

LATTICE SUMS THEN AND NOW

The study of lattice sums began when early investigators wanted to go from mechanical properties of crystals to the properties of the atoms and ions from which they were built (the literature of Madelung's constant). A parallel literature was built around the optical properties of regular lattices of atoms (initiated by Lord Rayleigh, Lorentz and Lorenz). For over a century many famous scientists and mathematicians have delved into the properties of lattices, sometimes unwittingly duplicating the work of their predecessors.

Here, at last, is a comprehensive overview of the substantial body of knowledge that exists on lattice sums and their applications. The authors also provide commentaries on open questions, and explain modern techniques which simplify the task of finding new results in this fascinating and ongoing field. Lattice sums in one, two, three, four and higher dimensions are covered.

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ENCYCLOPEDIA OF MATHEMATICS AND ITS APPLICATIONS

Lattice Sums Then and Now

J. M. BORWEIN

University of Newcastle, New South Wales

M. L. GLASSER

Clarkson University

R. C. McPHEDRAN

University of Sydney

J. G. WAN

University of Newcastle, New South Wales

I. J. ZUCKER

King's College London



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Knowledge of lattice sums has been built by many generations of researchers, commencing with Appell, Rayleigh, and Born. Two of the present authorship (MLG and IJZ) attempted the first comprehensive review of the subject 30 years ago. This inspired two more (JMB and RCM) to enter the field, and they have been joined by a member (JGW) of a new generation of enthusiasts in completing this second and greatly expanded compendium.

All five authors are certain that lattice sums will continue to be a topic of interest to coming generations of researchers, and that our successors will surely add to and improve on the results here.

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Foreword by Helaman and Claire Ferguson

The Borwein Award: Salt, the Sculpture, created in 2004

As sculptor, and also the inventor of the PSLQ integer relations algorithm, I described to the Canadian Mathematical Society the sculpture expressing the Madelung constant μ as follows:

$$\mu := \sum'_{n,m,p} \frac{(-1)^{n+m+p}}{\sqrt{n^2 + m^2 + p^2}}$$

This polished solid silicon bronze sculpture is inspired by the work of David Borwein, his sons and colleagues, on the conditional series above for salt, Madelung's constant. This series can be summed to give uncountably many constants; one is Madelung's constant for sodium chloride.

This constant is a period of an elliptic curve, a real surface in four dimensions. There are uncountably many ways to imagine that surface in three dimensions; one has negative Gaussian curvature and is the tangible form of this sculpture.

I will now explain some of the creative processes which led to this sculpture.

Actually, the inscription on the sculpture reads 'created in 2004' but, in the spirit of this book *Lattice Sums Then and Now*, the creation started much earlier. There are a couple of questions. First: why would a sculptor create a sculpture about NaCl, as in 'please pass the "nakkle"', sodium chloride or salt, a life-essential mineral? Second: why would a sculptor be interested in Madelung's constant, a conditionally convergent series, subject to special summability, giving the electrostatic potential of the interpenetrating lattices of sodium (Na^+) and chlorine (Cl^-) ions,

The equals sign in the above equation is misleading at this stage because the right-hand side is not defined as it stands. In fact, the right-hand side is a conditional series of infinitely many positive and negative terms which can be

rearranged to give any real number whatsoever (!); the commutative law holds for finitely many summands but does not hold for infinitely many summands.

I will answer these two questions raised above in order. First answer: I was born in the Humbolt Basin in the Rocky Mountains and spent the first five years of my life there. This basin contains the Great Salt Lake and huge areas of evaporated deposits of salt minerals. At age three I saw my natural mother killed by lightning and my natural father drafted into the Pacific theatre of World War II. Between ages three and five I was the ‘guest’ of a large extended family of aunts and uncles. After age five I was adopted by a carpenter and stone mason who lived in upstate New York. There I learned to work with my hands. I was a strange little grass orphan. The aunts wanted to mother me but the uncles had the pragmatic upper hand. How strange was I? One aunt, in particular, recalled that she came in the kitchen and found me at the kitchen table intent on sorting grains of salt. I had at that age some sort of microscopic vision; some of my own children told me they went through a sort of microscopic vision stage and later lost it, as did I. Those little cubettes of salt had a great fascination for me, a fascination not shared by sensible uncles. It was only much later that I learned to call the stuff Na^+Cl^- and that there was an interpenetrating pair of ion lattices underlying their cubical structure which I certainly could not see. Even so it was interesting to stack those grains of salt, the pre-Lego natural material I had to play with.

Second answer: I was an undergraduate at Hamilton College. My high school mathematics teacher Florence Deci, who appreciated my art as well as my



Figure 1 The David Borwein Distinguished Career Award of the Canadian Mathematical Society, created in 2004, is a bronze sculpture based on Benson’s formula for the Madelung constant. An exact copy is given to each award winner. Photograph by permission of the sculptor.

maths, had advised me to choose a liberal arts school so I could do both art and science. As a maths undergraduate I was fascinated by summability and conditionally convergent series. From my Hamilton chemistry professor Leland ‘Bud’ Cratty, I first heard about salt and its curious connection with a mathematical sum, Madelung’s constant. The non-commutativity of infinitely many summands was observed by Riemann in relation to the conditionally convergent series $\sum_{k \geq 1} (-1)^{k-1}/k$, which is supposed to be a representation of $\log 2 = 0.69314718\dots$; this value obtains by adding the terms in increasing k order, as is implicit in the convention of summation notation. Even worse in some respects, for Madelung’s series adding terms in increasing cubes gives a different answer than adding terms in increasing balls. So what is the true value, the value with which physicists like Born, Madelung, and Benson and mathematicians like the Borweins would be satisfied? Benson answered this most remarkably with

$$\mu = 12\pi \sum_{m \geq 0} \sum_{n \geq 0} \frac{1}{\cosh^2(\frac{\pi}{2} \sqrt{(2m+1)^2 + (2n+1)^2})},$$

which is an absolutely convergent series with all positive terms very rapidly decreasing, affording its evaluation to many decimal places:

$$\mu = 1.7475645946331821906362120355443974034851614366 \\ 2474175815282535076504\dots,$$

enough decimals to satisfy this sculptor. Subsequently, Borwein Crandall [2] and others have learned more and give an almost closed form for μ .

When the Borwein family asked me to do a sculpture about summability to celebrate the mathematics of David Borwein and his sons, particularly its application to Madelung’s constant, you can see that my art and science pump had been primed long ago in the deserts of the Rocky Mountains and the forests of the Finger Lakes of upstate New York. It is true that when the Borweins approached me about doing this sculpture, I had been celebrating mathematics with sculpture for decades. However, they approached me while I was in my negative-Gaussian-curvature phase and was carving granite, not salt, and would my geometric negative Gaussian curvature phase be inhospitable to the hard analysis about conditional triple sums over three-dimensional lattices?

It happened that I had developed a series of sculptures which involved two-dimensional lattice sums, specifically having to do with the planets and Kepler’s third law, i.e., that the squares of the orbital periods of the planets are proportional to the cubes of their radii, when this law is viewed in terms of elliptic complex curves or real tori in four and three real dimensions. For example, the planet Jupiter takes about $y = 11$ earth–sun years to elliptically orbit the sun at $x = 5$ earth–sun distances, and $11^2 = y^2 = x^3 - x + 1 = 5^3 - 5 + 1$ is a perfectly respectable \mathbb{Z} -rank-2 elliptic curve in the two complex dimensions of x and

y , which corresponds to four real dimensions. To get the planet Jupiter's elliptic curve into three real dimensions where I could expect to do sculpture required negative-Gaussian-curvature forms and lattice sums!

Some mathematical details behind my negative-Gaussian-curvature phase appeared in 'Sculpture inspired by work with Alfred Gray: Kepler elliptic curves and minimal surface sculptures of the planets' [3],² reflecting a keynote address by Helaman and Claire Ferguson for the Alfred Gray Memorial Congress on Homogeneous Spaces, Riemannian Geometry, Special Metrics, Symplectic Manifolds and Topology, held in September 2000 in Bilbao, Spain. This work actually made copious use of and reference to the Borwein brothers' *Pi and the AGM* [1],² an important resource for this negative-curvature phase of my sculpture.

