

Lattice sums arising from the Poisson equation

D H Bailey¹, J M Borwein², R E Crandall³ (1947-2012), I J Zucker⁴

¹ Lawrence Berkeley National Lab, Berkeley, CA 94720; University of California, Davis,
Department of Computer Science, Davis, CA 95616

E-mail: david@davidhbailey.com

Supported in part by the Director, Office of Computational and Technology Research,
Division of Mathematical, Information, and Computational Sciences of the U.S. Department
of Energy, under contract number DE-AC02-05CH11231.

² Centre for Computer Assisted Research Mathematics and its Applications (CARMA),
University of Newcastle, Callaghan, NSW 2308, Australia,

E-mail: jonathan.borwein@newcastle.edu.au

³ Center for Advanced Computation, Reed College, Portland OR

⁴ Department of Physics, Kings College London,

E-mail: jzucker@btinternet.com

Abstract: In recent times, attention has been directed to the problem of solving the Poisson equation, either in engineering scenarios (computational) or in regard to crystal structure (theoretical). Herein we study a class of lattice sums that amount to Poisson solutions, namely the n -dimensional forms

$$\phi_n(r_1, \dots, r_n) = \frac{1}{\pi^2} \sum_{m_1, \dots, m_n \text{ odd}} \frac{e^{i\pi(m_1 r_1 + \dots + m_n r_n)}}{m_1^2 + \dots + m_n^2}.$$

By virtue of striking connections with Jacobi ϑ -function values, we are able to develop new closed forms for certain values of the coordinates r_k , and extend such analysis to similar lattice sums. A primary result is that *for rational x, y , the natural potential $\phi_2(x, y)$ is $\frac{1}{\pi} \log A$ where A is an algebraic number*. Various extensions and explicit evaluations are given. Such work is made possible by number-theoretical analysis, symbolic computation and experimental mathematics, including extensive numerical computations using up to 20,000-digit arithmetic.

1. About this paper

In this paper, we analyze various generalized lattice sums [7], which have been studied for many years in the mathematical physics community, for example in [7, 13, 14] and a recent fascinating work on cyclotomic polylogarithms and corresponding multiple harmonic sums [1]. Recently our own interest has been triggered by some intriguing research in practical image processing techniques [9]. These developments have underscored the need to better understand the underlying theory behind both lattice sums and the associated Poisson potential functions.

To that end, we present a number of results, perhaps the most notable of which is the remarkable fact that, for rational x and y , the most natural two-dimensional Poisson potential function satisfies

$$\phi_2(x, y) = \frac{1}{\pi^2} \sum_{m, n \text{ odd}} \frac{\cos(m\pi x) \cos(n\pi y)}{m^2 + n^2} = \frac{1}{\pi} \log A, \quad (1)$$

where A is an *algebraic number*, or, in other words, the root of an integer polynomial, whose degree and coefficients depend on x and y .

In Section 2, we describe, consistent with [9], the underlying equations along with “natural” Madelung constants and relate them to the classical Madelung constants. In Section 3, we produce the solution ϕ_n which, especially with $n = 2$, provide the central objects of our study. In Section 4, we develop rapid methods of evaluating ϕ_n .

These fast methods are used in Section 5 to experimentally determine closed-form evaluations for $\phi_2(x, y)$ for some specific x and y , such as

$$\pi^2 \phi_2(1/5, 2/5) = \sum_{m, n \text{ odd}} \frac{\cos(m\pi/5) \cos(2n\pi/5)}{m^2 + n^2} \stackrel{?}{=} \frac{\pi}{16} \log 5. \quad (2)$$

We are also able to prove a few of the simpler evaluations (see Theorem 3 and Appendices I and III). From this and further computational evidence, we conjectured the algebraic result mentioned above in (1), which is stated and proven as Theorem 10 of Section 6. This result was made possible because earlier in Section 6 we relate ϕ_2 , and its counterpart sum over even integers ψ_2 , in terms of general Jacobean theta functions $\vartheta_k(z, q)$ for $k = 1, \dots, 4$. In Section 6.4, we also touch on generalizations to sums of the form

$$\phi_2(x, y, d) := \frac{1}{\pi^2} \sum_{m, n \text{ odd}} \frac{\cos(\pi m x) \cos(\pi n \sqrt{d} y)}{m^2 + dn^2}, \quad (3)$$

for rational $d > 0$.

In Section 7, we describe the quite extensive and challenging computational experiments we have undertaken, and summarize the results in tabular form. In Section 8, we briefly look at the state of our knowledge in three and four dimensions. Finally, in three Appendices, we present some additional details of our proofs via factorization of lattice sums.

2. Madelung entities

In a recent treatment of ‘natural’ Madelung constants [9] it is pointed out that the Poisson equation for an n -dimensional point-charge source,

$$\nabla^2 \Phi_n(\mathbf{r}) = -\delta(\mathbf{r}), \quad (4)$$

gives rise to an electrostatic potential—we call it the *bare-charge potential*—of the form

$$\Phi_n(\mathbf{r}) = \frac{\Gamma(n/2 - 1)}{4\pi^{n/2}} \frac{1}{r^{n-2}} =: \frac{C_n}{r^{n-2}}, \quad \text{if } n \neq 2, \quad (5)$$

$$\Phi_2(\mathbf{r}) = -\frac{1}{2\pi} \log r =: C_2 \log r, \quad (6)$$

where $r := |\mathbf{r}|$. Since this Poisson solution generally behaves as r^{2-n} , the previous work [9] defines a “natural” Madelung constant \mathcal{N}_n as (here, $m := |\mathbf{m}|$):

$$\mathcal{N}_n := C_n \sum'_{\mathbf{m} \in \mathbb{Z}^n} \frac{(-1)^{\mathbf{1} \cdot \mathbf{m}}}{m^{n-2}}, \quad \text{if } n \neq 2, \quad (7)$$

$$\mathcal{N}_2 := C_2 \sum'_{\mathbf{m} \in \mathbb{Z}^n} (-1)^{\mathbf{1} \cdot \mathbf{m}} \log m,$$

where in cases such as this log sum one must infer an analytic continuation [9], as the literal sum is quite non convergent. This \mathcal{N}_n coincides with the classical Madelung constant

$$\mathcal{M}_n := \sum'_{\mathbf{m} \in \mathbb{Z}^n} \frac{(-1)^{\mathbf{1} \cdot \mathbf{m}}}{m} \quad (8)$$

only for $n = 3$ dimensions, in which case $\mathcal{N}_3 = \frac{1}{4\pi} \mathcal{M}_3$. But in all other dimensions there is no obvious \mathcal{M}, \mathcal{N} relation.

A method for gleaning information about \mathcal{N}_n is to contemplate the Poisson equation with a crystal charge source, modeled after NaCl (salt) in the sense of alternating lattice charges:

$$\nabla^2 \phi_n(\mathbf{r}) = - \sum_{\mathbf{m} \in \mathbb{Z}^n} (-1)^{\mathbf{1} \cdot \mathbf{m}} \delta(\mathbf{m} - \mathbf{r}). \quad (9)$$

Accordingly—based on the Poisson equation (4)—solutions ϕ_n can be written in terms of the respective bare-charge functions Φ_n , as

$$\phi_n(\mathbf{r}) = \sum_{\mathbf{m} \in \mathbb{Z}^n} (-1)^{\mathbf{1} \cdot \mathbf{m}} \Phi_n(\mathbf{r} - \mathbf{m}). \quad (10)$$

2.1. Madelung variants

We have defined the classical Madelung constants (8) and the “natural Madelung constants (7). Following [9], we define a *Madelung potential*, now depending on a complex s and spatial

point $\mathbf{r} \in \mathbb{Z}^n$:

$$\mathcal{M}_n(s, \mathbf{r}) := \sum_{\mathbf{p} \in \mathbb{Z}^n} \frac{(-1)^{\mathbf{1} \cdot \mathbf{p}}}{|\mathbf{p} - \mathbf{r}|^s}, \quad (11)$$

We can write limit formulae for our Madelung variants, first the classical Madelung constant

$$\mathcal{M}_n := \lim_{\mathbf{r} \rightarrow \mathbf{0}} \left(\mathcal{M}_n(1, \mathbf{r}) - \frac{1}{r} \right) \quad (12)$$

$$= \sum'_{\mathbf{p} \in \mathbb{Z}^n} \frac{(-1)^{\mathbf{1} \cdot \mathbf{p}}}{p}, \quad (13)$$

and then the “natural” Madelung constant

$$\mathcal{N}_n := \lim_{\mathbf{r} \rightarrow \mathbf{0}} (\phi(\mathbf{r}) - \Phi(r)) \quad (14)$$

$$= C_n \sum'_{\mathbf{p} \in \mathbb{Z}^n} \frac{(-1)^{\mathbf{1} \cdot \mathbf{p}}}{p^{n-2}}. \quad (15)$$

For small even n this last sum is evaluable. For example, from [6, Eqn. (9.2.5)] we have

$$\sum'_{\mathbf{p} \in \mathbb{Z}^4} \frac{(-1)^{\mathbf{1} \cdot \mathbf{p}}}{p^{2s}} = (1 - 2^{2-s})(1 - 2^{1-s})\zeta(s)\zeta(s-1), \quad (16)$$

which with $s = 1$ yields

$$\mathcal{N}_4 = -\frac{1}{\pi^2} \log 2.$$

Similarly [6, Exercise 4b), p. 292] derives

$$\sum'_{\mathbf{p} \in \mathbb{Z}^8} \frac{(-1)^{\mathbf{1} \cdot \mathbf{p}}}{p^{2s}} = -16(1 - 2^{4-s})\zeta(s)\zeta(s-3), \quad (17)$$

which with $s = 3$ determines that

$$\mathcal{N}_8 = -\frac{4}{\pi^4} \zeta(3).$$

Generally, via the Mellin transform $M_s \vartheta_4^{2n}(q)$, see below, for small n values of \mathcal{N}_{2n} are similarly susceptible. For instance with G denoting Catalan’s constant

$$\mathcal{N}_6 = -\frac{1}{24\pi} - \frac{2G}{\pi^3},$$

given in [9]. The more complex value \mathcal{N}_2 is presented in (26).

2.2. Relation between crystal solutions ϕ_n and Madelung potentials

From (5), (10), and (11) we have the general relation for dimension $n \neq 2$,

$$\phi_n(\mathbf{r}) = C_n \mathcal{M}_n(n-2, \mathbf{r}). \quad (18)$$

Note that for the case $n = 3$, the solution ϕ_3 coincides with the classical Madelung potential $\mathcal{M}_3(1, \mathbf{r})$ in the sense

$$\phi_3(\mathbf{r}) = \frac{1}{4\pi} \mathcal{M}_3(1, \mathbf{r}),$$

because $C_3 = 1/(4\pi)$. Likewise, the ‘‘natural’’ and classical Madelung constants are related $4\pi \mathcal{N}_3 = \mathcal{M}_3$. The whole idea of introducing ‘natural’ Madelung constants \mathcal{N}_n is that this coincidence of radial powers for ϕ and \mathcal{M} potentials holds *only* in 3 dimensions. For example, in $n = 5$ dimensions, the summands for ϕ_5 and $\mathcal{M}_5(1, \cdot)$ involve radial powers $1/r^3$, as in

$$\phi_5(\mathbf{r}) = \frac{1}{8\pi^2} \mathcal{M}_5(3, \mathbf{r}).$$

3. The crystal solutions ϕ_n

In [9] it is argued that a solution to (9) is

$$\phi_n(\mathbf{r}) = \frac{1}{\pi^2} \sum_{\mathbf{m} \in \mathbb{O}^n} \frac{\prod_{k=1}^n \cos(\pi m_k r_k)}{m^2}, \quad (19)$$

where \mathbb{O} denotes the odd integers (including negative odds). These ϕ_n do give the potential within the appropriate n -dimensional crystal, in that ϕ_n vanishes on the surface of the cube $[-1/2, 1/2]^n$, as is required via symmetry within an NaCl-type crystal of any dimensions. To render this representation more explicit and efficient, we could write equivalently

$$\phi_n(\mathbf{r}) = \frac{2^n}{\pi^2} \sum_{m_1, \dots, m_n > 0, \text{ odd}} \frac{\cos(\pi m_1 r_1) \cdots \cos(\pi m_n r_n)}{m_1^2 + \cdots + m_n^2}.$$

It is also useful that—due to the symmetry inherent in having odd summation indices—we can cavalierly replace the cosine product in (19) with a simple exponential:

$$\phi_n(\mathbf{r}) = \frac{1}{\pi^2} \sum_{\mathbf{m} \in \mathbb{O}^n} \frac{e^{i\pi \mathbf{m} \cdot \mathbf{r}}}{m^2}. \quad (20)$$

This follows from the simple observation that $\prod \exp(\pi i m_k r_k) = \prod (\cos(\pi m_k r_k) + i \sin(\pi m_k r_k))$, so when the latter product is expanded out, the appearance of even a single *sin* term is annihilating, due to the bipolarity of every index m_k .

We observe that convergence of these conditionally convergent sums is by no means obvious but that results such as [7, Thm. 8.3 & Thm. 8.5] ensure that

$$\phi_n(\mathbf{r}, s) := \frac{1}{\pi^2} \sum_{\mathbf{m} \in \mathbb{O}^n} \frac{\prod_{k=1}^n \cos(\pi m_k r_k)}{m^{2s}}, \quad (21)$$

is convergent and analytic with abscissa σ_0 for $(n-1)/4 \leq \sigma_0 \leq (n-1)/2$ where $\text{Re}(s) = \sigma$. For the central case herein, summing over increasing spheres is analytic in two dimensions for $\sigma_0 \leq 23/73 < 1/2$ and in three dimensions for $\sigma_0 \leq 25/34 < 1$, but in general the best estimate we have is $\sigma_0 \leq n/2 - 1$, so for $n \geq 5$ to avoid ambiguity we work with the analytic continuation of (21) from the region of absolute convergence with $\sigma > n/2$. Indeed, all our transform methods are effectively doing just that.

4. Fast series for ϕ_n

From previous work [9] we know a computational series

$$\phi_n(\mathbf{r}) = \frac{1}{2\pi} \sum_{\mathbf{R} \in \mathbb{O}^{n-1}} \frac{\sinh(\pi R(1/2 - |r_1|)) \prod_{k=1}^{n-1} \cos(\pi R_k r_{k+1})}{R \cosh(\pi R/2)}, \quad (22)$$

suitable for any nonzero vector $\mathbf{r} \in [-1/2, 1/2]^n$. The previous work also gives an improvement in the case of $n = 2$ dimensions, namely the following form for which the logarithmic singularity at the origin has been siphoned off:

$$\phi_2(x, y) = \frac{1}{4\pi} \log \frac{\cosh(\pi x) + \cos(\pi y)}{\cosh(\pi x) - \cos(\pi y)} - \frac{2}{\pi} \sum_{\mathbf{m} \in \mathbb{O}^+} \frac{\cosh(\pi m x) \cos(\pi m y)}{m(1 + e^{\pi m})}. \quad (23)$$

These series, (22) and (23) are valid, respectively, for $r_1, x \in [-1, 1]$.

