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

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CAMBRIDGE
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Cambridge, New York, Melbourne, Madrid, Cape Town,
Singapore, São Paulo, Delhi, Mexico City

Cambridge University Press
The Edinburgh Building, Cambridge CB2 8RU, UK

Published in the United States of America by Cambridge University Press, New York

www.cambridge.org
Information on this title: www.cambridge.org/9781107039902

First published 2013

Printed and bound in the United Kingdom by the MPG Books Group

A catalogue record for this publication is available from the British Library

Library of Congress Cataloguing in Publication data

ISBN 978-1-107-03990-2 Hardback

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.

Contents

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 is 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 Madelungs 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 $\log 2 = 0.69314718\ldots$; 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:

$$\mu = 1.74756459463318219063621203554439740348516143662474175815282535076504\ldots,$$

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

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

where the decimals correspond to two-dimensional lattice sums for a lattice involving μ, with discriminant $-99932.555\ldots$ 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' 9438Cu + 430Si + 126Mn + 4Fe + Zn + Pb. I think of the 430Si + 126Mn + 4Fe + Zn + 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.

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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 Goettingen 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.

Acknowledgments. The authors would like to acknowledge the following: the late Nicolae Nicorovici, who created a TeX version of the original 1981 paper; the Canada Research Chair Programme, the Natural Science and Engineering Research Council of Canada, and the Australian Research Council, which have supported the research of Jon Borwein and Ross McPhedran over many years; also their many colleagues and students who have made important contributions – David McKenzie, Graham Derrick, Graeme Milton, David Dawes, Lindsay Botten, Sai Kong, Chris Poulton, James Yardley, Alexander Movchan, Natasha Movchan, and many others.

Chapter 1: The chapter authors wish to thank John Grindlay and Carl Benson for aid with the literature search.

Chapter 2: The chapter authors would like to thank Professor O. Knop for originally bringing our attention to the problems involved in lattice sums.

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.

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