What could be more natural than the conditional sum of a three-dimensional lattice as a period of a two-dimensional lattice to create a Madelung triply punctured torus immersed with negative Gaussian curvature in three-dimensional space? The Borwein Award sculpture emerged after considerable computational and sculptural work, which I will sketch next.

I had some number theoretical issues, which I discussed in detail with Jon Borwein. These involved the exponent in the denominator of the lattice sum, $s = \frac{1}{2}$ for the square root. As a function of the complex variable s , ought not the series $L_{\text{NaCl}}(s)$ have an analytic continuation to the whole plane, Riemann hypothesis, and even a functional equation? I thought it important to immerse the matter of salt symbolized by Madelung's constant as $L_{\text{NaCl}}(\frac{1}{2})$ in this larger world. Did it have an Euler product? The answers to these two questions are yes, no, yes, and no and appear in the writings of Jon Borwein and others elsewhere.

After much computation of $L_{\text{NaCl}}(s)$ for various values of s , I settled on $\mu = L_{\text{NaCl}}(\frac{1}{2})$ and an elliptic curve,

$$y^2 = 4x^3 - (32.6024622677216\dots)x - (70.6022720835820\dots)$$

where the decimals correspond to two-dimensional lattice sums for a lattice involving μ , with discriminant $-99932.555\dots$. The complex variables x, y are complex numbers in four real dimensions and the complex curve equation amounts to two real equations, so that the complex curve is really a surface in four dimensions. There is a dimension embargo (the Planck length is even harder to see than salt lattices!) on sculpture. Sculpture physically resides in spatial three dimensions, hence I enjoy the use of negative curvature to get the geometric surface in four dimensions into the spatial three dimensions where I have much experience.

While my aesthetic choice is to carve stone, my award sculptures are in polished silicon bronze. Silicon bronze is an alloy of copper with silicon and a few other things to improve flow and polishing. A typical recipe for silicon bronze is the 'molecule' $9438\text{Cu} + 430\text{Si} + 126\text{Mn} + 4\text{Fe} + \text{Zn} + \text{Pb}$. I think of the $430\text{Si} + 126\text{Mn} + 4\text{Fe} + \text{Zn} + \text{Pb}$ piece as being the 'stone' part. I wonder, is

there a Madelung constant for this molecule, there being many loose ions in this polycrystalline soup?

There are many steps in the casting of silicon bronze, but even before getting to those, I had much computation to do in placing the complex curve into three dimensions as a triply punctured torus. In the course of a computation and developing the computer graphics there are many choices to be made. My decision process is informed by my studio experience in the same way that looking at two-dimensional underwater video material is not at all the same after learning to scuba dive in a three-dimensional environment. This is not the place to discuss all these transitions; there are many. In Figure 2 some of them are shown: computer graphics, wire frame, clay, plaster. There are truly messy in between parts, especially making of the mould, the wax positive image, the ceramic shells to form a negative flask, and a hot dry throat embedded in sand in which to pour molten bronze; there is the high drama of the pouring of the bronze, the violence of smashing the ceramic flask to release the imprisoned bronze, then the hacking-off of air escape sprues, chasing away all evidence of what violence the bronze has experienced, grinding and sanding the bronze smooth enough to reveal the inevitable natural errors, which must be excavated and welded in kind to prepare for polishing. While the intermediate result is a beautiful polished bronze, shown in Figure 3, this is not the end.

I am carving into this silicon bronze the name of each recipient of this elegant CMS–SMC David Borwein Award, the provenance of the sculpture, and also in Figure 1 something about the sculpture relating to salt and summability. This is what is shown for the first recipient.

Art is always a social event in the end. In the case of this Borwein Award, the truly priceless part is the awarding of a silicon bronze to celebrate the distinguished careers of gifted people who have given substantial parts of their lives to creating new mathematics and even new mathematicians, as has David Borwein. So far these people have included:

2010: Nassif Ghoussoub

2008: Hermann Brunner

2006: Richard Kane



Figure 2 Stages in the design of 'Salt'.



Figure 3 The David Borwein Distinguished Career Award of the Canadian Mathematical Society. Photograph by permission of the sculptor.

I am honored that my mathematical sculpture is part of recognizing and celebrating mathematical lives.

References

- [1] J. M. Borwein and P. B. Borwein. *Pi and the AGM – A Study in Analytic Number Theory and Computational Complexity*. Wiley, New York, 1987.
- [2] J. M. Borwein and R. E. Crandall. Closed forms: what they are and why we care. *Not. Amer. Math. Soc.*, 60(1):60–65, 2013.
- [3] Helaman Ferguson and Claire Ferguson. Sculpture inspired by work with Alfred Gray: Kepler elliptic curves and minimal surface sculptures of the planets. *Contemp. Math.*, 288:39–53, 2000.

Preface

... Born decided to investigate the simple ionic crystal – rock salt (sodium chloride) – using a ring model. He asked Landé to collaborate with him in calculating the forces between the lattice points that would determine the structure and stability of the crystal. Try as they might, the mathematical expression that Born and Landé derived contained a summation of terms that would not converge. Sitting across from Born and watching his frustration, Madelung offered a solution. His interest in the problem stemmed from his own research in Göttingen on lattice energies that, six years earlier, had been a catalyst for Born and von Karman's article on specific heat. The new mathematical method he provided for convergence allowed Born and Landé to calculate the electrostatic energy between neighboring atoms (a value now known as the Madelung constant).¹ Their result for lattice constants of ionic solids made up of light metal halides (such as sodium and potassium chloride), and the compressibility of these crystals agreed with experimental results.²

The study of lattice sums is an important topic in mathematics, physics, and other areas of science. It is not a new field, dating back at least to the work of Appell in 1884, and has attracted contributions from some of the most eminent practitioners of science (Born and Landé [1], Rayleigh, Bethe, Hardy, ...). Despite this, it has not been widely recognised as an area with its own important tradition, results, and techniques. This has led to independent discoveries and rediscoveries of important formulae and methods and has impeded progress in some topics owing to the lack of knowledge of key results.

In order to solve this problem, Larry Glasser and John Zucker published in 1981 a seminal paper, the first comprehensive review of what was then known about the analytic aspects of lattice sums. This work was immensely valuable to many researchers, including the other authors of the present monograph, but now

¹ More exactly, this energy can be obtained from the Madelung constant.

² From [5], pp. 79–80. Max Born was the maternal grandfather of the singer and actress Olivia Newton-John. Actually, soon after this they discovered that they had forgotten to divide by 2 in the compressibility analysis. This ultimately led to the abandonment of the Bohr–Sommerfeld planar model of the atom.

is out of date and lacks the immediate electronic accessibility expected by today's researchers.

Hence, we have the genesis of the present project, the composition of this monograph. It contains a slightly corrected version of the 1981 paper of Glasser and Zucker as well as additions reflecting the progress of the subject since 1981. The authors hope it is sufficiently comprehensive in flavour to be of value to both experienced practitioners and those new to the field. However, as the study of lattice sums has applications in many diverse areas, the authors are well aware that important contributions may have been overlooked. They would thus welcome comments from readers regarding such omissions and hope that internet technology can make this a living and growing project rather than a static compendium.

The emphasis of the results collected here is on analytic techniques for evaluating lattice sums and results obtained using them. We will nevertheless touch upon numerical methods for evaluating sums and how these may be used in the spirit of experimental mathematics to discover new formulae for sums. Those interested primarily in numerical evaluation would do well to consult the relatively recent reviews of Moroz [7] and Linton [6].

Several chapters in this monograph are based on published material and, as such, we have tried to retain their original styles. In particular, we have not attempted to iron out the differences in notation. (we considered this option but decided it would be very likely to introduce more errors and difficulties than it removed). In particular, we alert the reader that several conventions of the summation notation are used liberally throughout the monograph: the symbol \sum may indicate either a single or a multiple sum and the variable(s) and range(s) of summation may be omitted when they are clear from the context. The reader is therefore advised to exercise caution when moving from chapter to chapter and to note that various notations are listed at the beginning of the index. The index uses bold font to indicate entries which are definitions and includes page numbers for the various tables.

We have made a full-hearted attempt to correct misprints in the original material. The end-of-chapter commentaries also direct the reader to more recent material and discussions of the source material. In the same spirit, each chapter has its own reference list while a complete bibliography is also provided at the end of the book.