For clarification, we give here the ($n = 3$)-dimensional case of the fast series:

$$\phi_3(x, y, z) = \frac{2}{\pi} \sum_{p, q > 0, \text{ odd}} \frac{\sinh\left(\frac{\pi}{2} \sqrt{p^2 + q^2} (1 - 2|x|)\right) \cos(\pi p y) \cos(\pi q z)}{\sqrt{p^2 + q^2} \cosh\left(\frac{\pi}{2} \sqrt{p^2 + q^2}\right)}. \quad (24)$$

Though it may not be manifest in this asymmetrical-looking series, it turns out that for any dimension n the $\phi_n(r_1, \dots, r_n)$ is *invariant under permutations and sign-flips*. For example, $\phi_3(x, y, z) = \phi_3(-y, z, -x)$ and so on. It thus behooves the implementor to consider x —which appears only in the first sum of (24)—to be the largest in magnitude of the three coordinates, for optimal convergence. A good numerical test case which we mention later is the exact evaluation $\phi_3(1/6, 1/6, 1/6) = \frac{\sqrt{3}}{4\pi}$, which we have confirmed to 500 digits.

With $n > 2$ it is not clear how best to isolate the ($\mathbf{r} = \mathbf{0}$) singularity in higher dimensions. One approach—possibly not optimal, is to derive [9]

$$\mathcal{N}_n = C_n \sum'_{\mathbf{m} \in \mathbb{Z}^{+(n-1)}} \frac{(-1)^{\mathbf{1} \cdot \mathbf{m}}}{m^{n-2}} - \frac{1}{\pi} \sum_{\mathbf{R} \in \mathbb{O}^{n-1}} \frac{1}{R(1 + e^{\pi R})}, \quad \text{if } n \neq 2 \quad (25)$$

then employ a fast series for the $C_n \sum'$ term [9]. In fact, it is often possible to give this \mathbf{m} -sum here a closed form [9], so that a great many \mathcal{N}_n are now resolved. (More generally speaking, we cannot yet resolve any of the $\mathcal{N}_{\text{odd } n > 1}$.)

4.1. Closed form for the “natural” Madelung constant \mathcal{N}_2

The ($n = 2$)-dimensional natural Madelung constant has also been resolved on the basis of (23) (see [9]), to take the value

$$\mathcal{N}_2 = \frac{1}{4\pi} \log \frac{4\Gamma^4(3/4)}{\pi^3}. \quad (26)$$

We remind ourselves that this closed form was achieved by contemplating the limiting process $\mathbf{r} \rightarrow \mathbf{0}$, and hence Coulomb-singularity removal.

We also record the following numerically effective Mellin transform for $n > 2$

$$\mathcal{N}_n = -\frac{1}{4\pi} \int_0^\infty (1 - \vartheta_4^n(e^{-\pi x})) x^{n/2-2} dx < 0, \quad (27)$$

where the integral is positive since $0 < \vartheta_4(q) < 1$ for $0 \leq q \leq 1$.

From this the large n behavior of \mathcal{N}_n may be estimated as

$$\mathcal{N}_n \asymp -\frac{\Gamma(n/2 - 1)}{\pi^{n/2}} \cdot \left(\frac{n}{2} - \frac{n(n-1)}{2^{n/2}} + \dots \right), \quad (28)$$

on approximating $\vartheta_4(q) = 1 - 2q + O(q^4)$ and $1 - x^n = -n(x-1) + n(n-1)/2(x-1)^2 + O((x-1)^3)$ and then integrating term-by-term. For instance, from (27) we compute

$$N_{100} = -8.6175767047403040779\dots \times 10^{37}$$

while the asymptotic (28) gives

$$\mathcal{N}_{100} \asymp -8.6175767047403038\dots \times 10^{37}.$$

Indeed, we can make effective estimates, as in:

Theorem 1 (Effective bounds on N_n). *For integer $n > 2$ we have*

$$-1 + \frac{n}{2^{n/2-1}} > \frac{\mathcal{N}_n}{\left(\frac{\Gamma(n/2-1)n}{\pi^{n/2}} \frac{n}{2} \right)} > -1. \quad (29)$$

Proof. Let $q := \exp(-\pi t)$ and note

$$1 - 2q \leq \vartheta_4(q) \leq 1 - 2q + 2q^4.$$

Now for any $x \in (0, 1)$ and positive integer n it is elementary that

$$1 - nx \leq (1 - x)^n \leq 1 - nx + n(n - 1)x^2/2.$$

Putting $x := \vartheta_4(q)$ here, knowing $x \in [1 - 2q, 1 - 2q + 2q^4]$ in the integral representation (27) quickly gives both bounds of the theorem. \square

Remark 2. Another approach to these effective error bounds is to note

$$\mathcal{N}_n = C_n \sum_{N \geq 1} \frac{r_n(N)(-1)^N}{N^{n/2-1}},$$

where $r_n(N)$ counts the number of n -square representations of N . Indeed, the first asymptotic terms in (28) arise immediately from the observation

$$r_n(1) = 2n,$$

as every representation of 1 is $(\pm 1)^2 + 0^2 + \dots + 0^2$, and similarly

$$r_n(2) = \frac{1}{2}n(n - 1) \cdot 4.$$

In this regard, the rapid decrease in asymptotic terms for large n makes intuitive sense. Indeed, in high dimensions, a “great deal” of the natural potential is due to charges that reside “near the origin.”

Also, applying the theta transform [6, Eqn. (2.3.2)] in (27) yields the analytically useful

$$\mathcal{N}_n = -\frac{1}{4\pi} \left\{ \frac{2}{n-2} - \int_0^1 \vartheta_4^n(e^{-\pi t}) t^{n/2-2} dt + \int_0^1 (t^{-n/2} - \vartheta_2^n(e^{-\pi t})) dt \right\}, \quad (30)$$

where numerical care is needed near the origin in the second integrand. \diamond

In the next section we derive certain closed forms and exhibit others determined experimentally—most of which we also indicate how to prove.

5. Closed forms for the ϕ_2 potential

Provably we have the following results which were established by factorization of lattice sums after being empirically discovered by the methods described in the next few sections.

Theorem 3. *We have*

$$\phi_2(1/3, 1/3) = \frac{1}{8\pi} \log(1 + 2/\sqrt{3}), \quad (31)$$

$$\phi_2(1/4, 1/4) = \frac{1}{4\pi} \log(1 + \sqrt{2}), \quad (32)$$

$$\phi_2(1/3, 0) = \frac{1}{8\pi} \log(3 + 2\sqrt{3}). \quad (33)$$

Proof. Consider for $s > 0$

$$\mathcal{V}_2(x, y; s) := \sum_{m, n=-\infty}^{\infty} \frac{\cos[\pi(2m+1)x] \cos[\pi(2n+1)y]}{[(2m+1)^2 + (2n+1)^2]^s}. \quad (34)$$

This \mathcal{V}_2 function will be related by normalization, as $\mathcal{V}_2(x, y; 1) = \pi^2 \phi_2(x, y)$. Treating it as some general lattice sum [6, 7], we derive (with some difficulty; more details are in Appendix I)

$$\begin{aligned} \mathcal{V}_2(1/3, 1/3; s) &= 2^{-1-s} \left[-(1 - 2^{-s})(1 - 3^{2-2s})L_1(s)L_{-4}(s) \right. \\ &\quad \left. + 3(1 + 2^{-s})L_{-3}(s)L_{12}(s) \right]. \end{aligned} \quad (35)$$

The L 's in (35) are various Dirichlet series, L_1 being the Riemann ζ function. Note that $(1 - 3^{2-2s})$ factors as $(1 + 3^{1-s})(1 - 3^{1-s})$ and $\lim_{s \rightarrow 1}(1 - 3^{1-s})L_1(s) = \log 3$, and that

$$L_{-4}(1) = \frac{\pi}{4}, \quad L_{-3}(1) = \frac{\sqrt{3}\pi}{9}, \quad L_{12}(1) = \frac{1}{\sqrt{3}} \log(2 + \sqrt{3}). \quad (36)$$

After gathering everything together we have

$$\phi_2(1/3, 1/3) = \frac{1}{\pi^2} \mathcal{V}_2(1/3, 1/3, 1) = \frac{1}{8\pi} \log \left(\frac{3 + 2\sqrt{3}}{3} \right),$$

which is (31).

More simply

$$\mathcal{V}_2(1/4, 1/4; s) = 2 \sum_{m, n=-\infty}^{\infty} \frac{(-1)^{m+n}}{[(4m-1)^2 + (4n-1)^2]^s} = 2^{1-s} L_{-8}(s) L_8(s) \quad (37)$$

is a familiar lattice sum [6, 7]. So with

$$L_{-8}(1) = \frac{\pi}{2\sqrt{2}} \quad \text{and} \quad L_8(1) = \frac{1}{\sqrt{2}} \log(1 + \sqrt{2}) \quad (38)$$

we derive

$$\phi_2(1/4, 1/4) = \frac{1}{4\pi} \log(1 + \sqrt{2}).$$

which is (32).

Likewise

$$\begin{aligned} \mathcal{V}_2(1/3, 0; s) = & 2^{-1-s} [(1 - 2^{-s})(1 - 3^{2-2s})L_1(s)L_{-4}(s) \\ & + 3(1 + 2^{-s})L_{-3}(s)L_{12}(s)] \end{aligned} \quad (39)$$

which yields

$$\phi_2(0, 1/3) = \frac{1}{16\pi} \log \left(3(2 + \sqrt{3})^2 \right) = \frac{\pi}{8} \log(3 + 2\sqrt{3}),$$

which is (33). □

Using the *integer relation method* PSLQ [5] to hunt for results of the form,

$$\exp(\pi\phi_2(x, y)) \stackrel{?}{=} \alpha, \quad (40)$$

for α algebraic we may obtain and further simplify many results such as:

Conjecture 4. *We have discovered and subsequently proven*

$$\phi_2(1/4, 0) \stackrel{?}{=} \frac{1}{4\pi} \log \alpha \quad \text{where} \quad \frac{\alpha + 1/\alpha}{2} = \sqrt{2} + 1$$

$$\phi_2(1/5, 1/5) \stackrel{?}{=} \frac{1}{8\pi} \log \left(3 + 2\sqrt{5} + 2\sqrt{5 + 2\sqrt{5}} \right),$$

$$\phi_2(1/6, 1/6) \stackrel{?}{=} \frac{1}{4\pi} \log \gamma \quad \text{where} \quad \frac{\gamma + 1/\gamma}{2} = \sqrt{3} + 1$$

$$\phi_2(1/3, 1/6) \stackrel{?}{=} \frac{1}{4\pi} \log \tau \quad \text{where} \quad \frac{\tau - 1/\tau}{2} = (2\sqrt{3} - 3)^{1/4}$$

$$\phi_2(1/8, 1/8) \stackrel{?}{=} \frac{1}{4\pi} \log \left(\frac{1 + \sqrt{2 - \sqrt{2}}}{\sqrt[4]{2} - 1} \right)$$

$$\phi_2(1/10, 1/10) \stackrel{?}{=} \frac{1}{4\pi} \log \mu \quad \text{where} \quad \frac{\mu + 1/\mu}{2} = 2 + \sqrt{5} + \sqrt{5 + 2\sqrt{5}}$$

where the notation $\stackrel{?}{=}$ indicates that we originally only had experimental (extreme-precision numerical) evidence of an equality.

Looking at (14) and (26), we can take the most valuable (in the sense of (x, y) being closest to the origin $(0, 0)$) of the above ϕ_2 evaluations, and attempt an approximation

$$\mathcal{N}_2 \approx \phi_2(1/10, 1/10) + \frac{1}{2\pi} \log \sqrt{1/100 + 1/100} = -0.09818\dots,$$

which is off of the correct analytic \mathcal{N}_2 value $-0.0982599931\dots$ by about 1 part in 1000.

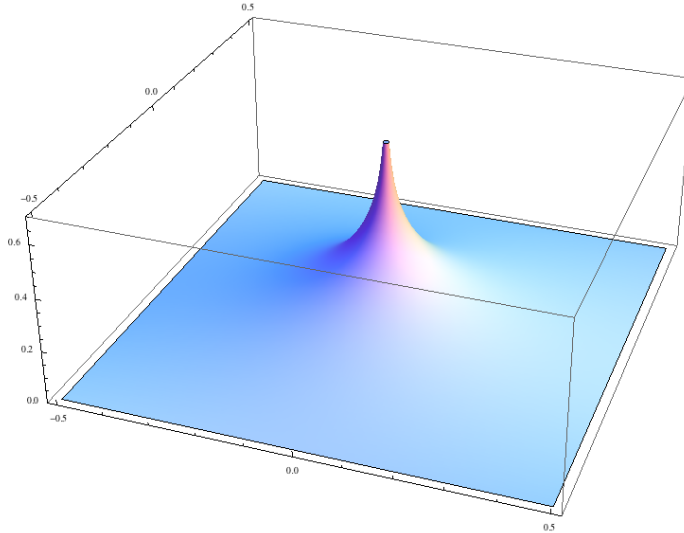


Figure 1. High-precision plot of the Monge surface $z = \phi_2(x, y)$, via fast series (23), showing the logarithmic origin singularity (plot adapted from [9]). In this plot, x, y range over the 2-cube $[-1/2, 1/2]^2$; from symmetry one only need know the ϕ_2 surface over an octant $1/2 > x \geq y > 0$, say. We are able to establish closed forms for heights on this surface above certain rational pairs (x, y) . As just one example, $\phi_2(1/4, 1/4) = \frac{1}{4\pi} \log(1 + \sqrt{2}) \approx 0.0701$.

Such hunts are made entirely practicable by (23). Note that for general x and y we have $\phi_2(y, x) = \phi_2(x, y) = -\phi_2(x, 1-y)$, so we can restrict searches to $1/2 > x \geq y > 0$, as illustrated in Figure 1.

