\,\middle|\, x\right)\Bigg|_{x=1/7^4} = \frac{49}{3\sqrt{3}\pi}\,. \tag{4}$$

Step 2. Convince yourself that identities of the wanted type are known in the literature. In fact, they are known for almost a century after Ramanujan's publication [15]; identity (1) is Eq. (42) there. Ramanujan did not indicate how he arrived at his series but left some hints that these series belong to what is now known as 'the theories of elliptic functions to alternative bases'. The first proofs of Ramanujan's identities and their generalisations were given by the Borweins [5] and Chudnovskys [8]. Those proofs are however too lengthy to be included here. Note that Ramanujan's list in [15] does not include the slowly convergent example

$$\sum_{n=0}^{\infty}\frac{\left(\frac{1}{2}\right)_n^3}{n!^3}(1+4n)\,(-1)^n=\left(1+4x\frac{\mathrm{d}}{\mathrm{d}x}\right){}_3F_2\left(\begin{matrix}\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}\\ 1,\ 1\end{matrix}\,\middle|\,x\right)\Bigg|_{x=-1}=\frac{2}{\pi}, \tag{5}$$

which was shown to be true by G. Bauer [3] already in 1859. Bauer's proof makes no reference to sophisticated theories and is much shorter, although does not seem to be generalisable to the other entries from [15]. In fact, D. Zeilberger assisted by his automatic collaborator S. B. Ekhad [9] came up in 1994 with a short proof of (5) verifiable by a computer. The key is a use of a simple telescoping argument (this part is completely automated by the great Wilf–Zeilberger (WZ) machinery [14]) and an advanced theorem due to Carlson [2, Chap. V]; the proof is reproduced in [21]. Quite recently, J. Guillera advocated [10–13] the method from [9] and significantly extended the outcomes; he showed, for example, that many other Ramanujan's identities for $1/\pi$ can be proven completely automatically. Note however that (1) is one of 'WZ resistant' identities. To overcome this technical difficulty, below we reduce the identity to the simpler one (5). (There is no warranty, of course, for (5) to exist. The comments below address this issue up to a certain point.)

Step 3. Use your favourite computer algebra system (CAS) to verify the hypergeometric identity

$${}_3F_2\left(\begin{matrix}\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}\\ 1,\ 1\end{matrix}\,\middle|\,x\right)=r\cdot{}_3F_2\left(\begin{matrix}\frac{1}{4},\ \frac{1}{2},\ \frac{3}{4}\\ 1,\ 1\end{matrix}\,\middle|\,y\right) \tag{6}$$

where $y=y(x)=-\frac{1}{1{,}024}x^3+O(x^4)$ and $r=r(x)=1+\frac{1}{8}x+\frac{27}{512}x^2+O(x^3)$ are algebraic functions determined by the equations

$$\begin{aligned}&(x^2-194x+1)^4y^4\\&\quad+16(4833x^6+2029050x^5+47902255x^4-92794388x^3\\&\qquad+47902255x^2+2029050x+4833)xy^3\\&\quad-96(3328x^6-623745x^5+3837060x^4-6470150x^3\\&\qquad+3837060x^2-623745x+3328)xy^2\\&\quad+256(1024x^6-1152x^5+225x^4-2x^3+225x^2-1152x+1024)xy+256x^4=0\end{aligned}$$

and

$$\begin{aligned}&(x^2-194x+1)^2r^8+4(61x^2+25798x+61)(x-1)r^6\\&\quad+486(41x^2-658x+41)r^4+551124(x-1)r^2+531{,}441=0.\end{aligned}$$

To do this you (and your CAS) are expected to use the linear differential equations (3) for the involved hypergeometric functions and generate any-order derivatives of y and r with respect to x by appealing to the implicit functional equations. To summarise, you have to check that both sides of (6) satisfy the same (third order) linear differential equation in x with algebraic function coefficients and then compare the first few coefficients in the expansions in powers of x. Note that $x = -1$ corresponds to $y = 1/7^4$ (cf. (5) vs. (4)), and this is the reason behind considering the sophisticated functional identity (6).
The task on this step does not look humanly pleasant, and there is a (casual) trick to verify (6) by parameterising x, y and r:

$$x = -\frac{4p(1-p)(1+p)^3(2-p)^3}{(1-2p)^6}, \quad y = \frac{16p^3(1-p)^3(1+p)(2-p)(1-2p)^2}{(1-2p+4p^3-2p^4)^4},$$
$$r = \frac{(1-2p)^3}{1-2p+4p^3-2p^4}.$$

Choosing $p = (1-\sqrt{45-18\sqrt{6}})/2$ we obtain $x = -1$ and $y = 1/7^4$. (The modular reasons behind this parametrisation can be found in [4, Lemma 5.5 on p. 111] where our p is the negative of the p there.)

Step 4. By differentiating identity (6) with respect to x and combining the result with (6) itself we see that

$$\left(a + bx\frac{\mathrm{d}}{\mathrm{d}x}\right) {}_3F_2\left(\begin{matrix}\frac12, \frac12, \frac12 \\ 1, 1\end{matrix} \,\middle|\, x\right) = \left(a + bx\frac{\mathrm{d}r}{\mathrm{d}x} + b\frac{rx}{y}\frac{\mathrm{d}y}{\mathrm{d}x}\cdot y\frac{\mathrm{d}}{\mathrm{d}y}\right)\cdot {}_3F_2\left(\begin{matrix}\frac14, \frac12, \frac34 \\ 1, 1\end{matrix} \,\middle|\, y\right); \tag{7}$$

again, the derivatives $\mathrm{d}y/\mathrm{d}x$ and $\mathrm{d}r/\mathrm{d}x$ are read from the implicit functional equations. An alternative (but simpler) way is using the parametrisations $x(p)$, $y(p)$ and $r(p)$. Taking $a = 1$, $b = 4$ and $x = -1$ in (7) you recognise the left-hand side as the familiar Bauer's (WZ easy) identity (5), while the right-hand side is nothing but the series in (4).