Chapter 1 originally appeared as [4]. Chapter 2 originally appeared as [3] and is reprinted with permission from the American Institute of Physics. Chapter 8 originally appeared as [2]: it was published in the *Transactions of the American Mathematical Society*, in vol. 350 (1998), © the American Mathematical Society 1998. Chapter 9 originally appeared as [8]: it was published in the *Journal of Statistical Physics*, in vol. 134 (2011), © Springer-Verlag 2011 with kind permission from Springer Science+Business Media.

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Chapter 9: The chapter author wishes to thank Geoff Joyce and Richard Delves, since without their input none of this could have been written. He also thanks Tony Guttmann for many pertinent comments.

Commentaries: We would like to thank Tony Guttmann, Roy Hughes, and Mathew Rogers for their valuable feedback on these.

Websiste. The authors are maintaining a website for the book at <http://www.carma.newcastle.edu.au/LatticeSums/>, at which updates and corrections can be received.

References

- [1] M. Born and A. Landé. The absolute calculation of crystal properties with the help of Bohr's atomic model. Part 2. *Sitzungsberichte der Königlich Preussischen Akademie der Wissenschaften*, pp. 1048–1068, 1918.
- [2] D. Borwein, J. M. Borwein, and C. Pinner. Convergence of Madelung-like lattice sums. *Trans. Amer. Math. Soc.*, 350:3131–3167, 1998.
- [3] D. Borwein, J. M. Borwein, and K. Taylor. Convergence of lattice sums and Madelung's constant. *J. Math. Phys.*, 26:2999–3009, 1985.
- [4] M. L. Glasser and I. J. Zucker. Lattice sums. In *Theoretical Chemistry, Advances and Perspectives*, vol. 5, eds. H. Eyring and D. Henderson, pp. 67–139, 1980.
- [5] N. T. Greenspan. *The End of the Certain World: The Life and Science of Max Born*. Basic Books, 2005.
- [6] C. M. Linton. Lattice sums for the Helmholtz equation. *SIAM Review*, 52:630–674, 2010.
- [7] A. Moroz. On the computation of the free-space doubly-periodic Green's function of the three-dimensional Helmholtz equation. *J. Electromagn. Waves Appl.*, 16:457–465, 2002.
- [8] I. J. Zucker. 70 years of the Watson integrals. *J. Stat. Phys.*, 143:591–612, 2011.

Bibliography

- Abramowitz, M. and I. A. Stegun. *Handbook of Mathematical Functions with Formulas, Graphs and Mathematical Tables*. Dover, New York, 1972.
- Adamchik, V. On the Hurwitz function for rational arguments. *Appl. Math. Comp.*, 187: 3–12, 2007.
- Adler, S. Generalized Ewald method for lattice sums. *Physica (Utrecht)*, 27:1193–1201, 1961.
- Andrews, G. E., R. Askey, and R. Roy. *Special Functions*. Cambridge University Press, Cambridge, 1999.
- Appell, P. Sur les transformations des équations différentielles linéaires. *C. R. Acad. Sci. Paris*, 91:211–214, 1880.
- Appell, P. Sur les fonctions de trois variables réelles satisfaisant à l'équation différentielle $\Delta F = 0$. *Acta Math.*, 4:313–374, 1884.
- Appell, P. Sur quelques applications de la fonction $Z(x, y, z)$ à la physique mathématique. *Acta Math.*, 8:265–294, 1886.
- Appell, P. Sur les fonctions harmoniques à trois groupes de périodes. *Rend. Circ. Mat. Palermo*, 22:361–370, 1906.
- Ayoub, R. *An Introduction to the Analytic Theory of Numbers*. American Mathematical Society, Providence, 1963.
- Bailey, D. H., J. M. Borwein, D. Broadhurst, and M. L. Glasser. Elliptic integral evaluations of Bessel moments and applications. *J. Phys. A: Math. Theor.*, 41:205203, 2008.
- Bailey, D. H., J. M. Borwein, R. E. Crandall, and I. J. Zucker. Lattice sums arising from the Poisson equation. 2012. Preprint.
- Bailey, W. N. A reducible case of the fourth type of Appell's hypergeometric functions of two variables. *Quart. J. Math. Oxford*, 4:305–308, 1933.
- Bailey, W. N. Some infinite integrals involving Bessel functions. *Proc. London Math. Soc.*, 40:37–48, 1935.
- Baldereschi, A., G. Senatore, and I. Oriani. Madelung energy of the Wigner crystal on lattices with non-equivalent sites. *Solid State Commun.*, 81:21–22, 1992.
- Barber, M. N. Cross-over phenomena in the asymptotic behaviour of lattice sums. *J. Phys. A.*, 10:2133–2142, 1977.

- Bellman, R. *A Brief Introduction to Theta Functions*. Holt, New York, 1961.
- Benson, G. C. A simple formula for evaluating the Madelung constant of a NaCl-type crystal. *Can. J. Phys.*, 34:888–890, 1956.
- Benson, G. C. and H. P. Schreiber. A method for the evaluation of some lattice sums occurring in calculations of physical properties of crystals. II. *Can. J. Phys.*, 33:529–533, 1955.
- Benson, G. C., H. P. Schreiber, and D. Patterson. An examination of the Verwey model for the lattice structure of the free surface of alkali halide crystals. *Can. J. Phys.*, 34:265–275, 1956.
- Benson, G. C. and F. van Zeggeren. Madelung constants of some cubic crystals. *J. Chem. Phys.*, 26:1083–1085, 1957.
- Berndt, B. C. *Ramanujan's Notebooks Part III*. Springer-Verlag, New York, 1991.
- Berndt, B. C., G. Lamb, and M. Rogers. Two dimensional series evaluations via the elliptic functions of Ramanujan and Jacobi. *Ramanujan Journal*, 2011.
- Bertaut, F. L'énergie électrostatique de réseaux ioniques. *J. Phys. Radium*, 13:499–505, 1952.
- Bertaut, F. C. R. *Hebd. Seances Acad. Sci.*, 239:234–235, 1954.
- Bertin, M. J. Mesure de Mahler d'hypersurfaces K^3 . *J. Number Theory*, 128:2890–2913, 2008.
- Bethe, H. Splitting of terms in crystals. *Ann. Phys. (Leipzig)*, 3:137, 1929.
- Birman, J. L. Effect of overlap on electrostatic lattice potentials in ionic crystals. *Phys. Rev.*, 97:897–902, 1955.
- Blakemore, J. S. *Solid State Physics*. Saunders, Philadelphia, 1969.
- Bogomolny, E. and P. Leboeuf. Statistical properties of the zeros of zeta functions – beyond the Riemann case. *Nonlinearity*, 7:1155–1167, 1994.
- Bonsall, L. and A. A. Maradudin. Some static and dynamical properties of a two-dimensional Wigner crystal. *Phys. Rev. B*, 15:1959–1973, 1977.
- Boon, M. and J. Zak. Coherent states and lattice sums. *J. Math. Phys.*, 19:2308–2311, 1978.
- Born, M. *Dynamik der Kristallgitter*. Teubner, Leipzig, 1916.
- Born, M. Über elektrostatische Gitterpotentiale. *Zeitschrift für Physik*, 7:124–140, 1921.
- Born, M. and M. Bradburn. The thermodynamics of crystal lattices. II. *Proc. Camb. Phil. Soc.*, 39:104–113, 1943.
- Born, M. and R. Fürth. The stability of crystal lattices. III. *Proc. Camb. Phil. Soc.*, 36:454–465, 1940.
- Born, M. and M. Göppert-Mayer. In *Handbuch der Physik* (S. Fliigge, ed.), vol. 24, Part 2, p. 707. Springer-Verlag, Berlin and New York, 1933.
- Born, M. and A. Landé. The absolute calculation of the crystal properties with the help of Bohr's atomic model. Part 2. In *Sitzungsberichte der Koniglich Preussischen Akademie der Wissenschaften*, pages 1048–1068, 1918.
- Born, M. and R. D. Misra. On the stability of crystal lattices. IV. *Proc. Camb. Phil. Soc.*, 36:466–478, 1940.
- Bornemann, F., D. Laurie, S. Wagon, and J. Waldvogel. *The SIAM 100-Digit Challenge*. SIAM, 2004.