The following hints at how much underlying algebraic structure there is:

Example 5 (Denominator of five). We record that

$$\phi_2(1/5, 1/5) \stackrel{?}{=} \log(\alpha)/\pi \quad \text{and} \quad \phi_2(2/5, 2/5) \stackrel{?}{=} \log(\beta)/\pi$$

where $\alpha > \beta$ are the positive roots of $x^{32} - 12x^{24} - 26x^{16} + 52x^8 + 1$. Similarly,

$$\phi_2(1/5, 0/5) \stackrel{?}{=} \log(\alpha)/\pi \quad \text{and} \quad \phi_2(2/5, 0/5) \stackrel{?}{=} \log(\beta)/\pi$$

share the positive roots of $x^{32} - 52x^{24} - 26x^{16} + 12x^8 + 1$. Moreover,

$$\phi_2(1/5, 2/5) \stackrel{?}{=} \frac{1}{16\pi} \log 5, \tag{41}$$

which is stunningly simple. Explicitly,

$$\sum_{0 < m, n \text{ odd}} \frac{\cos(m\pi/5) \cos(2n\pi/5)}{n^2 + m^2} \stackrel{?}{=} \frac{\pi \log 5}{64}. \tag{42}$$

This will be explained in Example 15. ◇

Example 6 (Denominator of six and more). Likewise,

$$\phi_2(1/6, 0) \stackrel{?}{=} \log(\alpha)/\pi$$

for α the largest root of

$$x^{16} - 4x^{14} + 4x^{12} - 4x^{10} - 2x^8 - 4x^6 + 4x^4 - 4x^2 + 1.$$

Similarly,

$$\phi_2(1/8, 0) \stackrel{?}{=} \log(\beta)/\pi \quad \text{and} \quad \phi_2(1/10, 0) \stackrel{?}{=} \log(\gamma)/\pi$$

for β, γ the largest roots respectively of

$$\begin{aligned} & x^{32} + 8(\sqrt{2} + 1)x^{28} - 12x^{24} - 8(\sqrt{2} + 1)x^{20} - 38x^{16} - 8(\sqrt{2} + 1)x^{12} \\ & - 12x^8 + 8(\sqrt{2} + 1)x^4 - 1 \end{aligned}$$

(the integer polynomial is of degree 64) and

$$x^8 - (\sqrt{5} + 1)x^6 - (5^{3/4} + 3 \cdot 5^{1/4} + \sqrt{5} + 1)x^4 - (\sqrt{5} + 1)x^2 + 1$$

(the integer polynomial is now degree 32). In each case the polynomial is palindromic. Again, the polynomial found for $x^{1/4}$ is simpler. For $1/6$ it is $x^8 - 8x^7 - 20x^6 - 56x^5 - 26x^4 - 56x^3 - 20x^2 - 8x + 1$.

Likewise,

$$\phi_2(1/3, 1/4) \stackrel{?}{=} \log(\sigma)/4\pi$$

for σ the largest root of

$$x^8 + 4x^7 - 4x^6\sqrt{3} - 4x^5 + (14 - 8\sqrt{3})x^4 - 4x^3 - 4x^2\sqrt{3} + 4x + 1.$$

We have also discovered that for $k = 1, 2, 3$ we have

$$\phi_2(k/7, k/7) \stackrel{?}{=} \frac{1}{8\pi} \log(\alpha_k)$$

where $\alpha_1 > \alpha_2 > \alpha_3$ are the positive roots of

$$\begin{aligned} & 7x^6 - (154 + 56\sqrt{7})x^5 - (1603 + 616\sqrt{7})x^4 + (9156 + 3472\sqrt{7})x^3 \\ & - (4431 + 1680\sqrt{7})x^2 - (4298 + 1624\sqrt{7})x - 8\sqrt{7} - 21. \end{aligned}$$

Also,

$$\phi_2(2/7, 1/7) \stackrel{?}{=} \frac{1}{16\pi} \log(\beta_1), \quad \phi_2(3/7, 2/7) \stackrel{?}{=} \frac{1}{16\pi} \log(\beta_2),$$

$$\text{and } \phi_2(3/7, 1/7) \stackrel{?}{=} \frac{1}{16\pi} \log(\beta_3),$$

where $\beta_1 > \beta_2 > \beta_3$ are the positive roots of

$$x^6 - 14x^5 - 3801x^4 + 9436x^3 - 1281x^2 - 238x - 7,$$

all of whose roots are real. Finally

$$\phi_2(1/7, 0) \stackrel{?}{=} \frac{1}{8\pi} \log(\gamma_1), \quad \phi_2(3/7, 0) \stackrel{?}{=} \frac{1}{8\pi} \log(\gamma_2)$$

$$\text{and } \phi_2(5/7, 0) \stackrel{?}{=} \frac{1}{8\pi} \log(\gamma_3),$$

where $\gamma_1 > \gamma_2 > \gamma_3$ are the positive roots of

$$x^6 - (98 + 40\sqrt{7})x^5 + (24\sqrt{7} + 147)x^4 + (308 + 48\sqrt{7})x^3 - (16\sqrt{7} - 119)x^2 + (14 - 8\sqrt{7})x - 8\sqrt{7} + 21.$$

Similar observations appeared to work for denominators of $3 \leq n \leq 15$. For instance, the quantity $\exp(4\pi\phi_2(1/13, 3/13))$ was found to be of degree 36 over $Q(\sqrt{3})$. \diamond

Remark 7 (Algebraicity). In light of our current evidence we conjecture that for x, y rational,

$$\phi_2(x, y) \stackrel{?}{=} \frac{\log \alpha}{\pi} \tag{43}$$

for α algebraic. Theorem 10 will prove this conjecture. \diamond

Remark 8. The proven results of Theorem 3 rely on the special structure of the series (35), (37) and (39). But conjecturally, as we have seen and will see below, much more is true and does not apparently rely on the complete factorizations [20] of (34) used above.

We might try to work backwards and find the expressions they came from for general s . However, $\phi_2(1/4, 0; s)$ in particular cannot be expressed in terms of Dirichlet series with *real* characters. This then is a candidate for the use of complex character Dirichlet series [7]. Moreover, (41) suggests another approach might be more fruitful. This is indeed so as Theorem 9 and its sequela show. \diamond

We note that Theorem 10 proves that all values should be algebraic but does not, a priori, establish the precise values we have found. This will be addressed in §6.2.

6. Madelung and “jellium” crystals and Jacobi ϑ -functions

We have studied

$$\phi_2(x, y) := \frac{1}{\pi^2} \sum_{a, b \in \mathbb{Z}} \frac{\cos(\pi ax) \cos(\pi by)}{a^2 + b^2}, \tag{44}$$

as a ‘natural’ potential for $n = 2$ dimensions in the Madelung problem. Here \mathbb{E} denotes the even integers. There is another interesting series, namely

$$\begin{aligned}\psi_2(x, y) &:= \frac{1}{4\pi^2} \sum'_{a,b \in \mathbb{Z}} \frac{\cos(2\pi ax) \cos(2\pi by)}{a^2 + b^2} \\ &= \frac{1}{\pi^2} \sum_{a,b \in \mathbb{E}} \frac{\cos(\pi ax) \cos(\pi by)}{a^2 + b^2},\end{aligned}\tag{45}$$

where \mathbb{E} denotes the even integers.

Now it is explained, and pictorialized in [9] that this ψ_2 function is the ‘natural’ potential for a classical *jellium* crystal and relates to Wigner sums [7]. This involves a positive charge at every integer lattice point, in a bath—a jelly—of uniform negative charge density. As such, the ψ functions satisfy a Poisson equation but with different source term [9].

Note importantly that ψ_2 satisfies *Neumann boundary conditions* on the faces of the Delord cube—in contrast with the Dirichlet conditions in the Madelung case.

Briefly, a fast series for ψ_n has been worked out [9] as:

$$\psi_n(\mathbf{r}) = \frac{1}{12} + \frac{1}{2}r_1^2 - \frac{1}{2}|r_1| + \frac{2^{n-3}}{\pi} \sum_{\mathbf{s} \in \mathbb{Z}^{+(n-1)}} \frac{\cosh(\pi S(1 - 2|r_1|)) \prod_{k=1}^{n-1} \cos(2\pi S_k r_{k+1})}{S \sinh(\pi S)},\tag{46}$$

valid on the Delord n -cube, i.e. for $\mathbf{r} \in [-1/2, 1/2]^n$.

6.1. Closed forms for ψ_2 and ϕ_2

Using the series (46) for high-precision numerics, it was discovered (see [9, Appendix]) that previous lattice-sum literature has harbored a longtime typographical issue for certain 2-dimensional sums, and that a valid closed form for ψ_2 is actually

$$\psi_2(x, y) = \frac{x^2}{2} + \frac{1}{4\pi} \log \left(\frac{\Gamma(1/4)}{\sqrt{8\pi} \Gamma(3/4)} \right) - \frac{1}{2\pi} \log |\vartheta_1(\pi(ix + y), e^{-\pi})|. \tag{47}$$

As for the Madelung scenario, it then became possible to cast ϕ_2 likewise in closed form, namely

$$\phi_2(x, y) = \frac{1}{4\pi} \log |\alpha(z)| \quad \text{where} \quad \alpha(z) := \frac{\vartheta_2^2(z, q) \vartheta_4^2(z, q)}{\vartheta_1^2(z, q) \vartheta_3^2(z, q)} \tag{48}$$

for $q := e^{-\pi}$, $z := \frac{\pi}{2}(y + ix)$. (See [9] and Appendix II for details.)

Now we observe that, using classical results [6, §2.6 Exercises 2 and 4] on theta functions (also described in [16]), we may also write

Theorem 9. For $z := \frac{\pi}{2}(y + ix)$

$$\phi_2(x, y) = \frac{1}{2\pi} \log \left| \frac{\vartheta_2(z, q)\vartheta_4(z, q)}{\vartheta_1(z, q)\vartheta_3(z, q)} \right| = \frac{1}{4\pi} \log \left| \frac{1 - \frac{\lambda(z)}{\sqrt{2}}}{1 - \frac{1/\lambda(z)}{\sqrt{2}}} \right|, \quad (49)$$

and

$$\psi_2(x, y) = -\frac{1}{4\pi} \log \left| 2\mu(2z) \left(\sqrt{2}\lambda(2z) - 1 \right) \right|, \quad (50)$$

where

$$\lambda(z) := \frac{\vartheta_4^2(z, e^{-\pi})}{\vartheta_3^2(z, e^{-\pi})} = \prod_{n=1}^{\infty} \frac{(1 - 2\cos(2z)q^{2n-1} + q^{4n-2})^2}{(1 + 2\cos(2z)q^{2n-1} + q^{4n-2})^2}, \quad (51)$$

and

$$\mu(z) := e^{-\pi x^2/2} \frac{\vartheta_3^2(z, e^{-\pi})}{\vartheta_3^2(0, e^{-\pi})} = q^{x^2/2} \prod_{n=1}^{\infty} \frac{(1 + 2\cos(2z)q^{2n-1} + q^{4n-2})^2}{(1 + q^{2n-1})^4} \quad (52)$$

with $q := e^{-\pi}$.

We recall the general ϑ -transform giving for all z with $\operatorname{Re} t > 0$

$$\vartheta_{3-k}(\pi z, e^{-t\pi}) = \sqrt{1/t} e^{-\pi z^2/t} \vartheta_{3+k}(i\pi z/t, e^{-\pi/t}) \quad (53)$$

for $k = -1, 0, 1$ (while $\vartheta_1(\pi z, e^{-t\pi}) = \sqrt{-1/t} e^{-\pi z^2/t} \vartheta_1(i\pi z/t, e^{-\pi/t})$). In particular with $t = 1$ we derive that

$$\vartheta_{3-k}(\pi(ix + y), e^{-\pi}) = e^{-\pi z^2} \vartheta_{3+k}(\pi(iy - x), e^{-\pi}), \quad (54)$$

which directly relates $|\mu(\pi(y + ix))|$ and $|\mu(\pi(x + iy))|$ in (52). Let

$$\kappa(z) := \frac{\vartheta_2^2(z, e^{-\pi})}{\vartheta_3^2(z, e^{-\pi})}. \quad (55)$$

Then

$$\kappa(ix + y) + \lambda(ix + y) = \sqrt{2} \quad (56)$$

or $1 - \sqrt{2}\kappa(ix + y) = \sqrt{2}\lambda(ix + y) - 1$, and (53) then shows

$$\lambda(ix + y) = \kappa(-x + iy) = \sqrt{2} - \lambda(-x + iy). \quad (57)$$

Likewise (49) is unchanged on replacing λ by κ .

Hence, it is equivalent to (43) to prove that for all $z = \frac{\pi}{2}(y + ix)$ with x, y rational $\lambda(z)$ in (51) is algebraic. Note also the natural occurrence of the factor of 4π in the rightmost term of (49).

Theorem 10 (Algebraic values of λ and μ). *For all $z = \frac{\pi}{2}(y + ix)$ with x, y rational the values of $\lambda(z)$ and $\mu(2z)$ in (51) are algebraic. It follows that $\phi_2(x, y) = \frac{1}{4\pi} \log \alpha$ with α algebraic. Similarly $\psi_2(x, y) = \frac{1}{4\pi} \log \beta$ for β algebraic.*

Proof. (As suggested by Wadim Zudilin)

For λ , fix an integer $m > 1$. The addition formulas for the ϑ 's as given in [6, §2.6]

$$\vartheta_3(z+w, q)\vartheta_3(z-w, q)\vartheta_3^2(0, q) = \vartheta_3^2(z, q)\vartheta_3^2(w, q) + \vartheta_1^2(z, q)\vartheta_1^2(w, q) \quad (58)$$

$$\vartheta_4(z+w, q)\vartheta_4(z-w, q)\vartheta_4^2(0, q) = \vartheta_4^2(z, q)\vartheta_4^2(w, q) - \vartheta_1^2(z, q)\vartheta_1^2(w, q) \quad (59)$$

$$\begin{aligned} \vartheta_1(z+w, q)\vartheta_1(z-w, q)\vartheta_2(0, q)\vartheta_3(0, q) &= \vartheta_1(z, q)\vartheta_4(z, q)\vartheta_2(w, q)\vartheta_3(w, q) \\ &\quad + \vartheta_1(w, q)\vartheta_4(w, q)\vartheta_2(z, q)\vartheta_3(z, q) \end{aligned} \quad (60)$$

along with (56) allow one to write $\lambda(mz)$ algebraically in terms of $\lambda(z)$ in the same way that Weierstrass $\wp(mz)$ is in terms of $\wp(z)$. (We give the details below for μ .) We thus have an algebraic equation

$$\Omega_m(\lambda(z), \lambda(mz)) = 0. \quad (61)$$

for all z . Take m to be the denominator of x, y . Then mz is in $(\pi/2)(\mathbb{Z} + \mathbb{Z}i)$ and the double periodicity of λ —periods of λ are π and πi —allows us to conclude that $\lambda(mz) \in \{0, \lambda(0), 1/\lambda(0), \infty\}$, and these are algebraic numbers. In conjunction with (61) we are done.