Comments. The story exposed above is general enough to be used in other situations for proving *some* other formulae for $1/\pi$. The setup can be as follows. Assume we already have an identity

$$\left(a + bx\frac{\mathrm{d}}{\mathrm{d}x}\right)F(x)\bigg|_{x=x_0} = \mu,$$

where a, b, x_0 and μ are certain (simple or at least arithmetically significant) numbers, and $F(x)$ is an (arithmetic) series. Furthermore, assume we have a transformation $F(x) = rG(y)$ with $r = r(x)$ and $y = y(x)$ differentiable at $x = x_0$. Then

$$\left(\hat{a} + \hat{b}y\frac{\mathrm{d}}{\mathrm{d}y}\right)G(y)\bigg|_{y=y_0} = \mu,$$

where

$$\hat{a} = a + bx\frac{\mathrm{d}r}{\mathrm{d}x}\bigg|_{x=x_0}, \quad \hat{b} = b\frac{rx}{y}\frac{\mathrm{d}y}{\mathrm{d}x}\bigg|_{x=x_0}, \quad \text{and} \quad y = y_0.$$

There is, of course, no magic in this result: it is just the standard 'chain rule'.

The applicability of this simple argument heavily rests on existence of transformations like (6). This in turn is based on the modular origin [5, 6, 8, 21] of Ramanujan's identities for $1/\pi$: any such identity can be written in the form

$$\left(a + bx\frac{\mathrm{d}}{\mathrm{d}x}\right)F(x)\bigg|_{x=x_0} = \frac{c}{\pi}, \qquad a, b, c, x_0 \in \overline{\mathbb{Q}}, \tag{8}$$

where $F(x)$ is an *arithmetic hypergeometric series* [23] satisfying a third order linear differential equation. In other words, for a certain modular function $x = x(\tau)$ (not uniquely defined!) the function $F(x(\tau))$ is a modular form of weight 2. The theory of modular forms provides us with the knowledge that any two modular forms are algebraically dependent; thus, whenever we have another arithmetic hypergeometric series $G(y)$ and a related modular parametrisation $y = y(\tau)$, the modular functions $y(\tau)$ and $G(y(\tau))/F(x(\tau))$ are algebraic over $\mathbb{Q}[x(\tau)]$. Another warrants of the theory is an algebraic dependence over $\mathbb{Q}$ of $x(\tau)$ and $x((A\tau + B)/(C\tau + D))$ for any $\left(\begin{smallmatrix} A & B \\ C & D \end{smallmatrix}\right) \in SL_2(\mathbb{Q})$. On the other hand, there is no other source known for such algebraic dependency; the functions $x(\tau)$ and $x(A\tau)$, $A > 0$, are algebraically dependent if and only if A is rational.

The above arithmetic constraints impose the natural restriction on τ_0 from the upper half-plane $\operatorname{Re}\tau > 0$ to satisfy $x(\tau_0) = x_0$ in (8). Namely, τ_0 is an (imaginary) quadratic irrationality, $\tau_0 \in \mathbb{Q}[\sqrt{-d}]$ for some positive integer d. But then $(A\tau_0 + B)/(C\tau_0 + D)$ belongs to the same quadratic extension of $\mathbb{Q}$ for any $\left(\begin{smallmatrix} A & B \\ C & D \end{smallmatrix}\right) \in SL_2(\mathbb{Q})$, so whatever transformation $F(x) = rG(y)$ (of modular origin) we use, the modular arguments of $x(\tau)$ and $y(\tau)$ have to be tied by an $SL_2(\mathbb{Q})$ linear-fractional transform. In the examples (4) and (5) we have both arguments belonging to $\mathbb{Q}[\sqrt{-2}]$, therefore an algebraic transformation must exist, and this is confirmed by (6) mapping the corresponding $x(\tau_0) = -1$ into $y(3\tau_0) = 1/7^4$ where $\tau_0 = (1 + \sqrt{-2})/2$. There is however no way known to 'translate' identities (4) and (5) to either

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

or

$$\sum_{n=0}^{\infty} \frac{\left(\frac{1}{6}\right)_n\left(\frac{1}{2}\right)_n\left(\frac{5}{6}\right)_n}{n!^3}(13591409 + 545140134n)\cdot\frac{(-1)^n}{53360^{3n+2}} = \frac{3}{2\sqrt{10005}\pi},$$

as the corresponding modular arguments lie in the fields $\mathbb{Q}[\sqrt{-3}]$ and $\mathbb{Q}[\sqrt{-163}]$, respectively. We refer the interested reader to [6] for exhausting lists of 'rational' (in the sense of x_0) identities which express $1/\pi$ by means of general hypergeometric-type series; the details of the modular machinery are greatly explained there.

In a sense, to make the 'translation method' work we first should carefully examine the underlying modular parametrisations. On the other hand, there are situations when we know (or can produce [1]) the algebraic transformations without having modularity at all. These are particularly useful in the context of similar formulae for $1/\pi^2$ recently discovered by Guillera [10, 11, 13].

There is a p-adic counterpart of the Ramanujan-type identities for $1/\pi$ and $1/\pi^2$ which we review in [22]. It seems likely that the algebraic transformation machinery is generalisable to those situations as well but, for the moment, no single example of this is known.

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