- Borwein, D. and J. M. Borwein. A note on alternating series in several dimensions. *Amer. Math. Mon.*, 93:531–539, 1985.
- Borwein, D. and J. M. Borwein. Some exponential and trigonometric lattice sums. *J. Math. Anal. Appl.*, 188:209–5218, 1994.
- Borwein, D., J. M. Borwein, and C. Pinner. Convergence of Madelung-like lattice sums. *Trans. Amer. Math. Soc.*, 350:3131–3167, 1998.
- Borwein, D., J. M. Borwein, and R. Shail. Analysis of certain lattice sums. *J. Math. Anal. Appl.*, 143:126–137, 1989.
- Borwein, D., J. M. Borwein, R. Shail, and I. J. Zucker. Energy of static electron lattices. *J. Phys. A: Math. Gen.*, 21:1519–1531, 1988.
- Borwein, D., J. M. Borwein, and K. Taylor. Convergence of lattice sums and Madelung’s constant. *J. Math. Phys.*, 26:2999–3009, 1985.
- Borwein, J. M. and D. H. Bailey. *Mathematics by Experiment: Plausible Reasoning in the 21st Century*, 2nd edition. A. K. Peters, 2008.
- Borwein, J. M. and P. B. Borwein. *Pi and the AGM – A Study in Analytic Number Theory and Computational Complexity*. Wiley, New York, 1987.
- Borwein, J. M., P. B. Borwein, and F. G. Garvan. Some cubic modular identities of Ramanujan. *Trans. Amer. Math. Soc.*, 343:35–47, 1994.
- Borwein, J. M. and K.-K. S. Choi. On the representations of $xy + yz + zx$. *Exp. Math.*, 9:153–158, 2000.
- Borwein, J. M. and A. S. Lewis. Partially-finite convex programming in L^1 : entropy maximization. *SIAM J. Optimization*, 3:248–267, 1993.
- Borwein, J. M., A. Straub, and J. G. Wan. Three-step and four-step random walk integrals. *Exp. Math.*, 2013.
- Borwein, J. M., A. Straub, J. G. Wan, and W. Zudilin. Densities of short uniform random walks. *Can. J. Math.*, 64:961–990, 2012, with an appendix by Don Zagier.
- Borwein, J. M. and J. Vanderwerff. *Convex Functions: Constructions, Characterizations and Counterexamples*. Encyclopedia of Mathematics and Applications, vol. 109, Cambridge University Press, 2010.
- Borwein, J. M. and I. J. Zucker. Elliptic integral evaluation of the Gamma function at rational values of small denominator. *IMA J. Numer. Anal.*, 12:519–526, 1992.
- Borwein, J. M. and R. E. Crandall. Closed forms: what they are and why we care. *Not. Amer. Math. Soc.*, 60(1):60–65, 2013.
- Boyd, D. W. Mahler’s measure and special values of L -functions. *Exp. Math.*, 7:37–82, 1998.
- Broadhurst, D. Elliptic integral evaluation of a Bessel moment by contour integration of a lattice Green function. 2008. Preprint: arXiv:0801.0891v1.
- Brown, E. and C. J. Parry. The imaginary bicyclic biquadratic fields with class number 1. *J. Reine Angew. Math.*, 266:118–120, 1974.
- Buhler, J. P. and R. E. Crandall. On the convergence problem for lattice sums. *J. Phys. A: Math. Gen.*, 23:2523–2528, 1990.
- Burrows, E. L. and S. F. A. Kettle. Madelung constants and other lattice sums. *J. Chem. Ed.*, 52:58–59, 1975.

- Campbell, E. S. Existence of a well defined specific energy for an ionic crystal – justification of Eward’s formulae and of their use to deduce equations for multipole lattices. *J. Phys. Chem. Solids*, 24:197, 1963.
- Cayley, A. *The Collected Mathematical Papers, vol. 1*. Cambridge University Press, 1889.
- Cayley, A. *An Elementary Treatise on Elliptic Functions*, 2nd edition. Deighton, Bell and Co., 1895.
- Chaba, A. N. and R. K. Pathria. Evaluation of a class of lattice sums in arbitrary dimensions. *J. Math. Phys.*, 16:1457–1460, 1975.
- Chaba, A. N. and R. K. Pathria. Evaluation of lattice sums using Poisson’s summation formula. 2. *J. Phys. A*, 9:1411–1423, 1976a.
- Chaba, A. N. and R. K. Pathria. Evaluation of lattice sums using Poisson’s summation formula. 3. *J. Phys. A*, 9:1801–1810, 1976b.
- Chaba, A. N. and R. K. Pathria. Evaluation of lattice sums using Poisson’s summation formula. 4. *J. Phys. A*, 10:1823–1832, 1977.
- Chen, L. C. and F. Y. Wu. The random cluster model and a new integration identity. *J. Phys. A: Math. Gen.*, 38:6271–6276, 1005.
- Chin, S. K., N. A. Nicorovici, and R. C. McPhedran. Green’s function and lattice sums for electromagnetic scattering by a square array of cylinders. *Phys. Rev. E*, 49, 1994.
- Chowla, S. An extension of Heilbronn’s class number theorem. *Quart. J. Math. Oxford*, 5:304–307, 1934.
- Clausen, T. Ueber die fälle wenn die Reihe $y = 1 + \frac{\alpha\beta}{1-\gamma}x + \dots$ ein quadrat von der Form $y = 1 + \frac{\alpha'\beta'\gamma'}{1-\delta'\epsilon'}x + \dots$ hat. *J. Math.*, 3:89–95, 1828.
- Clausius, R. *Die Mechanische Behandlung der Electricität*. Braunschweig, Vieweg, 1879.
- Cockayne, E. Comment on ‘stability of the Wigner electron crystal on the perovskite lattice’. *J. Phys: Condens. Matter*, 3:8757, 1991.
- Cohn, H. *A Classical Invitation to Algebraic Numbers and Class Fields*. Springer-Verlag, Berlin and New York, 1978.
- Coldwell-Horsfall, R. A. and A. A. Maradudin. Zero point energy of an electron lattice. *J. Math. Phys.*, 1:395–404, 1960.
- Colquitt, D. J., M. J. Nieves, I. S. Jones, A. B. Movchan, and N. V. Movchan. Localisation for an infinite line defect in an infinite square lattice. Preprint, *arXiv*, 1208.1871v2:1–24, 2012.
- Conrey, J. B. The Riemann hypothesis. *Not. AMS*, 50:341–353, 2003.
- Courant, R. Über partielle Differenzengleichung. In *Proc. Atti Congresso Internazionale Dei Matematici, Bolgna*, vol. 3, pp. 83–89, 1929.
- Courant, R., K. Friedrichs, and H. Lewy. Über die partiellen Differenzengleichung der mathematischen Physik. *Math. Ann.*, 100:32–74, 1928.
- Crandall, R. E. New representations for the Madelung constant. *Exp. Math.*, 8:367–379, 1999.
- Crandall, R. E. The Poisson equation and ‘natural’ Madelung constants. 2012. Preprint.
- Davies, H. Poisson’s partial differential equation. *Quart. J. Math.*, 6:232–240, 1955.
- De Wette, F. W. Electric field gradients in point-ion and uniform-background lattices. *Phys. Rev.*, 123:103, 1961.
- De Wette, F. W. and G. E. Schacher. Internal fields in general dipole lattices. *Phys. Rev. A*, 137:78–91, 1965.