For μ . For $u, v \in \mathbb{Z}$ we have [6, §2.6] that $\vartheta_3(z + \pi u + \pi i) = q^{-1}e^{-2iz}\vartheta_3(z)$, hence

$$\vartheta_3(z + \pi u + \pi iv) = q^{-v^2}e^{-2viz}\vartheta_3(z) = e^{\pi v^2 - 2viz}\vartheta_3(z). \quad (62)$$

We now assume that $z = \pi(y + ix) \in \pi(\mathbb{Q} + i\mathbb{Q})$, so that any quotient $\vartheta_j(z)/\vartheta_k(z)$ is an algebraic number. For any such z we set

$$f(z) = e^{-\pi x^2} \frac{\vartheta_3(z)}{\vartheta_3(0)}.$$

Now (58) can be re-written as

$$\frac{f(z_1 - z_2)f(z_1 + z_2)}{f(z_1)^2 f(z_2)^2} = 1 + \left(\frac{\vartheta_1(z_1)}{\vartheta_3(z_1)}\right)^2 \left(\frac{\vartheta_1(z_2)}{\vartheta_3(z_2)}\right)^2, \quad (63)$$

the right-hand side being *algebraic*. Since $f(0) = 1$, application of (63) with $z_1 = z_2 = z$ implies that $f(z)$ is algebraic over $K_2 := \overline{\mathbb{Q}}(f(2z))$; then inductive use (63) with $z_1 = (m-1)z$ and $z_2 = z$ shows $f(z)$ is algebraic over $K_m := \overline{\mathbb{Q}}(f(mz))$ for any m .

Now choose m such that $mz = \pi(Y + iX) \in \pi(\mathbb{Z} + i\mathbb{Z})$. By (62) for $z = 0$, $u = Y$ and $v = X (= mx)$,

$$\vartheta_3(mz) = e^{\pi X^2} \vartheta_3(0) = e^{\pi(mx)^2} \vartheta_3(0);$$

in other words, $f(mz) = 1$. But then $K_m = \overline{\mathbb{Q}}$ and by the above $f(z)$ is algebraic. Finally $f(2z)^2 = \mu(2z)$. \square

This will also work for any singular value: $\tau = \sqrt{-d}$ and $q = \exp(2\pi i\tau)$ and so may apply to sums with $n^2 + dm^2$ in the denominator, as we see in the next section.

6.2. Explicit equations for degree 2, 3, 5

We illustrate the complexity of Ω_m by first considering $m = 2, 3$.

Example 11 ($\lambda(2z)$ and $\lambda(3z)$). We also have various other consequences of Liouville's principle such as the following which were used in Theorem 9:

$$\vartheta_3^2(z, e^{-\pi}) = \sqrt{2} \vartheta_4^2(z, e^{-\pi}) - \vartheta_1^2(z, e^{-\pi}) \quad (64)$$

$$\vartheta_2^2(z, e^{-\pi}) = \vartheta_4^2(z, e^{-\pi}) - \sqrt{2} \vartheta_1^2(z, e^{-\pi}). \quad (65)$$

Setting $z = w$ in (58) and (59) on division we have

$$\lambda(2z)^{1/2} = 2^{3/4} \frac{\vartheta_4^4(z, e^{-\pi}) - \vartheta_1^4(z, e^{-\pi})}{\vartheta_3^4(z, e^{-\pi}) + \vartheta_1^4(z, e^{-\pi})}, \quad (66)$$

and so letting $\tau(z) = \vartheta_1^2(z, e^{-\pi})/\vartheta_3^2(z, e^{-\pi})$ we obtain Ω_2 in the form

$$\tau(z) = \sqrt{2}\lambda(z) - 1 \quad (67)$$

$$\lambda(2z) = 2^{3/2} \left(\frac{\lambda^2(z) - \tau^2(z)}{1 + \tau^2(z)} \right)^2, \quad (68)$$

where we have used (64). Iteration yields Ω_{2^n} . We may write (66) as

$$\Omega_2(x, y) = 2(x^4 + 1)^2 y^2 + 8(x^7 - x^5 - x^3 + x)y - x^8 + 12x^6 - 38x^4 + 12x^2 - 1, \quad (69)$$

for $x = \lambda(z), y = \lambda(2z)$. The inverse iteration is

$$x = \frac{2^{3/4} + \sqrt{y} - \sqrt{\sqrt{2} - y}}{\sqrt[4]{2} + \sqrt{2}\sqrt{y}}. \quad (70)$$

From this one may recursively compute $\lambda(z/2^n)$ from $\lambda(z)$ and watch the tower of radicals grow.

Correspondingly, we may use $2z \pm z$ in (58) and (59) to obtain

$$\lambda(3z) = 2 \frac{(\lambda(2z)\lambda(z) - \tau(2z)\tau(z))^2}{(1 + \tau(2z)\tau(z))^2 \lambda(z)}, \quad (71)$$

where $\tau(z), \tau(2z), \lambda(2z)$ are given by (67) and (68). After simplification we obtain

$$\lambda(3z) = \lambda(z) \left(\frac{\lambda^4(z) - 6\lambda^2(z) + 6\sqrt{2}\lambda(z) - 3}{3\lambda^4(z) - 6\sqrt{2}\lambda^3(z) + 6\lambda^2(z) - 1} \right)^2. \quad (72)$$

We can then determine that

$$\begin{aligned} \Omega_3(x, y) = & (81x^{16} - 648x^{14} + 1836x^{12} - 2376x^{10} + 1782x^8 - 792x^6 + 204x^4 \\ & - 24x^2 + 1)y^2 + (-18x^{17} + 264x^{13} - 768x^{11} + 916x^9 - 768x^7 \\ & + 264x^5 - 18x)y + x^{18} - 24x^{16} + 204x^{14} - 792x^{12} + 1782x^{10} \\ & - 2376x^8 + 1836x^6 - 648x^4 + 81x^2. \end{aligned}$$

In addition, since we have an algebraic relation $\alpha = \frac{1-\lambda/\sqrt{2}}{1-1/\lambda/\sqrt{2}}$ this allows us computationally to prove the evaluation of $\phi_2(x/2, y/2)$ and $\phi_2(x/3, y/3)$ once $\phi_2(x, y)$ is determined as it is for the cases of Theorem 3. \diamond

We may perform the same work inductively for $d = 2n + 1$ using $(n + 1)z \pm nz$ to obtain Ω_5 and so on. The inductive step is

$$\lambda((2n + 1)z) = \frac{2}{\lambda(z)} \left(\frac{\lambda((n + 1)z)\lambda(nz) - \tau((n + 1)z)\tau(nz)}{1 + \tau((n + 1)z)\tau(nz)} \right)^2. \quad (73)$$

In Example 17 we give the explicit formula for $\lambda(5z)$ as a rational function in $\lambda(z)$. Alternatively, integer relation methods can be used to empirically determine Ω_d for reasonably small degree d .

Example 12 (Empirical computation of Ω_d). Given z and $x = \lambda(z), y = \lambda(dz)$, we compute $x^j y^k$ for $0 \leq j \leq J, 0 \leq k \leq K$ up to degree J, K and look for a relation to precision D . This is a potential candidate for Ω_d . If $\Omega_d(\lambda(w), \lambda(dw)) \approx 0$ at a precision significantly greater than D and for various choices of w , we can reliably determine Ω_d this way. For $d = 2$, it is very easy to recover (69) in this fashion. For $3 \leq d \leq 5$ we had a little more difficulty. We show the equation for $\lambda(5z)$ in (77) and $\lambda(7z)$ in (94). \diamond

Example 13 (Products). Let $\Lambda(y) := \lambda((y + i \cdot 0)\pi/2)$. Then inspection of infinite-product forms for ϑ ratios yields the following λ -product identity. For any positive odd integer d ,

$$\Lambda\left(\frac{2}{d}\right) \cdot \Lambda\left(\frac{4}{d}\right) \cdots \Lambda\left(\frac{d-1}{d}\right) = \frac{\vartheta_3(0, e^{-\pi})\vartheta_4(0, e^{-d\pi})}{\vartheta_4(0, e^{-\pi})\vartheta_3(0, e^{-d\pi})} = 2^{1/4} \sqrt{k'_{d^2}}, \quad (74)$$

where $k' = \sqrt{1 - k^2}$ and k_{d^2} is the d^2 -singular value—itsself an algebraic number that can be given closed forms [6, 7]. This shows the intricate manner in which natural-potential value sets such as $\{\phi_2(0, 2/7), \phi_2(0, 4/7), \phi_2(0, 6/7)\}$ are interrelated. For example

$$k_{25}^2 = \frac{(\sqrt{5} - 2)^2(3 - 2 \cdot 5^{1/4})^2}{2}.$$

Correspondingly

$$2k_{49}k'_{49} = \left(\frac{7^{1/4} - \sqrt{4 + \sqrt{7}}}{2} \right)^{12}.$$

More subtle variations on this kind of computation are possible. \diamond

Remark 14 (Incomplete Landen transformation). Moreover, we have access to Landen's transformation [6, Thm. 2.5] namely

$$\frac{\vartheta_4(2z, e^{-2\pi})}{\vartheta_4(0, e^{-2\pi})} = \frac{\vartheta_4(z, e^{-\pi})\vartheta_3(z, e^{-\pi})}{\vartheta_4(0, e^{-\pi})\vartheta_3(0, e^{-\pi})},$$

for all z .

Example 15. We conclude this subsection by proving the empirical evaluation of (41), namely

$$\phi_2(1/5, 2/5) \stackrel{?}{=} \frac{1}{4\pi} \log 5^{1/4}. \quad (75)$$

Let $w = \frac{\pi}{10}(1 + 2i)$ so that

$$\phi_2(2/5, 1/5) = \frac{\log |\alpha(w)|}{4\pi} \quad \text{while} \quad -\phi_2(2/5, 1/5) = \frac{\log |\alpha(2w)|}{4\pi}$$

since $\phi_2(2/5, 4/5) = -\phi_2(2/5, 1/5)$. We may—with help from a computer algebra system—solve for the stronger requirement that $\alpha(2w) = -\alpha(w)$ using Example 11. We obtain

$$\alpha(2w) = \sqrt{\frac{2i-1}{5}}$$

so that $|\alpha(2w)| = 5^{-1/4}$ and $|\alpha(w)| = 5^{1/4}$, as required. To convert this into a proof we can make an a priori estimate of the degree and length of $\alpha(w)$ —using (68), (72) and (73) while $\lambda(5w) = 1$ —and then perform a high precision computation to show no other algebraic number could approximate the answer well enough. The underlying result we appeal to [6, Exercise 8, p. 356] is given next in Theorem 16.

In this particular case, we use $P(\alpha) = \alpha^4 + 2\alpha^2 + 5$ with $\ell = 8, d = 4$ and need to confirm that $|P(\alpha)| < 5^{D/4}L^{-3}8^{-D}$. A very generous estimate of $L < 10^{12}$ and $D < 10^3$ shows it is enough to check $|P(\alpha(w))| \leq 10^{-765}$. This is very easy to confirm. Relaxing to $L < 10^{100}, D < 10^4$ requires verifying $|P(\alpha(w))| \leq 10^{-7584}$. This takes only a little longer. \diamond

Recall that the *length* of a polynomial is the sum of the absolute value of the coefficients.

Theorem 16 (Determining a zero). *Suppose P is an integral polynomial of degree D and length L . Suppose that α is algebraic of degree d and length ℓ . Then either $P(\alpha) = 0$ or*

$$|P(\alpha)| \geq \frac{\max\{1, |\alpha|\}^D}{L^{d-1}\ell^D}.$$

Example 17 ($\lambda(5z)$). Making explicit the recipe for $\lambda(5z)$ we eventually arrive at:

$$\begin{aligned} \lambda(5z) &= \lambda(z) \frac{(\lambda^4(z) - 4\sqrt{2}\lambda^3(z) + 14\lambda^2(z) - 10\sqrt{2}\lambda(z) + 5)^2}{(5\lambda^4(z) - 10\sqrt{2}\lambda^3(z) + 14\lambda^2(z) - 4\sqrt{2}\lambda(z) + 1)^2} \\ &\times \frac{(\lambda^8(z) + 4\sqrt{2}\lambda^7(z) - 32\lambda^6(z) + 36\sqrt{2}\lambda^5(z) - 34\lambda^4(z) + 4\sqrt{2}\lambda^3(z) + 8\lambda^2(z) - 4\sqrt{2}\lambda(z) + 1)^2}{(\lambda^8(z) - 4\sqrt{2}\lambda^7(z) + 8\lambda^6(z) + 4\sqrt{2}\lambda^5(z) - 34\lambda^4(z) + 36\sqrt{2}\lambda^3(z) - 32\lambda^2(z) + 4\sqrt{2}\lambda(z) + 1)^2}. \end{aligned} \quad (76)$$

This shows how generous our estimates were in Example 15. Equation (76) may be written as

$$\lambda(5z) = \lambda(z) \frac{Q_5(\lambda(z))}{\widehat{Q}_5(\lambda(z))} \quad (77)$$

for an integer polynomial of degree 64 Here \widehat{Q}_5 reverses the coefficients of Q_5 and so is a renormalized reciprocal polynomial. For $n = 3$ in (71) this is also the case with Q_3 of degree 16. The case of $n = 2$ is slightly different.

The corresponding Ω_5 polynomial for degree 5 is:

$$\begin{aligned}
\Omega_5(x, y) = & -625x^2 + 23000x^4 - 336900x^6 + 2602520x^8 - 12245586x^{10} + 40127080x^{12} \\
& - 108682580x^{14} + 276123880x^{16} - 635900495x^{18} + 1237910128x^{20} \\
& - 2092012680x^{22} + 3279149040x^{24} - 4660484540x^{26} + 5424867280x^{28} \\
& - 4748415048x^{30} + 2986413520x^{32} - 1322491935x^{34} + 411477560x^{36} \\
& - 92161140x^{38} + 15610488x^{40} - 1998610x^{42} + 174920x^{44} - 11620x^{46} \\
& + 200x^{48} - x^{50} + 50xy + 1280x^3y - 20888x^5y - 148480x^7y + 4242660x^9y \\
& - 28815360x^{11}y + 95275720x^{13}y - 151372544x^{15}y - 76498770x^{17}y \\
& + 1124451840x^{19}y - 3330728240x^{21}y + 5935590400x^{23}y - 7143431048x^{25}y \\
& + 5935590400x^{27}y - 3330728240x^{29}y + 1124451840x^{31}y - 76498770x^{33}y \\
& - 151372544x^{35}y + 95275720x^{37}y - 28815360x^{39}y + 4242660x^{41}y \\
& - 148480x^{43}y - 20888x^{45}y + 1280x^{47}y + 50x^{49}y - y^2 + 200x^2y^2 - 11620x^4y^2 \\
& + 174920x^6y^2 - 1998610x^8y^2 + 15610488x^{10}y^2 - 92161140x^{12}y^2 \\
& + 411477560x^{14}y^2 - 1322491935x^{16}y^2 + 2986413520x^{18}y^2 - 4748415048x^{20}y^2 \\
& + 5424867280x^{22}y^2 - 4660484540x^{24}y^2 + 3279149040x^{26}y^2 - 2092012680x^{28}y^2 \\
& - 108682580x^{30}y^2 + 40127080x^{32}y^2 - 12245586x^{34}y^2 + 2602520x^{36}y^2 \\
& + 1237910128x^{38}y^2 - 635900495x^{40}y^2 + 276123880x^{42}y^2 - 336900x^{44}y^2 \\
& + 23000x^{46}y^2 - 625x^{48}y^2.
\end{aligned} \tag{78}$$

◇

In similar fashion we can now computationally confirm all of the other exact evaluations in Conjecture 4 and Example 6. For example, we know that $|\alpha(\pi(1/3 + i/3))| = |1/\alpha(\pi/2(2/3 + 2i/3))|$. This solves to produce $-\alpha(\pi/2(1/3 + i/3))^2 = 1 + 2/3\sqrt{3}$ and establishes (31) of Theorem 3. Now Example 11 can be used to produce $\alpha(\pi/2(1/6 + i/6))$ is as given in Conjecture 4. This also applies to $\psi_2(1/8, 1/8)$ of the next subsection and so on.