- Delves, R. T. and G. S. Joyce. On the Green function for the anisotropic simple cubic lattice. *Ann. Phys.*, 291:71–133, 2001.
- Delves, R. T. and G. S. Joyce. Exact product form for the anisotropic simple cubic lattice Green function. *J. Phys. A: Math. Theor.*, 39:4119–4145, 2006.
- Delves, R. T. and G. S. Joyce. Derivation of exact product forms for the simple cubic lattice Green function using Fourier generating functions and Lie group identities. *J. Phys. A: Math. Theor.*, 40:8329–8343, 2007.
- Deninger, C. Deligne periods of mixed motives, K -theory and the entropy of certain Z^n -actions. *J. Amer. Math. Soc.*, 10:259–281, 1997.
- Dickson, L. E. *An Introduction to the Theory of Numbers*. Dover, New York, 1957.
- Dietz, B. and K. Zyczkowski. Level-spacing distributions beyond the Wigner surmise. *Z. Phys. Condens. Matter*, 84:157–158, 1991.
- Domb, C. On multiple returns in the random walk problem. *Proc. Camb. Phil. Soc.*, 50:586–591, 1954.
- Doyle, P. G. and L. J. Snell. *Random Walks and Electric Networks*. Carus Mathematical Monographs, 1984.
- Duffin, R. J. Discrete potential theory. *Duke Math. J.*, 20:233–251, 1953.
- Emersleben, O. Zetafunktionen und elektrostatische Gitterpotentiale. I. *Phys. Z.*, 24:73–80, 1923a.
- Emersleben, O. Zetafunktionen und elektrostatische Gitterpotentiale. II. *Phys. Z.*, 24:97–104, 1923b.
- Emersleben, O. Die elektrostatische Gitterenergie eines neutralen ebenen, insbesondere alternierenden quadratischen Gitters. *Z. Phys.*, 127:588–609, 1950a.
- Emersleben, O. Über die Berechnung der Gitterenergie endlicher Kristallstücke. *Z. Angew. Math. Mech.*, 30:252–254, 1950b.
- Emersleben, O. *Math. Nachr.*, 4:468–480, 1951.
- Emersleben, O. *Z. Phys. Chem.*, 194:170–190, 1952.
- Emersleben, O. Über Summen Epsteinscher Zetafunktionen regelmäßig verteilter ‘unterer’ Parameter. *Math. Nachr.*, 13:59–72, 1954.
- Emersleben, O. Über Funktionalgleichungen zwischen Epsteinscher Zetafunktionen gleichen Arguments. *Math. Nachr.*, 44:205–230, 1970.
- Engblom, S. Gaussian quadratures with respect to discrete measures. *Uppsala University Technical Reports*, 7:1–17, 2006.
- Epstein, P. Zur Theorie allgemeiner Zetafunktionen. *Math. Ann.*, 56:615–644, 1903.
- Evjen, H. On the stability of certain heteropolar crystals. *Phys. Rev.*, 39:675–687, 1932.
- Ewald, P. Die Berechnung optischer und elektrostatischer Gitterpotentiale. *Ann. Phys.*, 64:253–287, 1921.
- Ferguson Helaman and Claire Ferguson. Sculpture inspired by work with Alfred Gray: Kepler elliptic curves and minimal surface sculptures of the planets. *Contemp. Math.*, 288:39–53, 2000.
- Fetter, A. L. Evaluation of lattice sums for clean type-II superconductors. *Phys. Rev. B*, 11:2049–2052, 1975.
- Foldy, L. L. Electrostatic stability of Wigner and Wigner–Dyson lattices. *Phys. Rev. B*, 17:4889–4894, 1978.

- Folsom, A., W. Kohnen, and S. Robins. Conic theta functions and their relations to theta functions. 2011. Preprint.
- Forrester, P. J. and M. L. Glasser. Some new lattice sums including an exact result for the electrostatic potential within the NaCl lattice. *J. Phys. A*, 15:911–914, 1982.
- Fuchs, K. A quantum mechanical investigation of the cohesive forces of metallic copper. *Proc. Roy. Soc. London A*, 151:585–602, 1935.
- Fumi, F. G. and M. P. Tosi. On the Naor relations between Madelung constants for cubic ionic lattices. *Phil. Mag.*, 2:284, 1957.
- Fumi, F. G. and M. P. Tosi. Extension of the Madelung method for the evaluation of lattice sums. *Phys. Rev.*, 117:1466–1468, 1960.
- Garnett, J. C. M. Colours in metal glasses and in metallic films. *Phil. Trans. Roy. Soc. London*, 203:385–420, 1904.
- Glaisher, J. W. L. *Messenger of Mathematics*, 24:27, 1895.
- Glasser, M. L. A Watson sum for a cubic lattice. *J. Math. Phys.*, 13:1145, 1972.
- Glasser, M. L. Evaluation of lattice sums. I. Analytic procedures. *J. Math. Phys.*, 14:409–413, 1973a.
- Glasser, M. L. The evaluation of lattice sums. II. Number-theoretic approach. *J. Math. Phys.*, 14:701–703, 1973b.
- Glasser, M. L. The evaluation of lattice sums. III. Phase modulated sums. *J. Math. Phys.*, 15:188–189, 1974.
- Glasser, M. L. Evaluation of lattice sums. IV. A five-dimensional sum. *J. Math. Phys.*, 16:1237–1238, 1975.
- Glasser, M. L. Definite integrals of the complete elliptic integral K . *J. Res. NBS.*, 80B:313–323, 1976.
- Glasser, M. L. and G. Lamb. A lattice spanning tree entropy function. *J. Phys. A: Math. Gen.*, 38:L471–L475, 2005.
- Glasser, M. L. and E. Montaldi. Staircase polygons and recurrent lattice walks. *Phys. Rev. E.*, 48:2339–2342, 1993.
- Glasser, M. L. and V. E. Wood. A closed form evaluation of the elliptical integral. *Math. Comput.*, 25:535–536, 1971.
- Glasser, M. L. and F. Y. Wu. On the entropy of spanning trees on a large triangular lattice. *Ramanujan Journal*, 10:205–214, 2005.
- Glasser, M. L. and I. J. Zucker. Extended Watson integrals for the cubic lattices. *Proc. Nat. Acad. Sci. USA*, 74:1800–1801, 1977.
- Glasser, M. L. and I. J. Zucker. Lattice sums. In *Theoretical Chemistry, Advances and Perspectives*, eds H. Eyring and D. Henderson, vol. 5, pp. 67–139, 1980.
- Gordon, B. Some identities in combinatorial analysis. *Quart. J. Math.*, 12:285–290, 1961.
- Goursat, E. Sur l'équation différentielle linéaire qui admet pour intégrale la série hypergéométrique. *Ann. Sci. École Norm. Sup.*, 10:S3–S142, 1881.
- Graovac, A., H. J. Monkhorst, and M. L. Glasser. Computation of Fourier transform quantities in Hartree–Fock calculations for simple crystals. *Int. J. Quantum Chem.*, 9:243–259, 1975.
- Greenspan, N. T. *The End of the Certain World: The Life and Science of Max Born*. Basic Books, 2005.

- Guillera, J. and M. Rogers. Ramanujan series upside-down. preprint. Submitted for publication on 18 June 2012.
- Guttman, A. J. Lattice Green functions in all dimensions. *J. Phys. A: Math. Theor.*, 43:305205, 2010.
- Guttman, A. J. and T. Prellberg. Staircase polygons, elliptic integrals, Heun functions, and lattice Green functions. *Phys. Rev. E.*, 47:R2233–R2236, 1993.
- Guttman, A. J. and M. Rogers. An integral arising from the chiral $sl(n)$ Potts model. Preprint.
- Guttman, A. J. and M. Rogers. Spanning tree generating functions and Mahler measures. *J. Phys. A.*, to appear.
- Guy, R. K. Gauss' lattice point problem. In *Unsolved Problems in Number Theory, 2nd edition*. Springer-Verlag, New York, 1994.
- Hall, G. E. Asymptotic properties of generalized Chaba and Pathria lattice sums. *J. Math. Phys.*, 17:259–260, 1976a.
- Hall, G. E. Weak phase transitions in asymptotic properties of lattice sums. *J. Stat. Phys.*, 14:521–524, 1976b.
- Hall, G. E. Order relations for lattice sums from order relations for theta functions. *J. Phys. Chem. Solids*, 38:367–373, 1977.
- Hardy, G. H. On some definite integral considered by Mellin. *Messenger of Mathematics*, 49:85–91, 1919.
- Hardy, G. H. and M. Riesz. *The General Theory of Dirichlet Series*. Cambridge Tracts in Mathematics and Mathematical Physics, Cambridge University Press, 1915.
- Hardy, G. H. and E. M. Wright. *An Introduction to the Theory of Numbers, 4th edition*. Clarendon, Oxford, 1960.
- Harris, F. E. and H. J. Monkhorst. Electronic-structure studies of solids. I. Fourier representation method for Madelung sums. *Phys. Rev. B*, 2:4400–4405, 1970.
- Hautot, A. A new method for the evaluation of slowly convergent series. *J. Math. Phys.*, 15:1722–1727, 1974.
- Hautot, A. New applications of Poisson's summation formula. *J. Phys. A*, 8:853–862, 1975.
- Heller, W. R. and A. Marcus. A note on the propagation of excitation in an idealized crystal. *Phys. Rev.*, 84:809–813, 1951.
- Hioe, F. T. A Green's function for a cubic lattice. *J. Math. Phys.*, 19:1064–1067, 1978.
- Hirschhorn, M., F. Garvan, and J. M. Borwein. Cubic analogues of the Jacobian theta function $\Theta(q, z)$. *J. Math. Phys.*, 19:1064, 1978.
- Højendahl, K. K. *Dan. Vidensk. Selsk. Mat. Fys. Medd.*, 16:135, 1938.
- Hoskins, C. S., M. L. Glasser, and E. R. Smith. Half-space electrostatic sums. *J. Phys. A*, 10:879–884, 1977.
- Hove, J. and J. A. Krumhansl. The evaluation of lattice sums for cubic crystals. *Phys. Rev.*, 92:569–572, 1953.
- Hund, F. Versuch einer Ableitung der Gittertypen aus der Vorstellung des isotropen polarisierbaren Ions. *Z. Phys.*, 34:833–857, 1925.
- Hund, F. Vergleich der elektrostatischen Energien einiger Ionengitter. *Z. Phys.*, 94:11–21, 1935.
- Huxley, M. N. Exponential sums and lattice points II. *Proc. London Math. Soc.*, 66:279–301, 1993.