6.3. Evaluation of $\psi_2(x, y)$

We observe also that the classical lattice evaluation

$$\sum'_{m,n \in \mathbb{Z}} \frac{(-1)^{m+n}}{m^2 + n^2} = -\pi \log(2),$$

see [6, Eqn. (9.2.4)] shows that $\psi_2(1/2, 1/2) = -\frac{\log 2}{4\pi}$, and similarly $\psi_2(1/2, 0) = \psi_2(0, 1/2) = -\frac{\log 2}{8\pi}$.

Example 18 (Some empirical evaluations). We obtain experimentally that

$$\psi_2(1/3, 1/3) \stackrel{?}{=} \frac{\log\left(\frac{2\sqrt{3}-3}{3}\right)}{3 \cdot 8\pi}, \quad \psi_2(1/4, 1/4) \stackrel{?}{=} -\frac{\log 2}{4 \cdot 4\pi},$$

while

$$\psi_2(1/5, 1/5) \stackrel{?}{=} \frac{\log\left(-\frac{709}{2} + \frac{319}{2}\sqrt{5} + 3\sqrt{28090 - 12562\sqrt{5}}\right)}{5 \cdot 8\pi},$$

and

$$\psi_2(1/6, 1/6) \stackrel{?}{=} \frac{\log(2 + \sqrt{3})}{6 \cdot 2\pi}.$$

So we are off to the races again.

By techniques like those of Appendix I we can establish a subset of such results:

$$\psi_2(1/4, 1/4) = -\frac{\log 2}{4 \cdot 4\pi}, \quad \psi_2(1/4, 0) = \frac{\log \frac{4+3\sqrt{2}}{2}}{4 \cdot 4\pi},$$

and

$$\psi_2(1/6, 1/6, 1) = \frac{\log(2 + \sqrt{3})}{2 \cdot 6\pi},$$

via explicit lattice sum factorization. But the other cases, perhaps unsurprisingly in light of (50), seem more recondite than for ϕ_2 . Details are given in Appendix III. \diamond

6.4. “Compressed” potentials

Yet another solution to the Poisson equation with crystal charge source, for $d > 0$, is

$$\phi_2(x, y, d) := \frac{1}{\pi^2} \sum_{m, n \in \mathbb{O}^2} \frac{\cos(\pi m x) \cos(\pi n \sqrt{d} y)}{m^2 + dn^2}. \quad (79)$$

This is the potential inside a crystal compressed by $1/\sqrt{d}$ on the y -axis, in the sense that the Delord-cube now becomes the cuboid $\{x, y\} \in [-1/2, 1/2] \times [-1/(2\sqrt{d}), 1/(2\sqrt{d})]$. Indeed, $\phi_2(x, y, d)$ vanishes on the faces of this 2-cuboid (rectangle) for $d > 0$ and integer.

Along the same lines as involve the analysis of (22), we can posit a fast series

$$\phi_2(x, y, d) = \frac{1}{\pi\sqrt{d}} \sum_{R \in \mathbb{O}^+} \frac{\sinh(\pi R \sqrt{d} (1/2 - |x|)) \cos(\pi R \sqrt{d} y)}{R \cosh(\pi R \sqrt{d} / 2)}, \quad (80)$$

valid on the Delord cuboid, i.e. $x \in [-1/2, 1/2]$, $y \in [-1/(2\sqrt{d}), 1/(2\sqrt{d})]$.

Moreover, the log-accumulation technique of [9, Appendix] (see also our Appendix II) may be used as with Theorem 9 to obtain:

Theorem 19 (ϑ -representation for compressed potential). *For the compressed potential we have*

$$\phi_2(x, y, d) = \frac{1}{2\sqrt{d}\pi} \log \left| \frac{\vartheta_2(z, q)\vartheta_4(z, q)}{\vartheta_1(z, q)\vartheta_3(z, q)} \right|, \quad (81)$$

where $q := \exp(-\pi\sqrt{d})$ and $z := \frac{1}{2}\pi\sqrt{d}(y + ix)$.

Note that this theorem is consistent with $d = 1$, in the sense $\phi_2(x, y, 1) = \phi_2(x, y)$. In addition, for integers $a, b \geq 1$ we have:

$$a^2 \phi_2 \left(ax, ay, \frac{b^2}{a^2} \right) := \frac{1}{\pi^2} \sum_{m \in a\mathbb{O}, n \in b\mathbb{O}} \frac{\cos(\pi mx) \cos(\pi ny)}{m^2 + n^2}. \quad (82)$$

Moreover, for each positive rational d there is an analogue of Theorem 10 in which $1/\sqrt{2}$ is replaced by the d -th singular value k_d [6, 7]. Thus $k_2 = \sqrt{2} - 1$, $k_3 = (\sqrt{3} - 1)/\sqrt{2}$, and $k_4 = (\sqrt{2} - 1)^2$. Precisely, we set

$$\begin{aligned} \lambda_d(z) &:= \frac{\vartheta_4^2(z, \exp(-\pi\sqrt{d}))}{\vartheta_3^2(z, \exp(-\pi\sqrt{d}))} & \kappa_d(z) &:= \frac{\vartheta_2^2(z, \exp(-\pi\sqrt{d}))}{\vartheta_3^2(z, \exp(-\pi\sqrt{d}))} \\ \tau_d(z) &:= \frac{\vartheta_1^2(z, \exp(-\pi\sqrt{d}))}{\vartheta_3^2(z, \exp(-\pi\sqrt{d}))} \end{aligned} \quad (83)$$

and we have

$$k'_d \lambda_d(z) + k_d \kappa_d(z) = 1,$$

(see [6, Prop. 2.1]), while

$$k_d \lambda_d(z) - k'_d \kappa_d(z) = \tau_d(z).$$

Thus,

$$\phi_2(x, y, d) = \frac{1}{4\sqrt{d}\pi} \log \left| \frac{1 - k'_d \lambda_d(z)}{1 - k'_d / \lambda_d(z)} \right|, \quad (84)$$

and we may now study λ_d exclusively. We specify the details in a separate paper [2]. For now we record only the the equation for $\lambda_d(2z)$.

Example 20 ($\lambda_d(2z)$). As for $\lambda(2z)$, which is the case $d = 1$, we have

$$\tau_d(z) = \frac{\lambda_d(z) - k'_d}{k_d} \quad (85)$$

$$\lambda_d(2z) = k'^{-3}_d \left(\frac{\lambda_d^2(z) - \tau_d^2(z)}{1 + \tau_d^2(z)} \right)^2. \quad (86)$$

This becomes

$$\lambda_d(2z) = k'_d \left(\frac{1 + \lambda_d^2(z) - 2\lambda_d(z)/k'_d}{1 + \lambda_d^2(z) - 2\lambda_d(z) \cdot k'_d} \right)^2, \quad (87)$$

and $\lambda_d(0) = k'_d$. \diamond

We record: $\phi_2(x, 1/4, 4) = 0$ for all x and have several sample evaluations:

$$\phi_2(1/3, \sqrt{2}/3, 2) \stackrel{?}{=} \frac{-1}{8\sqrt{2}\pi} \log(9 - 6\sqrt{2}) \quad (88)$$

$$\phi_2(1/3, \sqrt{3}/3, 3) \stackrel{?}{=} \frac{-1}{8\sqrt{3}\pi} \log 3 \quad (89)$$

$$\phi_2(1/3, 1/3, 4) \stackrel{?}{=} \frac{1}{16\pi} \log \left(\sqrt{3} (2 + \sqrt{3}) (\sqrt{2} - \sqrt{3})^2 \right) \quad (90)$$

$$\begin{aligned} \phi_2(1/4, 1/4, 9) \stackrel{?}{=} & \frac{1}{48\pi} \log \left(\frac{1}{4} (3 + 5\sqrt{3} - 4\sqrt{2}) (\sqrt{3} - 1)^3 (1 + \sqrt{2})^2 \right. \\ & \left. \cdot (\sqrt{3} - \sqrt{2})^2 \right). \end{aligned} \quad (91)$$

In general we anticipate similarly algebraic evaluations for $\phi_2(a/c, \sqrt{kb}/c, k)$ for nonnegative integer values of a, b, c, k

7. Computation techniques and results

7.1. Discovery of minimal polynomials for algebraic numbers in $\phi_2(x, y)$ and $\psi_2(x, y)$

The experimental evaluations of $\phi_2(x, y)$ and $\psi_2(x, y)$ presented in the previous two sections, along with numerous others summarized in Table 1, 2 and 3 below, were, in most cases, obtained by the following computational procedure:

- (i) Given a positive integer d , select a conjectured polynomial degree m and a precision level P . For $\phi_2(x, y)$, we typically set the numeric precision level P somewhat greater than $0.5m^2$ digits (see Tables 1 and 2), while for $\psi_2(x, y)$, we set P somewhat greater than $3m^2$ (see Table 3).
- (ii) Given the rationals $x = j/d$ and $y = k/d$, compute $\phi_2(x, y)$ to P -digit precision using formula (23), terminating the infinite series when the terms are consistently less than the “epsilon” of the arithmetic being used. The functions \cosh and \sin can be evaluated using well-known well-known schemes based on argument reductions and infinite series [5, pg. 218–235]. Alternatively (which is faster), compute $\phi_2(x, y)$ via formula (49). Evaluate the four theta functions indicated using the very rapidly convergent formulas given in [6, pg. 52] or [15]. Similarly, compute $\psi_2(x, y)$ using formulas (50), (51) and (52).
- (iii) Generate the $(m + 1)$ -long vector $(1, \alpha, \alpha^2, \dots, \alpha^m)$, where either $\alpha = \exp(8\pi\phi_2(x, y))$ or $\alpha = \exp(8\pi\psi_2(x, y))$ as appropriate. Note: we have found that without the eight here, the degree of the resulting polynomial would be eight times as high (but the larger polynomials were in fourth or eighth powers). Given the very rapidly escalating computational cost of

higher degrees, many of the results listed in Tables 1 and 2 would not be feasible without this factor.

- (iv) Apply the PSLQ algorithm (we actually employed the two-level multipair variant of PSLQ [3]) to find a nontrivial $(m + 1)$ -long integer vector $A = (a_0, a_1, a_2, \dots, a_m)$ such that $a_0 + a_1\alpha + a_2\alpha^2 + \dots + a_m\alpha^m = 0$, if such a vector exists. PSLQ (or one of its variants) either finds a vector A , which then is the vector of coefficients of an integer polynomial satisfied by α (certified to the “epsilon” of the numerical precision used), or else exhausts precision without finding a relation, in which case the algorithm nonetheless provides a lower bound on the Euclidean norm of the coefficients of any possible degree- m integer polynomial A satisfied by α .
- (v) If no relation is found, try again with a larger value of m and correspondingly higher precision. If a relation is found, try with somewhat lower m , until the minimal m is found that produces a numerically significant relation vector A . Here “numerically significant” means that the relation holds to at least 100 digits beyond the level of precision required to discover it. To obtain greater assurance that the polynomial produced by this process is in fact the minimal polynomial for α , use the polynomial factorization facilities in *Mathematica* or *Maple* to attempt to factor the resulting polynomial.

Our computations required up to 20,000-digit precision, and, for large degrees and correspondingly high precision levels, were rather expensive (over 100 processor-hours in some cases). We employed the ARPREC arbitrary precision software [4].

Table 1 below shows results for in our results to find the minimal polynomial for $\exp(8\pi\phi_2(1/d, 1/d))$ for various positive integers d . In this table, runs noted with an asterisk were obtained by Andrew Mattingly. Table 2 shows similar data for $\exp(8\pi\phi_2(1/d, q/d))$, where in each case $q \geq 2$ is chosen to be the smallest integer coprime with d . Table 3 shows similar data for $\exp(8\pi\psi_2(1/d, 1/d))$.

The number of zeroes $z(d)$ among the minimal polynomial coefficients, the numeric precision level P , the run time in seconds T , and the approximate base-10 logarithm M of the absolute value of the central coefficient, are also shown in the tables, together with the ratio $(\log_{10} M)/m(d)$. Note that this ratio tends to be highly consistent within each table, at least for successful runs. The notation “Failed” means that we were unable to find a polynomial for the specific case, in which case the entry in the column $\log_{10} M$ is the base-10 logarithm of the norm bound produced by the PSLQ program for that run (shown in bold), and the last column gives this value divided by $m(d)$.

As Jason Kimberley has observed empirically, in Table 1 the degree of the polynomial $m(d)$ appears to be given for odd primes by $m(4k + 1) = (2k) \cdot (2k)$ and $m(4k + 3) = (2k + 2) \cdot (2k + 1)$. If we set $m(2) = 1/2$, for notational convenience, then it seems that for any prime factorization

of an integer greater than 2:

$$m \left(\prod_{i=1}^k p_i^{e_i} \right) \stackrel{?}{=} 4^{k-1} \prod_{i=1}^k p_i^{2(e_i-1)} m(p_i). \quad (92)$$

This sequence now appears as <http://oeis.org/A218147> in the *Online Encyclopedia of Integer Sequences*.

With regards to the run times listed (given to 0.01 second accuracy), it should be recognized that like all computer run times, particularly in a multicore or multiprocessor environment, they are only repeatable to two or three significant digits. They are listed here only to emphasize the extremely rapid increase in computational cost as the degree m and corresponding precision level P increase.

Remark 21. With regards to the results in Tables 1, 2 and 3, we observe the following:

- (i) We observe that with a few exceptions (as noted in Examples 5 and 6) the minimal polynomial for $\exp(8\pi\phi_2(1/d, q/d))$, where q is the smallest integer coprime with d , as given in Table 2, appears to have the same degree as the minimal polynomial for $\exp(8\pi\phi_2(1/d, 1/d))$, as given in Table 1. We have confirmed this in Table 2 and noted that the polynomials are typically dense. In Table 2, we mark in italics those which have a lower degree than the corresponding entry in Table 1.
- (ii) Although the degree of the minimal polynomial for $\exp(8\pi\psi_2(1/d, 1/d))$ (from Table 3) is, in most cases, the same as the corresponding degree for $\exp(8\pi\phi_2(1/d, 1/d))$ (from Table 1), the coefficients of the polynomials in Table 3 are much larger. For example, in the case $d = 17$, the central coefficient of the degree-64 minimal polynomial for $\exp(8\pi\psi_2(1/17, 1/17))$ is approximately 2.936×10^{218} , as compared with approximately 1.736×10^{28} for $\exp(8\pi\phi_2(1/17, 1/17))$.
- (iii) We also observe that for each d , $\exp(8\pi\phi_2(k/d, k/d))$ appears to satisfy the same minimal polynomial as $\exp(8\pi\phi_2(1/d, 1/d))$, whenever $(k, d) = 1$. We have confirmed this in every successful case listed in Table 1, namely for all integers up to 32 except 27, 29 and 31.
- (iv) Similarly, the constants $\exp(8\pi\phi_2(j/d, k/d))$ appear to share the same minimal polynomial (or the alternating sign equivalent) for all $0 < j < k \leq d/2$ and k with $(j, d) = (k, d) = (j, k) = 1$. We have checked this for all successful cases in Table 1.
- (v) A sample of the extraordinarily large polynomials that we obtained is shown in Table 4.
- (vi) In all cases we checked the polynomials split once over an appropriate quadratic extension field.
- (vii) In Table 1, note that in each of the three cases for which we failed to find a relation, the base-10 logarithm of the norm bound divided by $m(d)$ is significantly larger than the values for $(\log_{10} M)/m(q)$ for the successful cases. This suggests that the minimal polynomials

d	$m(d)$	$z(d)$	P	T	$\log_{10} M$	$\frac{\log_{10} M}{m(d)}$
3	2	0	400			
4	2	0	400			
5	4	0	400	0.40	1.4150	0.3537
6	4	0	400	0.39	0.7782	0.1945
7	12	0	400	0.71	5.0489	0.4207
8	8	0	400	0.43	3.2989	0.4124
9	18	0	400	1.81	7.6477	0.4249
10	8	0	400	0.54	2.6571	0.3321
11	30	0	1000	28.50	12.9873	0.4329
12	16	0	400	1.22	6.7880	0.4243
13	36	0	1000	44.04	15.6385	0.4344
14	24	0	1000	12.37	9.7245	0.4052
15	32	0	1000	34.58	12.8370	0.4012
16	32	0	1000	29.62	13.8452	0.4327
17	64	0	4000	3387.71	28.2396	0.4412
18	36	0	2000	274.60	13.8718	0.3853
19	90	0	6000	19559.37	39.8456	0.4427
20	32	0	2000	222.87	13.9705	0.4366
21	96	0	6000	25210.51	42.4696	0.4424
22	60	0	3000	1748.19	25.8002	0.4300
23	132	0	12000	212634.54	58.7280	0.4449
24	64	0	3000	2224.42	28.1624	0.4400
25	100	0	8000	58723.90	44.0690	0.4407
26	72	0	4000	4961.57	30.9611	0.4300
27*	162		19500	128074.00	72.1946	0.4456
28	96	0	8000	46795.52	42.5098	0.4428
29*	196		19500	145388.00	87.4974	0.4464
30	64	0	3000	2208.95	27.2294	0.4255
31	144		12000	Failed	79.4119	0.5515
32	128	0	10000	163662.83	56.8932	0.4445

Table 1. PSLQ runs to recover minimal polynomials satisfied by $\exp(8\pi\phi_2(1/d, 1/d))$. Here $m(d)$ is the degree, $z(d)$ is the number of zero coefficients, P is the precision level in digits, T is the run time in seconds, and $\log_{10} M$ is the size in digits of the central coefficient. In cases where we failed to find a minimal polynomial, the next-to-last column gives the base-10 logarithm of the norm bound produced by PSLQ (shown in bold), and the last column gives this value divided by $m(d)$.

d	q	$m(d, q)$	$z(d, q)$	P	T	$\log_{10} M$	$\frac{\log_{10} M}{m(d, q)}$
3	2	2	1	400			
4	3	2	0	400			
5	2	<i>2</i>	1	400	0.05		
6	5	4	0	400	0.48	0.7782	0.1945
7	2	12	6	400	0.61	3.9748	0.3312
8	3	<i>4</i>	0	400	0.57	1.4150	0.3537
9	2	18	0	400	2.15	4.9247	0.2736
10	3	<i>4</i>	0	400	0.79	0.3010	0.0753
11	2	30	0	1000	35.46	8.9251	0.2975
12	5	<i>8</i>	0	1000	14.79	2.7649	0.3456
13	2	36	0	1000	57.66	11.7334	0.3259
14	3	24	0	1000	23.15	7.1480	0.2978
15	2	32	0	1000	44.09	9.9373	0.3105
16	3	32	0	1000	34.17	10.5043	0.3283
17	2	64	0	3000	2937.12	20.8611	0.3260
18	5	36	0	2000	622.89	9.4009	0.2611
19	2	90	0	4000	11261.72	28.4757	0.3164
20	3	32	0	2000	706.11	10.7876	0.3371
21	2	96	0	6000	19324.80	30.4115	0.3168
22	3	60	0	3000	2634.11	18.2712	0.3045
23	2	132	0	12000	163121.04	42.3745	0.3210
24	5	<i>32</i>	0	3000	2298.24	10.1475	0.3171
25	2	100	0	8000	45993.38	30.6394	0.3064
26	3	72	0	4000	6650.19	22.5268	0.3129
27	2	144		12000	Failed	79.4592	0.5518
28	3	96	0	8000	47313.98	31.1368	0.3243
29	2	144		12000	Failed	79.5120	0.5522
30	5	64	0	3000	2641.60	22.6747	0.3543
31	2	144		12000	Failed	79.5970	0.5528
32	3	128	0	12000	142227.49	41.4107	0.3235

Table 2. PSLQ runs to recover minimal polynomials satisfied by $\exp(8\pi\phi_2(1/d, q/d))$, where q is the smallest integer coprime with d . Here $m(d, q)$ is the degree (shown in italics if different from entry in Table 1), $z(d, q)$ is the number of zero coefficients, P is the precision level in digits, T is the run time in seconds, and $\log_{10} M$ is the size in digits of the central coefficient. In cases where we failed to find a minimal polynomial, the next-to-last column gives the base-10 logarithm of the norm bound produced by PSLQ (shown in bold), and the last column gives this value divided by $m(d, q)$.

d	$m(d)$	$z(d)$	P	T	$\log_{10} M$	$\frac{\log_{10} M}{m(d)}$
3	2	0	400			
4	1	0	400			
5	4	0	400	0.04	3.7782	0.9446
6	2	0	400	0.04	2.2878	1.1439
7	12	0	400	0.14	16.4171	1.3681
8	5	0	400	0.03	6.1960	1.5490
9	18	0	1000	12.18	32.3999	1.8000
10	4	0	400	0.05	8.7028	2.1757
11	30	0	4000	97.51	66.6944	2.2231
12	16	0	1000	0.35	20.1865	2.5233
13	36	0	6000	227.17	94.9054	2.6363
14	24	0	2000	9.3803	33.3200	2.7767
15	32	0	6000	184.68	96.8105	3.0253
16	16	0	1000	9.25	52.2196	3.2637
17	64	0	20000	40311.96	218.4678	3.4136
18	18	0	2000	12.75	64.8446	3.6025
19	90	0	20000	Failed	163.0918	1.8121
20	17	0	2000	12.1360	64.1039	4.0065

Table 3. PSLQ runs to recover minimal polynomials satisfied by $\exp(8\pi\psi_2(1/d, 1/d))$. Here $m(d)$ is the degree, $z(d)$ is the number of zero coefficients, P is the precision level in digits, T is the run time in seconds, and $\log_{10} M$ is the size in digits of the central coefficient. In the one case where we failed to find a minimal polynomial, the next-to-last column gives the base-10 logarithm of the norm bound produced by PSLQ (shown in bold), and the last column gives this value divided by $m(d)$.

for these cases have degrees higher than 144, and that significantly more computation will be required to recover them. Indeed, formula (92) predicts $m(27) = 162$, $m(29) = 196$ and $m(31) = 240$, so that unwittingly our failed cases confirm (92).

A similar conclusion holds for the failed cases in Table 2. However, in Table 3, in the one case of failure, the last-column bold value is less than the corresponding figure for most of the successful cases. But given that the degrees in Table 3 are, in most cases, the same as corresponding entries in Table 1, it seems likely that $\exp(8\pi\psi_2(1/19, 1/19))$ does satisfy a minimal polynomial of degree 90, as listed in the table, although evidently more than 20,000-digit precision will be required to recover the vector of coefficients.

$$\begin{aligned}
& -1 + 21888\alpha + 5893184\alpha^2 + 15077928064\alpha^3 - 3696628330464\alpha^4 - 287791501240448\alpha^5 - 30287462976198976\alpha^6 \\
& + 4426867843186404992\alpha^7 - 554156920878198587888\alpha^8 + 10731545733669133574528\alpha^9 \\
& + 120048731928709050250048\alpha^{10} + 4376999211577765512726656\alpha^{11} - 279045693458194222125366432\alpha^{12} \\
& + 18747586287780118903854334848\alpha^{13} - 643310226865188446831485766208\alpha^{14} \\
& + 12047117225922787728443496655488\alpha^{15} - 117230595100328033884939566091384\alpha^{16} \\
& + 667772184328316952814362214365568\alpha^{17} - 4130661734713288144037409932696512\alpha^{18} \\
& + 7231362623938964765274946226530432\alpha^{19} - 1891420571205861612091802761809141088\alpha^{20} \\
& + 38770881730553471470590641060872686464\alpha^{21} - 577943965397394779947709633563006963008\alpha^{22} \\
& + 6279796382074485140847650604801614559872\alpha^{23} - 50438907678331243798448849245156136801232\alpha^{24} \\
& + 305806320133365055812520453224169520739712\alpha^{25} - 1441007171934715336769224848138270812591296\alpha^{26} \\
& + 5554617356232728647085822946642640269497472\alpha^{27} - 20280024430170705107000630261773759070647328\alpha^{28} \\
& + 99541720739995105011861264308551867164583808\alpha^{29} - 754081464712315412970559119390477134883548736\alpha^{30} \\
& + 6271958646895434365874802435136411922022336128\alpha^{31} - 45931349314815625339442690290912948480194150172\alpha^{32} \\
& + 280907040806572157908285324812126135484630889344\alpha^{33} - 1427273782916972532576299009596755423149111059136\alpha^{34} \\
& + 6055180299673737231932804443230077408291723908736\alpha^{35} - 21609910939164553316101994301952988793013291135584\alpha^{36} \\
& + 65433275736596914909292838375737685959952141180288\alpha^{37} - 169928170513492897108417040254326115991438719391296\alpha^{38} \\
& + 385709310577705218843549196766620216295554031550592\alpha^{39} - 801233230832691550861608914233661767474963249815792\alpha^{40} \\
& + 1706210557291030772074402183123327251333271061516160\alpha^{41} - 4421210594351357102505784181831242174063263551938496\alpha^{42} \\
& + 14444199585866329915643888187597383540233619718619776\alpha^{43} - 50968478530199956388487913417905125665738409426112032\alpha^{44} \\
& + 169891313454945514927724813351516976839425267825908096\alpha^{45} - 506612996672385619931633440490993959534203673546181440\alpha^{46} \\
& + 1330573388204326565144545192834096788469932897185696896\alpha^{47} - 3069501638444045841407951432645059776135089489403138888\alpha^{48} \\
& + 6226636397646752257692349351542872634032398917736673152\alpha^{49} - 11133383491631126059761752734485434504397040890449485504\alpha^{50} \\
& + 17601823309919260471943648355479182983209248554083752576\alpha^{51} - 24723027443995082126054012492323603544226813344022687712\alpha^{52} \\
& + 31141043717679289808081270766611355726695735914995681664\alpha^{53} - 35982430389670551550204799905599476866868765647852189248\alpha^{54} \\
& + 40292583920117898286863491450657424717015372825433076864\alpha^{55} - 48512188214363976290470868896252008979896310883132967248\alpha^{56} \\
& + 69275112214095149977288310632868535966705567728055958400\alpha^{57} - 114516830148561378617778209682642099604147034577152904128\alpha^{58} \\
& + 195760470467323759899736578743283333538805684128806803072\alpha^{59} - 317349593507106729834513764473487031789280056911012860320\alpha^{60} \\
& + 468944248086031450001465269696090117959962662732817675648\alpha^{61} - 622467103741378906100611838210632752408312516281305008960\alpha^{62} \\
& + 738516443137003178837650661261546833168555909499151978624\alpha^{63} - 781916756680856373187881889706233393197646662361906135622\alpha^{64} \\
& + 738516443137003178837650661261546833168555909499151978624\alpha^{65} - 622467103741378906100611838210632752408312516281305008960\alpha^{66} \\
& + 468944248086031450001465269696090117959962662732817675648\alpha^{67} - 317349593507106729834513764473487031789280056911012860320\alpha^{68} \\
& + 195760470467323759899736578743283333538805684128806803072\alpha^{69} - 114516830148561378617778209682642099604147034577152904128\alpha^{70} \\
& + 69275112214095149977288310632868535966705567728055958400\alpha^{71} - 48512188214363976290470868896252008979896310883132967248\alpha^{72} \\
& + 40292583920117898286863491450657424717015372825433076864\alpha^{73} - 35982430389670551550204799905599476866868765647852189248\alpha^{74} \\
& + 31141043717679289808081270766611355726695735914995681664\alpha^{75} - 24723027443995082126054012492323603544226813344022687712\alpha^{76} \\
& + 17601823309919260471943648355479182983209248554083752576\alpha^{77} - 11133383491631126059761752734485434504397040890449485504\alpha^{78} \\
& + 6226636397646752257692349351542872634032398917736673152\alpha^{79} - 3069501638444045841407951432645059776135089489403138888\alpha^{80} \\
& + 1330573388204326565144545192834096788469932897185696896\alpha^{81} - 506612996672385619931633440499093959534203673546181440\alpha^{82} \\
& + 169891313454945514927724813351516976839425267825908096\alpha^{83} - 50968478530199956388487913417905125665738409426112032\alpha^{84} \\
& + 14444199585866329915643888187597383540233619718619776\alpha^{85} - 4421210594351357102505784181831242174063263551938496\alpha^{86} \\
& + 1706210557291030772074402183123327251333271061516160\alpha^{87} - 801233230832691550861608914233661767474963249815792\alpha^{88} \\
& + 385709310577705218843549196766620216295554031550592\alpha^{89} - 169928170513492897108417040254326115991438719391296\alpha^{90} \\
& + 65433275736596914909292838375737685959952141180288\alpha^{91} - 21609910939164553316101994301952988793013291135584\alpha^{92} \\
& + 6055180299673737231932804443230077408291723908736\alpha^{93} - 1427273782916972532576299009596755423149111059136\alpha^{94} \\
& + 280907040806572157908285324812126135484630889344\alpha^{95} - 45931349314815625339442690290912948480194150172\alpha^{96} \\
& + 6271958646895434365874802435136411922022336128\alpha^{97} - 754081464712315412970559119390477134883548736\alpha^{98} \\
& + 99541720739995105011861264308551867164583808\alpha^{99} - 20280024430170705107000630261773759070647328\alpha^{100} \\
& + 5554617356232728647085822946642640269497472\alpha^{101} - 1441007171934715336769224848138270812591296\alpha^{102} \\
& + 305806320133365055812520453224169520739712\alpha^{103} - 50438907678331243798448849245156136801232\alpha^{104} \\
& + 6279796382074485140847650604801614559872\alpha^{105} - 577943965397394779947709633563006963008\alpha^{106} \\
& + 38770881730553471470590641060872686464\alpha^{107} - 1891420571205861612091802761809141088\alpha^{108} \\
& + 7231362623938964765274946226530432\alpha^{109} - 4130661734713288144037409932696512\alpha^{110} \\
& + 667772184328316952814362214365568\alpha^{111} - 117230595100328033884939566091384\alpha^{112} \\
& + 12047117225922787728443496655488\alpha^{113} - 643310226865188446831485766208\alpha^{114} \\
& + 18747586287780118903854334848\alpha^{115} - 279045693458194222125366432\alpha^{116} \\
& + 4376999211577765512726656\alpha^{117} + 120048731928709050250048\alpha^{118} + 10731545733669133574528\alpha^{119} \\
& - 554156920878198587888\alpha^{120} + 4426867843186404992\alpha^{121} - 30287462976198976\alpha^{122} \\
& - 287791501240448\alpha^{123} - 3696628330464\alpha^{124} + 15077928064\alpha^{125} + 5893184\alpha^{126} + 21888\alpha^{127} - \alpha^{128}
\end{aligned}$$

Table 4. Minimal polynomial discovered by PSLQ for $\alpha = \exp(8\pi\phi_2(1/32, 1/32))$.