- Iwata, G. Evaluation of the Watson integral of a face-centered lattice. *Nat. Sci. Report, Ochanomizu University*, 20:13–18, 1969.
- Jacobi, C. G. *Fundamenta Nova Theoriae Functionum Ellipticarum*. Königsberg, 1829.
- Jacobi, C. G. *Gesammelte Werke, vol. 3*. Chelsea, New York, 1969.
- Jones, D. S. *Generalized Functions*. McGraw-Hill, New York, 1966.
- Jones, J. E. On the determination of molecular fields. III. From crystal measurements and kinetic theory data. *Proc. Roy. Soc. London A*, 106:709–718, 1924.
- Jones, J. E. and B. M. Dent. Cohesion at a crystal surface. *Trans. Faraday Soc.*, 24:92–108, 1928.
- Jones, J. E. and A. E. Ingham. On the calculation of certain crystal potential constants, and on the cubic crystal of least potential energy. *Proc. Roy. Soc. London A*, 107:636–653, 1925.
- Joyce, G. S. Lattice Green function for the anisotropic face centred cubic lattice. *J. Phys. C*, 4:L53–L56, 1971.
- Joyce, G. S. Lattice Green function for the simple cubic lattice. *J. Phys. A*, 5:L65–L68, 1972.
- Joyce, G. S. On the simple cubic lattice Green function. *Phil. Trans. Roy. Soc. London*, A273:583–610, 1973.
- Joyce, G. S. On the cubic lattice Green functions. *Proc. Roy. Soc. London*, A455:463–477, 1994.
- Joyce, G. S. On the cubic modular transformation and the cubic lattice Green functions. *J. Math. A: Math. Gen.*, 31:5105–5115, 1998.
- Joyce, G. S. Singular behaviour of the cubic lattice Green functions and associated integrals. *J. Phys. A: Math. Gen.*, 34:3831–3839, 2001.
- Joyce, G. S. Application of Mahler measure theory to the face-centred cubic lattice Green function at the origin and its associated logarithmic integral. *J. Phys. A: Math. Theor.*, 45:285001, 2012.
- Joyce, G. S. and R. T. Delves. Exact product forms for the simple cubic lattice Green functions: I. *J. Phys. A: Math. Gen.*, 37:3645–3671, 2004.
- Joyce, G. S. and R. T. Delves. Exact product forms for the simple cubic lattice Green functions: II. *J. Phys. A: Math. Gen.*, 37:5417–5447, 2004.
- Joyce, G. S., R. T. Delves, and I. J. Zucker. Exact evaluation of the Baxter–Bazhanov Green function. *J. Phys. A: Math. Gen.*, 31:1781–1790, 1998.
- Joyce, G. S., R. T. Delves, and I. J. Zucker. Exact evaluation for the anisotropic face-centred and simple cubic lattices. *J. Phys. A: Math. Gen.*, 36:8661–8672, 2003.
- Joyce, G. S. and I. J. Zucker. Evaluation of the Watson integral and associated logarithmic integral for the d -dimensional hypercubic lattice. *J. Phys. A*, 34:7349–7354, 2001.
- Joyce, G. S. and I. J. Zucker. On the evaluation of generalized Watson integrals. *Proc. AMS*, 133:71–81, 2004.
- Kac, V. G. Infinite-dimensional algebras, Dedekind's η -function, classical Möbius function and the very strange formula. *Adv. Math.*, 30:85–136, 1978.
- Kanamori, J., T. Moriya, K. Motizuki, and T. Nagamiya. Methods of calculating the crystalline electric field. *J. Phys. Soc.*, 10:93–102, 1956.

- Kanemitsu, S., Y. Tanigawa, K. Tsukada, and M. Yoshimoto. Chapter 9 in Crystal symmetry viewed as zeta symmetry. *Zeta Functions, Topology and Quantum Physics*. Springer, 2005.
- Kanemitsu, S. and H. Tsukada. *The Legacy of Alladi Ramakrishnan in the Mathematical Sciences: Crystal symmetry viewed as zeta symmetry II*. Springer, 2010.
- Kendall, J. The abnormality of strong electrolytes and the ionization theory of Ghosh. *J. Am. Chem. Soc.*, 44:717–738, 1922.
- Kittel, C. *Introduction to Solid State Physics*. Wiley, New York, 1953.
- Köhler, G. Some eta-identities arising from theta series. *Math. Scand.*, 66:147–154, 1990.
- Kornfeld, H. Die Berechnung elektrostatischer Potentiale und der Energie von Dipol- und Quadrupolgittern. *Z. Phys.*, 22:27–43, 1924.
- Krätzel, E. Bemerkungen zu einem Gitterpunkte. *Math. Ann.*, 179:90–96, 1969.
- Krätzel, E. and W. Nowak. Lattice points in large convex bodies, II. *Acta Arith.*, 62:285–295, 1992.
- Krazer, A. and E. Prym. *Neue Grundlagen einer Theorie der Allgemeinen Thetafunktionen*. Teubner, Leipzig, 1893.
- Kummer, E. E. Über die hypergeometrische Reihe. *J. Reine Angew. Math.*, 15:39–83, 127–172, 1836.
- Landau, E. Über eine Aufgabe aus der Theorie der quadratischen Formen. *Wien. Sitzungsber.*, 124:445–468, 1915.
- Landau, E. Zur analytischen Zahlentheorie der definiten quadratischen Formen (über Gitterpunkte in mehrdimensionalen Ellipsoiden). *S. B. Preuss. Akad. Wiss.*, 458–476, 1915.
- Landau, E. Über Gitterpunkte in mehrdimensionalen Ellipsoiden. *Math. Zeit.*, 21:126–132, 1924.
- Landau, E. Über Gitterpunkte in mehrdimensionalen Ellipsoiden. Zweite Abhandlung. *Math. Zeit.*, 24:299–310, 1926.
- Landau, E. *Vorlesungen über Zahlentheorie*, vol. 2, Part 8, Chapter 6 Chelsea, New York, 1955.
- Landauer, R. Electrical conductivity in inhomogeneous media. In *Proc. American Institute of Physics Conf.*, vol. 40, pp. 2–45, 1978.
- Landé, A. *Verh. Dtsch. Phys. Ges.*, 20:217, 1918.
- Lin, Y. K. Staggered ice-rule vertex model on the Kagome lattice. *J. Phys. A: Math. Gen.*, 8:1899–1919, 1975.
- Linton, C. M. Lattice sums for the Helmholtz equation. *SIAM Review*, 52:630–674, 2010.
- Lorentz, H. A. *The Theory of Electrons*. B. G. Teubner, Leipzig, 1909. Reprint: Dover, New York, 1952.
- Lorenz, L. Bidrag til titalienes teori. *Tidsskrift Math.*, 1:97–114, 1871.
- Lorenz, L. *Wiedemannsche Ann.*, 11:70, 1880.
- Mackenzie, J. K. General relation between lattice sums. *J. Chem. Phys.*, 26:1769, 1957.
- Mackenzie, J. K. A simple formula for evaluating the Madelung constant of a NaCl-type crystal. *Can. J. Phys.*, 35:500–501, 1957.
- Madelung, E. Das elektrische Feld in Systemen von regelmäßig angeordneten Punktladungen. *Phys. Z.*, 19:524–533, 1918.

- Madras, N., C. E. Soteris, S. G. Whittington, *et al.* The free energy of a collapsing branched polymer. *J. Phys. A: Math. Gen.*, 23:5327–5350, 1990.
- Maradudin, A. A., E. W. Montroll, G. H. Weiss, R. Herman, and W. H. Miles. *Green's Functions for Monatomic Simple Cubic Lattices*. Acadèmie Royale de Belgique, 1960.
- Maradudin, A. A. and G. H. Weiss. A method for evaluating lattice sums. *Can. J. Phys.*, 37:170–173, 1959.
- Martin, Y. and K. Ono. Eta-quotients and elliptic curves. *Proc. Amer. Math. Soc.*, 125:3169–3176, 1997.
- McCrea, W. H. A problem on random paths. *Math. Gazette*, 20:311–317, 1936.
- McCrea, W. H. and F. J. W. Whipple. Random paths in two and three dimensions. *Proc. Roy. Soc. Edinburgh*, 60:281–298, 1940.
- McKean, P. and V. Moll. *Elliptic Curves: Function Theory, Geometry, Arithmetic*. Cambridge University Press, New York, 1997.
- McNeil, M. B. Electrostatic energies calculated by plane-wise summation. *J. Phys. C*, 3:2020–2021, 1970.
- McPhedran, R. C., L. C. Botten, N. P. Nicorovici, and I. J. Zucker. Systematic investigation of two-dimensional static array sums. *J. Math. Phys.*, 48:033501, 2007.
- McPhedran, R. C., L. C. Botten, N. P. Nicorovici, and I. J. Zucker. On the Riemann property of angular lattice sums and the one-dimensional limit of two-dimensional lattice sums. *Proc. Roy. Soc. A*, 464:3327–3352, 2008.
- McPhedran, R. C., L. C. Botten, D. J. Williamson, and N. A. Nicorovici. The Riemann hypothesis and the zero distribution of angular lattice sums. *Proc. Roy. Soc. London A*, 467:2462–2478, 2011.
- McPhedran, R. C., G. H. Smith, N. A. Nicorovici, and L. C. Botten. Distributive and analytic properties of lattice sums. *J. Math. Phys.*, 45:2560–2578, 2004.
- Miller, J. Jr. *Lie Theory and Special Functions*. Academic Press, New York, 1968.
- Misra, R. On the stability of crystal lattices. II. *Proc. Camb. Phil. Soc.*, 36:173–182, 1940.
- Mityushev, V. V. Transport properties of doubly-periodic arrays of circular cylinders. *Z. Angew. Math. Mech.*, 77:115–120, 1997.
- Mityushev, V. V. and P. M. Adler. Longitudinal permeability of spatially periodic rectangular arrays of circular cylinders. I. A single cylinder in the unit cell. *Z. Angew. Math. Mech.*, 82:335–345, 2002.
- Molière, G. Z. *Kristallogr.*, 101:383, 1939.
- Monien, H. Gaussian quadrature for sums: a rapidly convergent summation scheme. *Math. Comp.*, 79:857–869, 2010.
- Montaldi, E. The evaluation of Green's functions for cubic lattices, revisited. *Lettera al Nuovo Cimento*, 30:403–409, 1981.
- Montroll, E. W. Theory of the vibration of simple cubic lattices with nearest neighbor interaction. In *Proc. 3rd Berkeley Symp. on Math. Stats. and Probability*, 3:209–246, 1956.
- Moroz, A. On the computation of the free-space doubly-periodic Green's function of the three-dimensional Helmholtz equation. *J. Electromagn. Waves Appl.*, 16:457–465, 2002.

- Mossotti, O. F. *Memorie di Matematica e di Fisica della Società Italiana delle Scienze Residente in Modena*, 24:49–74, 1850.
- Movchan, A. B., N. A. Nicorovici, and R. C. McPhedran. Green's tensors and lattice sums for elastostatics and elastodynamics. *Proc. Roy. Soc. London A*, 453:643–662, 1997.
- Naor, P. Linear dependence of lattice sums. *Z. Kristallogr. Kristallgeom.*, 110:112–126, 1958.
- Nicholson, M. M. Surface tension in ionic crystals. *Proc. Roy. Soc. London A*, 228:490–510, 1955.
- Nicorovici, N. A., C. G. Poulton, and R. C. McPhedran. Analytical results for a class of sums involving Bessel functions and square arrays. *J. Math. Phys.*, 37:2043–2052, 1996.
- Nijboer, B. R. A. and F. W. de Wette. On the calculation of lattice sums. *Physica (Utrecht)*, 23:309–321, 1957.
- Nijboer, B. R. A. and F. W. de Wette. The internal field in dipole lattices. *Physica (Utrecht)*, 24:422–431, 1958.
- Novák, B. Über eine Methode der Ω -abschätzungen. *Czech. Math. J.*, 21:257–279, 1971.
- Novák, B. New proofs of a theorem of Edmund Landau. *Acta Arith.*, 31:101–105, 1976.
- Olver, F. W. J., D. W. Lozier, R. F. Boisvert, and C. W. Clark. *NIST Digital Handbook of Mathematical Functions*, 2012.
- Ornstein, L. S. and F. Zernike. Magnetische eigenschappen van cubische Kristalnetten. *Proc. K. Akad. Wet. Amst.*, 21:911, 1918.
- Peng, H. W. and S. C. Powers. On the stability of crystal lattices. VIII. Stability of rhombohedral Bravais lattices. *Proc. Camb. Phil. Soc.*, 38:67–81, 1942.
- Perrins, W. T., D. R. McKenzie, and R. C. McPhedran. Transport properties of regular arrays of cylinders. *Proc. Roy. Soc. London A*, 369:207–225, 1979.
- Peters, M. The Diophantine equation $xy + yz + xz = n$ and indecomposable binary quadratic forms. *Exp. Math.*, 13:273–274, 2004.
- Petkovsek, M., H. Wilf, and D. Zeilberger. *A = B*. A. K. Peters, Wellesley, 1996.
- Placzek, G., B. R. A. Nijboer, and L. van Hove. Effect of short wavelength interference on neutron scattering by dense systems of heavy nuclei. *Phys. Rev.*, 82:392–403, 1951.
- Pólya, G. Über eine Aufgabe der Wahrscheinlichkeitstheorie betreffend die Irrfahrt im Strassennetz. *Math. Ann.*, 84:149–60, 1921.
- Poulton, C. G., L. C. Botten, R. C. McPhedran, and A. B. Movchan. Source-neutral Green's functions for periodic problems and their equivalents in electromagnetism. *Proc. Roy. Soc. London A*, 455:1107–1123, 1999.
- Prudnikov, A. P., Y. A. Brychkov, and O. I. Marichev. *Integrals and Series. 1. Elementary Functions*. Gordon and Breach, New York, 1986.
- Ramanujan, S. Modular equations and approximations to π . *Quart. J. Math.*, 45:350–372, 1914.
- Ramanujan, S. On certain arithmetical functions. *Trans. Camb. Phil. Soc.*, 22:159–184, 1916.
- Rashid, M. A. Lattice Green's functions for cubic lattices. *J. Math. Phys.*, 21:2549–2552, 1980.