7.2. Numerical discovery of $\Omega_m(x, y)$ polynomials

In our analysis of the $\Omega_m(x, y)$ polynomials, we employed the following computational strategy. Freely extrapolating from the cases $m = 2$ and $m = 3$, we hypothesized that these polynomials are all of the form

$$\Omega_m(x, y) \stackrel{?}{=} P_m(x, y) = p_0(x) + p_1(x)y + p_2(x)y^2, \quad (93)$$

where $p_0(x)$ and $p_2(x)$ have only even powers of x and are of degree $2m^2$, while $p_1(x)$ has only odd powers of x and is of degree $2m^2 + 1$. Note that the total number of terms of $P_m(x, y)$ is thus $3(m^2 + 1)$. With this reckoning in mind, we arbitrarily selected some real z , such as $z = 1$, then numerically computed $x = \lambda(z)$, $y = \lambda(mz)$ and all $3(m^2 + 1)$ terms of $P_m(x, y)$ to very high precision. This $3(m^2 + 1)$ -long vector was then input to a PSLQ program, which produced a vector of integers, which then are the coefficients of $P(x, y)$, and, thus, of $\Omega_m(x, y)$. This procedure successfully recovered plausible $\Omega_m(x, y)$ polynomials up to $m = 7$, which run required 4000-digit arithmetic and 7.5 processor-hours computer run time. The next case of interest, $m = 11$, would require much higher precision and many times more computer run time. After computer-algebraic massaging we recovered

$$\lambda(7z) \stackrel{?}{=} \lambda(z) \left(\frac{Q_7(\lambda(z))}{\widehat{Q}_7(\lambda(z))} \right)^2 \quad (94)$$

where

$$\begin{aligned} Q_7(x) = & x^{24} - 196x^{22} + 1764\sqrt{2}x^{21} - 16422x^{20} + 48888\sqrt{2}x^{19} - 200732x^{18} \\ & + 290052\sqrt{2}x^{17} - 559993x^{16} + 243936\sqrt{2}x^{15} + 544152x^{14} - 1480248\sqrt{2}x^{13} \\ & + 3758860x^{12} - 3331440\sqrt{2}x^{11} + 4457992x^{10} - 2298072\sqrt{2}x^9 + 1821407x^8 \\ & - 543648\sqrt{2}x^7 + 231532x^6 - 29484\sqrt{2}x^5 - 70x^4 + 1848\sqrt{2}x^3 - 812x^2 \\ & + 84\sqrt{2}x - 7, \end{aligned}$$

and \widehat{Q}_7 reverses the coefficients of Q_7 , as was the case with (71) and (77).

8. Closed forms for $n = 3, 4$ dimensions

The only nontrivial closed form evaluation of ϕ_3 of which we are aware is that of Forrester and Glasser [10, 6, 7]. Namely

$$\begin{aligned} 4\pi\phi_3(\mathbf{1}/\mathbf{6}) &= \mathcal{M}_3(1, \mathbf{1}/\mathbf{6}) = \sum_{\mathbf{m} \in \mathbb{Z}^3} \frac{(-1)^{\mathbf{1} \cdot \mathbf{m}}}{|\mathbf{m} - \mathbf{1}/\mathbf{6}|} \\ &= \sqrt{3}. \end{aligned}$$

A careful search for closed forms $\phi_3(\mathbf{r})$ seems called for.

We also have access to a splitting algorithm for very high precision computation of ϕ_n values. (See [9, Sec 3.5] and [8] for relevant series forms.) Thence, to 1000 places

$$\phi_4(1/6, 1/6, 1/6, 1/6) =$$

```
0.1598295944178901737538686709387968761639933022144751037391120691681838842744\
209064806793412115298503409343583548679702288709168670207456499599800486154108\
308165030043936153109658545566067935390541166323196740557596875085706590081648\
013179231342864216112479518653976132625873221005912039529813868011734049817551\
508567833965177341021725140962373469383292594983556975941002041270309026720362\
867404154000999515556155877859315248933268525767350366384980561471158844878559\
022481927005081171952246111536064311228653311696791690164965431933924469708502\
754419428439446777269398123987112367163919553812864963576841446876027640005161\
786754254941372509144587265751232911776700205737574810405772940786524434341685\
453710838983862891142087879809840401056128726071492273488926720130803026529300\
965224446071196799462710004752411247479068658082206364885402729179680334639994\
151615502429422728361803516635947997086766657240209621800578398634855864575107\
587329752224597845527919791870348445538391351719323110622750092965479047671053\
688923350047856706156573591954178209161393651658651971850621985132438367289973\
2877520923444250719180858848398553109463938921...
```

Recall that we have closed forms for $\phi_2(\mathbf{1}/6)$ and $\phi_3(\mathbf{1}/6)$. Should one have intuition as to what shape a closed form for the above $\phi_4(\mathbf{1}/6)$ might take, this provides substantial data.

8.1. The problem of inversion

The inverse problem is interesting. For example, for $n > 1$, what points in the cube $[-1/2, 1/2]^n$ have $\phi_n = 1$? (Note that every nonnegative real value of ϕ_n must occur on this cube; moreover there will be contours of equipotential, so that we expect $\phi_n(\mathbf{r}) = c$ for constant $c \in [0, \infty)$ to have uncountably many solutions \mathbf{r} .) Take

$$a := 0.21321087149714956794918011030024508,$$

whence the fast series methods can be used to show

$$\phi_3(a, a, a) = 1.000000000000000000000000(2) \dots$$

Acknowledgements The authors thank many colleagues, but especially Wadim Zudilin, for fruitful discussions about lattice sums and theta functions.

- [1] J. Ablinger, J. Blumlein and C. Schneider, “Harmonic Sums and Polylogarithms Generated by Cyclotomic Polynomials,” *J. Math. Phys.* **52** (2011), 102301.
- [2] D.H. Bailey and J.M. Borwein, “Compressed lattice sums arising from the Poisson equation.” Submitted to special volume of *Boundary Value Problems* in honour of Hari Srivastava, December 2012.
- [3] D.H. Bailey and D.J. Broadhurst, “Parallel integer relation detection: Techniques and applications,” *Mathematics of Computation*, **70** 236 (2000), 1719–1736.
- [4] D.H. Bailey, Y. Hida, X.S. Li and B. Thompson, “ARPREC: An arbitrary precision computation package,” Sept 2002, available at <http://crd-legacy.lbl.gov/dhbailey/dhbpapers/arprec.pdf>. The ARPREC software itself is available at <http://crd-legacy.lbl.gov/dhbailey/mpdist>.
- [5] J.M. Borwein and D.H. Bailey, *Mathematics by Experiment: Plausible Reasoning in the 21st Century* A.K. Peters Ltd, 2004, ISBN: 1-56881-136-5. Second expanded edition, 2008.
- [6] J.M. Borwein and P. B. Borwein, *Pi and the AGM*, John Wiley & Sons, New York, 1987.
- [7] J. Borwein, L. Glasser, R. McPhedran, J. Wan and J. Zucker, *Lattice Sums: Then and Now*. Cambridge University Press. To appear, 2013.
- [8] R. Crandall, “Unified algorithms for polylogarithms, L-functions, and zeta variants,” in *Algorithmic reflections: Selected works*, PSIPress, Portland, 2011. Also downloadable at <http://www.psipress.com>.
- [9] R. Crandall, “The Poisson equation and ‘natural’ Madelung constants,” preprint (2012).
- [10] P.J. Forrester and M.L. Glasser, “Some new lattice sums including an exact result for the electrostatic potential within the NaCl lattice,” *J. Phys. A* **15** (1982), 911–914.
- [11] M.L. Glasser, “The evaluation of lattice sums. III. Phase modulated sums,” *J. Math. Phys.* **15** 188 (1974), 188–189.
- [12] M.L. Glasser and I.J. Zucker, “Lattice Sums,” pp. 67–139 in *Perspectives in Theoretical Chemistry: Advances and Perspectives*, Vol. 5 (Ed. H. Eyring). New York: Academic Press, 1980.
- [13] S. Kanemitsu, Y. Tanigawa, H. Tsukada and M. Yoshimoto, “Crystal symmetry viewed as zeta symmetry,” pp. 91–130 in T. Aoki, S. Kanemitsu, M. Nakahara and Y. Ohno, eds., *Zeta Functions, Topology and Quantum Physics*, Springer, New York, 2005 (reprinted 2010).
- [14] S. Kanemitsu and H. Tsukada, “Crystal symmetry viewed as zeta symmetry II,” pp. 275–292 in K. Alladi, J.R. Klauder and C.R. Rao, eds., *The Legacy of Alladi Ramakrishnan in the Mathematical Sciences*, Springer, New York, 2010.
- [15] E. Weisstein, “Jacobi theta functions,” *MathWorld*, available at <http://mathworld.wolfram.com/JacobiThetaFunctions.html>.
- [16] E.T. Whittaker and G.N. Watson, *A Course of Modern Analysis*, 4th edition, Cambridge University Press, 1946.
- [17] I.J. Zucker, “Exact values for some lattice sums in 2, 4, 6 and 8 dimensions,” *J. Phys. A.* **7** (1974), 1568–1575 .
- [18] I.J. Zucker, “Functional equations for poly-dimensional zeta functions and the evaluation of Madelung constants,” *J. Phys. A.*, **9** (1976), 499–505.
- [19] I.J. Zucker, “Some infinite series of exponential and hyperbolic functions,” *SIAM J. Math.*, **15**, 2 (1984) , 406–413.
- [20] I.J. Zucker, “A systematic way of converting infinite series into infinite products,” *J. Phys. A.*, **20** (1987), L13-L17.
- [21] I.J. Zucker, “Further relations amongst infinite series and products: II. The evaluation of three-dimensional lattice sums,” *J. Phys. A.*, **23** (1990), 117–132.
- [22] I.J. Zucker and R.C. McPhedran. “Dirichlet L -series with real and complex characters and their application to solving double sums,” *Proc.Roy.Soc.Lond. A* **464** (2008), 1405–1422.

Appendix A.

We return to

$$\mathcal{V}_2(x, y; s) = \sum_{m, n=-\infty}^{\infty} \frac{\cos[\pi(2m+1)x] \cos[\pi(2n+1)y]}{[(2m+1)^2 + (2n+1)^2]^s},$$

reminding ourselves of the normalization $\phi_2(x, y) = \frac{1}{\pi^2} \mathcal{V}_2(x, y; 1)$. First we decouple the double sum into a product of two single sums using the Mellin transform as defined by

$$\Gamma(s)M_s[f(t)] := \int_0^{\infty} t^{s-1} f(t) dt$$

so

$$\mathcal{V}_2(x, y; s) = M_s \left(\sum_{m=-\infty}^{\infty} q^{(2m+1)^2} \cos[\pi(2m+1)x] \sum_{n=-\infty}^{\infty} q^{(2n+1)^2} \cos[\pi(2n+1)y] \right) \quad (\text{A.1})$$

where $q = e^{-t}$. Note that in terms of classical theta functions [6, Ch. 2] we can write

$$\sum_{m=-\infty}^{\infty} q^{(2m+1)^2} \cos[\pi(2m+1)x] = \vartheta_2(q^4, x).$$

Appendix A.1. Specific values of x and y

We can find the q -series in (A.1) for various values of x, y .

For $x = 0$ we have

$$\sum_{m=-\infty}^{\infty} q^{(2m+1)^2} \cos[\pi(2m+1)x] = 2 (q + q^9 + q^{25} + q^{49} + q^{81} + q^{121} + q^{169} \dots) = \vartheta_2(q^4).$$

For $x = 1/4$ we have

$$\sum_{m=-\infty}^{\infty} q^{(2m+1)^2} \cos[\pi(2m+1)x] = \frac{2}{\sqrt{2}} (q - q^9 - q^{25} + q^{49} + q^{81} - q^{121} - q^{169} \dots) = \frac{1}{\sqrt{2}} \vartheta_5(q^4).$$

So

$$\mathcal{V}_2(1/4, 1/4; s) = M_s \frac{1}{2} \vartheta_5^2(q^4) = M_s \vartheta_2(q^8) \vartheta_4(q^8) = 2^{-3s} M_s \vartheta_2 \vartheta_4 = 2^{1-s} L_{-8}(s) L_8(s),$$

see [17, Table 1].