- Rayleigh, Lord. On the influence of obstacles arranged in rectangular order upon the properties of a medium. *Phil. Mag.*, 34:481–502, 1892.
- Redlack, A. and J. Grindlay. The electrostatic potential in a finite ionic crystal. *Can. J. Phys.*, 50:2815–2825, 1972.
- Redlack, A. and J. Grindlay. Coulombic potential lattice sums. *J. Phys. Chem. Solid*, 36:73–82, 1975.
- Riesz, M. Sur un théorème de la moyenne et ses applications. *Acta Univ. Hungaricae Franc.-Jos.*, 1:114–126, 1923.
- Rodriguez-Villegas, F. Modular Mahler measures I. In *Topics in Number Theory*, pp. 17–48. Kluwer, Dordrecut, 1999.
- Rogers, M. New ${}_5F_4$ hypergeometric transformations, three-variable Mahler measures, and formulas for $1/\pi$. *Ramanujan Journal*, 18:327–340, 2009.
- Rogers, M. Hypergeometric formulas for lattice sums and Mahler measures. *IMRN*, 17:4027–4058, 2011.
- Rogers, M., J. G. Wan, and I. J. Zucker. Moments of elliptical integrals and critical L -values. In preparation, 2013.
- Rogers, M. and W. Zudilin. From L -series of elliptic curves to Mahler measures. *Compositio Math.*, 148:385–414, 2012.
- Rosengren, A. On the number of spanning trees for the 3d simple cubic lattice. *J. Phys. A: Math. Gen.*, 20:L923–L927, 1987.
- Rudge, W. E. Generalized Ewald potential problem. *Phys. Rev.*, 181:1020–1024, 1969.
- Sakamoto, Y. Madelung constants of simple crystals expressed in terms of Born's basic potentials of 15 figures. *J. Chem. Phys.*, 28:164–165, 1958.
- Sakamoto, Y. *J. Sci. Hiroshima Univ.*, 27:111, 1964.
- Sakamoto, Y. *J. Sci. Hiroshima Univ.*, 38:239–270, 1974.
- Schoeneberg, B. *Elliptic Modular Functions*. Springer-Verlag, New York, 1974.
- Selberg, A. and S. Chowla. On Epstein's zeta function (I). *Proc. Nat. Acad. Sci. USA*, 35:371–374, 1949.
- Selberg, A. and S. Chowla. On Epstein's zeta-function. *J. Reine Angew. Math.*, 227:86–110, 1967.
- Sherman, J. Crystal energies of ionic compounds and thermochemical applications. *Chem. Rev.*, 11:93–170, 1932.
- Sholl, C. A. The calculation of electrostatic energies of metals by plane-wise summation. *Proc. Phys. Soc.*, 92:434–445, 1967.
- Shrock, R. and F. Y. Wu. Spanning trees on graphs and lattices in d -dimensions. *J. Phys. A: Math. Gen.*, 33:3881–3902, 2000.
- Smith, H. J. S. *Report on the Theory of Numbers*. Chelsea, New York, 1865.
- Srivastava, H. M. and J. Choi. *Series Associated with the Zeta and Related Functions*. Kluwer, Dordrecht, 2001.
- Stepanets, G. F. and A. A. Lopatkin. *Russ. J. Phys. Chem.* (Engl. Transl.), 41:1481–1484, 1967.
- Stewart, I. *How to Cut a Cake and Other Mathematical Conundrums*. Oxford University Press, 2006.
- Takahasi, U. and Y. Sakamoto. *J. Sci. Hiroshima Univ.*, 24:118–130, 1960.
- Taylor, P. R. On the Riemann zeta function. *Quart. J. Oxford*, 16:1–21, 1945.

- Temperley, H. N. V. Combinatorics. In *Proc. Oxford Conf. on Combinatorial Mathematics*, pp. 356–357, 1972.
- Tikson, M. Tabulation of an integral arising in the theory of cooperative phenomena. *J. Res. Nat. Bur. Stds.*, 50:177–178, 1953.
- Titchmarsh, E. C. *The Theory of the Riemann Zeta Function*. Oxford University Press, London and New York, 1951.
- Topping, J. On the mutual potential energy of a plane network of doublets. *Proc. Roy. Soc. London A*, 114:67–72, 1927.
- Tosi, M. P. Cohesion of ionic solids in the Born model. *Solid State Phys.*, 16:1, 1964.
- Tyagi, S. New series representation for the Madelung constant. *Progr. Theor. Phys.*, 114:517–521, 2005.
- van der Hoff, B. M. E. and C. L. Benson. A method for the evaluation of some lattice sums occurring in calculations of physical properties of crystals. *Can. J. Phys.*, 31:1087–1094, 1953.
- van Peype, W. F. Zür Theorie der magnetischen anisotropen kubischer Kristalle beim absoluten Nullpunkt. *Physica*, 5:465–82, 1938.
- Waddington, T. C. Lattice energies and their significance in inorganic chemistry. *Adv. Inorg. Chem. Radiochem.*, 1:157, 1959.
- Walfisz, A. Über Gitterpunkte in mehrdimensionalen Ellipsoiden. *Math. Zeit.*, 19:300–307, 1924.
- Walfisz, A. Convergence abscissae of certain Dirichlet series. *Akad. Nauk Gruzin. SSR. Trudy Tbiliss. Mat. Inst. Razmadze*, 22:33–75, 1956.
- Wan, J. G. Moments of products of elliptic integrals. *Adv. Appl. Math.*, 48:121–141, 2012.
- Watson, G. N. The expansion of products of hypergeometric functions. *Quart. J. Math.*, 39:27–51, 1908.
- Watson, G. N. *A Treatise on the Theory of Bessel Functions*. Cambridge University Press, Cambridge, 1922.
- Watson, G. N. Three triple integrals. *Quart. J. Math. Oxford*, 10:266–276, 1939.
- Whittaker, E. T. and G. N. Watson. *A Course of Modern Analysis, 4th edition*. Cambridge University Press, 1946.
- Wigner, E. P. On the interaction of electrons in metals. *Phys. Rev.*, 46:1002–1011, 1934.
- Wilton, J. R. A series of Bessel functions connected with the theory of lattice points. *Proc. London Math. Soc.*, 29:168–188, 1928.
- Wu, F. Y. Number of spanning trees on a lattice. *J. Phys. A: Math. Gen.*, 10:L113–115, 1977.
- Zucker, I. J. Exact results for some lattice sums in 2, 4, 6 and 8 dimensions. *J. Phys. A*, 7:1568–1575, 1974.
- Zucker, I. J. Madelung constants and lattice sums for invariant cubic lattice complexes and certain tetragonal structures. *J. Phys. A*, 8:1734–1745, 1975.
- Zucker, I. J. New Jacobian θ functions and the evaluation of lattice sums. *J. Math. Phys.*, 16:2189–2191, 1975.
- Zucker, I. J. Functional equations for poly-dimensional zeta functions and the evaluation of Madelung constants. *J. Phys. A: Math. Gen.*, 9:499–505, 1976.
- Zucker, I. J. The evaluation in terms of Γ -functions of the periods of elliptic curves admitting complex multiplication. *Math. Proc. Camb. Phil. Soc.*, 82:111–118, 1977.

- Zucker, I. J. The summation of series of hyperbolic functions. *SIAM J. Math. Anal.*, 10:192–206, 1979.
- Zucker, I. J. Some infinite series of exponential and hyperbolic functions. *SIAM J. Math. Anal.*, 15:406–413, 1984.
- Zucker, I. J. Further relations amongst infinite series and products II. The evaluation of 3-dimensional lattice sums. *J. Phys. A.*, 23:117–132, 1990.
- Zucker, I. J. Stability of the Wigner electron crystal on the perovskite lattice. *J. Phys.: Condens. Matter*, 3:2595–2596, 1991.
- Zucker, I. J. 70 years of the Watson integrals. *J. Stat. Phys.*, 143:591–612, 2011.
- Zucker, I. J. and R. C. McPhedran. Problem 11294. *Amer. Math. Monthly*, 114:452, 2007.
- Zucker, I. J. and M. M. Robertson. Some properties of Dirichlet L -series. *J. Phys. A.*, 9:1207–1214, 1976.
- Zucker, I. J. and M. M. Robertson. Systematic approach to the evaluation of $\sum_{(m,n \neq 0,0)}(am^2 + bmn + cn^2)^{-s}$. *J. Phys. A*, 9:1215–1225, 1976.
- Zucker, I. J. and M. M. Robertson. Further aspects of the evaluation of $\sum_{(m,n \neq 0,0)}(am^2 + bmn + cn^2)^{-s}$. *Math. Proc. Camb. Phil. Soc.*, 95:5–13, 1984.
- Zvengrowski, P. and F. Saidak. On the modulus of the Riemann zeta function in the critical strip. *Math. Slovaca*, 53:145–272, 2003.

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