For $x = 1/3$ we have

$$\sum_{m=-\infty}^{\infty} q^{(2m+1)^2} \cos[\pi(2m+1)x] = q - 2q^9 + q^{25} + q^{49} - 2q^{81} + q^{121} + \dots = \frac{1}{2} [\vartheta_2(q^4) - 3\vartheta_2(q^{36})].$$

Thus

$$\begin{aligned} \mathcal{V}_2(1/3, 1/3; s) &= M_s 2^{-2} [\vartheta_2(q^4) - 3\vartheta_2(q^{36})]^2 = M_s 2^{-2-2s} [\vartheta_2 - 3\vartheta_2(q^9)]^2 \\ &= M_s 2^{-2-2s} [\vartheta_2^2 - 6\vartheta_2\vartheta_2(q^9) + 9\vartheta_2^2(q^9)] \end{aligned} \quad (\text{A.2})$$

Now [17] provides

$$M_s \vartheta_2^2 = 2^{2s+1} (1 - 2^{-s}) L_1(s) L_{-4}(s)$$

while

$$M_s 9 \vartheta_2^2(q^9) = 2^{2s+1} 3^{2-2s} (1 - 2^{-s}) L_1(s) L_{-4}(s).$$

All that is needed now to resolve (A.2) is $M_s \vartheta_2 \vartheta_2(q^9)$.

Appendix A.2. More theta manipulations

Two known results are required. These are

$$\begin{aligned} M_s [\vartheta_3 \vartheta_3(q^9) - 1] &= \\ &= (1 + 3^{1-2s}) L_1(s) L_{-4}(s) + L_{-3}(s) L_{12}(s), \end{aligned} \quad (\text{A.3})$$

$$\begin{aligned} M_s [\vartheta_3 \vartheta_3(q^{36}) + \vartheta_3(q^4) \vartheta_3(q^9) - 2] &= (1 - 2^{-s} + 2^{1-2s}) (1 + 3^{1-2s}) L_1(s) L_{-4}(s) \\ &+ (1 + 2^{-s} + 2^{1-2s}) L_{-3}(s) L_{12}(s), \end{aligned} \quad (\text{A.4})$$

where (A.3) may be found in [17], while (A.4) was communicated by Mark Watkins of Bristol, see [22, 7]. From (A.3) it is simple to deduce that

$$M_s [\vartheta_4 \vartheta_4(q^9) - 1] = -(1 - 2^{1-s}) (1 + 3^{1-2s}) L_1(s) L_{-4}(s) - (1 + 2^{1-s}) L_{-3}(s) L_{12}(s).$$

Now

$$\begin{aligned} \vartheta_2(q^4) \vartheta_2(q^{36}) &= \frac{1}{4} [\vartheta_3 - \vartheta_4] [\vartheta_3(q^9) - \vartheta_4(q^9)] = \frac{1}{4} [\vartheta_3 \vartheta_3(q^9) + \vartheta_4 \vartheta_4(q^9) - \vartheta_3 \vartheta_4(q^9) - \vartheta_4 \vartheta_3(q^9)] \\ \vartheta_3 \vartheta_3(q^{36}) + \vartheta_3(q^4) \vartheta_3(q^9) &= \frac{1}{2} \{ \vartheta_3 [\vartheta_3(q^9) + \vartheta_4(q^9)] + [\vartheta_3 + \vartheta_4] \vartheta_3(q^9) \} \\ &= \frac{1}{2} [2\vartheta_3 \vartheta_3(q^9) + \vartheta_3 \vartheta_4(q^9) + \vartheta_4 \vartheta_3(q^9)]. \end{aligned} \quad (\text{A.5})$$

Thus, we have

$$2\vartheta_2(q^4) \vartheta_2(q^{36}) + \vartheta_3 \vartheta_3(q^{36}) + \vartheta_3(q^4) \vartheta_3(q^9) = \frac{3}{2} \vartheta_3 \vartheta_3(q^9) + \frac{1}{2} \vartheta_4 \vartheta_4(q^9).$$

Taking Mellin transforms of both sides of this equation gives us

$$\begin{aligned}
 2^{1-2s} M_s \vartheta_2 \vartheta_2(q^9) &= -(1 - 2^{-s} + 2^{1-2s})(1 + 3^{1-2s}) L_1(s) L_{-4}(s) \\
 &\quad - (1 + 2^{-s} + 2^{1-2s}) L_{-3}(s) L_{12}(s) \\
 &\quad + \frac{3}{2} [(1 + 3^{1-2s}) L_1(s) L_{-4}(s) + L_{-3}(s) L_{12}(s)] \\
 &\quad + \frac{1}{2} [-(1 - 2^{1-s})(1 + 3^{1-2s}) L_1(s) L_{-4}(s) - (1 + 2^{1-s}) L_{-3}(s) L_{12}(s)],
 \end{aligned} \tag{A.6}$$

and eventually

$$M_s \vartheta_2 \vartheta_2(q^9) = 2^s [(1 - 2^{-s})(1 + 3^{1-2s}) L_1(s) L_{-4}(s) - (1 + 2^{-s}) L_{-3}(s) L_{12}(s)]. \tag{A.7}$$

Finally one arrives at

$$\mathcal{V}_2(1/3, 1/3; s) = 2^{-1-s} [-(1 - 2^{-s})(1 - 3^{2-2s}) L_1(s) L_{-4}(s) + 3(1 + 2^{-s}) L_{-3}(s) L_{12}(s)],$$

which is (35).

Recall that $(1 - 3^{2-2s})$ factors as $(1 + 3^{1-s})(1 - 3^{1-s})$, that $\lim_{s \rightarrow 1} (1 - 3^{1-s}) L_1(s) = \log 3$, and that

$$L_{-4}(1) = \frac{\pi}{4}, \quad L_{-3}(1) = \frac{\sqrt{3}\pi}{9}, \quad L_{12}(1) = \frac{1}{\sqrt{3}} \log(2 + \sqrt{3}).$$

Gathering everything together we also have

$$\mathcal{V}_2(1/3, 1/3; 1) = \frac{\pi}{8} \log\left(\frac{3 + 2\sqrt{3}}{3}\right),$$

as asserted in (31). Similarly

$$\mathcal{V}_2(0, 1/3; s) = M_s 2^{-1} \vartheta_2(q^4) [\vartheta_2(q^4) - 3\vartheta_2(q^{36})] = M_s 2^{-1-2s} [\vartheta_2^2 - 3\vartheta_2 \vartheta_2(q^9)]$$

which finally gives

$$\mathcal{V}_2(0, 1/3; s) = 2^{-1-s} [(1 - 2^{-s})(1 - 3^{2-2s}) L_1(s) L_{-4}(s) + 3(1 + 2^{-s}) L_{-3}(s) L_{12}(s)].$$

It is also possible to obtain (A.3) and (A.7) from [6, §4.7].

Remark 22. The \mathcal{V}_2 lattice sum can be given a fast series

$$\begin{aligned}
 \mathcal{V}_2(x, y; s) &:= \sum_{m, n \in \mathbb{O}} \frac{\cos(\pi m x) \cos(\pi n y)}{(m^2 + n^2)^s} \\
 &= \frac{2^{3/2-s} \pi^s}{\Gamma(s)} \sum_{\substack{n \in \mathbb{O}^+ \\ u \in \mathbb{Z}}} (-1)^u \left(\frac{|u+x|}{n}\right)^{s-1/2} K_{1/2-s}(\pi n |u+x|) \cos(\pi n y),
 \end{aligned} \tag{A.8}$$

where K_ν is a standard modified Bessel function. For $s = 1$ this series collapses somewhat further into π^2 times our series (23) for Poisson potential ϕ_2 .

Appendix B.

As explained in reference [9], there has been a typographical issue propagated since 1974 [11, 12, 7] concerning the forms (46), (47). When the literature entries are corrected, we obtain the present formula (47) as a Poisson solution for the jellium scenario.

This successful development for ψ_2 can be echoed to develop a ϑ -representation for our Madelung solution $\phi_2(x, y)$, as follows. The $(n = 2)$ -dimensional instance of (22) is

$$\phi_2(x, y) = \frac{1}{\pi} \sum_{p \in \mathbb{O}^+} \frac{\sinh\left(\pi p \left(\frac{1}{2} - |x|\right)\right) \cos(\pi p y)}{p \cosh(\pi p/2)}.$$

We cast this into a double series by expanding the sinh/cosh exponentials, then to employ the odd-sum formula

$$\sum_{d \in \mathbb{O}^+} \frac{u^d}{d} = \frac{1}{2} \log \frac{1+u}{1-u}.$$

On defining $z = \pi(y + ix)/2$, $q := e^{-\pi}$, one has after some tedium, and setting $z^* = x + iy$, that

$$\begin{aligned} \phi_2(x, y) &:= \frac{1}{4\pi} \log \left(\frac{1 + e^{2iz}}{1 - e^{2iz}} \cdot \frac{1 + e^{2iz^*}}{1 - e^{2iz^*}} \right) \\ &+ \frac{1}{4\pi} \sum_{u \geq 1} (-1)^u \log \left(\frac{1 + 2 \cos(2z) q^u + q^{2u}}{1 - 2 \cos(2z) q^u + q^{2u}} \cdot \frac{1 + 2 \cos(2z^*) q^u + q^{2u}}{1 - 2 \cos(2z^*) q^u + q^{2u}} \right). \end{aligned}$$

Happily, the u -sum can be written as the log of an infinite product, and then the classical product formulae for Jacobi ϑ -functions may be used, giving in straightforward fashion our (48).

It is interesting that experimental mathematics has been used here not to develop a formula, but to “debug” one. Fast series were found not to agree with older ϑ representations; moreover, the same extreme-precision numerics fully verify our solutions $\phi_2(x, y)$ and $\psi_2(x, y)$, in the respective forms (48) and (47).

Appendix C.

We turn to evaluation of ψ_2 without the $1/4\pi^2$ factor, i.e.,

$$\mathcal{W}_2(x, y, s) := \sum'_{m, n \in \mathbb{Z}} \frac{\cos(2\pi m x) \cos(2\pi n y)}{(m^2 + n^2)^s}.$$

As before decouple the double sum into a product of two single sums using the Mellin transform defined by

$$\Gamma(s) M_s[f(t)] = \int_0^\infty t^{s-1} f(t) dt$$

so

$$\mathcal{W}_2(x, y, s) = M_s \left[\sum_{m=-\infty}^{\infty} q^{m^2} \cos(2\pi mx) \sum_{n=-\infty}^{\infty} q^{n^2} \cos(2\pi ny) \right],$$

where $q = e^{-t}$, and the case where $m = n = 0$ has to be excluded. Then

$$\begin{aligned} \mathcal{W}_2(x, y, s) = M_s \left[4 \sum_{m=1}^{\infty} q^{m^2} \cos(2\pi mx) \sum_{n=1}^{\infty} q^{n^2} \cos(2\pi ny) \right. \\ \left. + 2 \sum_{m=1}^{\infty} q^{m^2} \cos(2\pi mx) + 2 \sum_{n=1}^{\infty} q^{n^2} \cos(2\pi ny) \right]. \end{aligned} \quad (\text{C.1})$$

Again we can identify the q -series for a few individual cases of x and y .

For $x = 0$ we have

$$\sum_{m=1}^{\infty} q^{m^2} = q + q^4 + q^9 + q^{16} + q^{25} + q^{36} + q^{49} \dots = \frac{(\theta_3 - 1)}{2}.$$

For $x = 1/2$ we have

$$\sum_{m=1}^{\infty} q^{m^2} \cos(\pi m) = -q + q^4 - q^9 + q^{16} - q^{25} + q^{36} - q^{49} \dots = \frac{(\theta_4 - 1)}{2}.$$

For $x = 1/4$ we have

$$\sum_{m=1}^{\infty} q^{m^2} \cos(\pi m/2) = -q^4 + q^{16} - q^{36} + q^{64} - q^{100} + q^{144} \dots = \frac{[\theta_4(q^4) - 1]}{2}.$$

Using (C.1) we find

$$\mathcal{W}_2(0, 0, s) = M_s(\theta_3^2 - 1) = 4\zeta(s)L_{-4}(s) \quad (\text{C.2})$$

$$\mathcal{W}_2(1/2, 1/2, s) = M_s(\theta_4^2 - 1) = -4(1 - 2^{1-s})\zeta(s)L_{-4}(s) = -\pi \log 2, \text{ for } s = 1. \quad (\text{C.3})$$

$$\mathcal{W}_2(0, 1/2, s) = M_s(\theta_3\theta_4 - 1) = -4 \cdot 2^{-s}(1 - 2^{1-s})\zeta(s)L_{-4}(s) = -\frac{\pi \log 2}{2}, \text{ for } s = 1. \quad (\text{C.4})$$

These of course are well-known.

But we can now add

$$\begin{aligned} \mathcal{W}_2(1/4, 1/4, s) &= M_s [\theta_4^2(q^4) - 1] = -4 \cdot 2^{-2s}(1 - 2^{1-s})\zeta(s)L_{-4}(s) = -\frac{\pi \log 2}{4}, \text{ for } s = 1. \\ \mathcal{W}_2(0, 1/4, s) &= M_s [\theta_3\theta_4(q^4) - 1] = M_s \{ [[\theta_3(q^4) + \theta_2(q^4)] \theta_4(q^4) - 1] \} \\ &= M_s\theta_2(q^4)\theta_4(q^4) + M_s [\theta_3(q^4)\theta_4(q^4) - 1] \\ &= 2L_{-8}(s)L_8(s) - 4 \cdot 2^{-3s}(1 - 2^{1-s})\zeta(s)L_{-4}(s). \end{aligned} \quad (\text{C.5})$$

When $s = 1$

$$\mathcal{W}_2(0, 1/4, 1) = \frac{\pi}{4} \log \frac{(4 + 3\sqrt{2})}{2}.$$

Similarly

$$\begin{aligned} \mathcal{W}_2(1/2, 1/4, s) &= M_s [\theta_4 \theta_4(q^4) - 1] = M_s \{ [\theta_3(q^4) - \theta_2(q^4)] \theta_4(q^4) - 1 \} \\ &= M_s [\theta_3(q^4) \theta_4(q^4) - 1] - M_s \theta_2(q^4) \theta_4(q^4) \\ &= -4 \cdot 2^{-3s} (1 - 2^{1-s}) \zeta(s) L_{-4}(s) - 2 L_{-8}(s) L_8(s). \end{aligned} \quad (\text{C.6})$$

and we have

$$\mathcal{W}_2(1/2, 1/4, 1) = -\frac{\pi}{4} \log(4 + 3\sqrt{2}).$$

It is possible to express the q -series found when $x = 1/3$ in terms of theta functions. For $x = 1/3$

$$\begin{aligned} \sum_{m=1}^{\infty} q^{m^2} \cos(2\pi m/3) &= -\frac{1}{2} (q + q^4 - 2q^9 + q^{16} + q^{25} - 2q^{36} + q^{49} + q^{64} - 2q^{81} \dots) \\ &= \frac{1}{2} \left[3\theta_2(q^{36}) - \frac{(\theta_3 - 1)}{2} \right], \end{aligned} \quad (\text{C.7})$$

but going further has in this case proven intractable.

For $x = 1/6$ we have

$$\begin{aligned} \sum_{m=1}^{\infty} q^{m^2} \cos(\pi m/3) &= -\frac{1}{2} (q - q^4 - 2q^9 - q^{16} + q^{25} + 2q^{36} + q^{49} - q^{64} - 2q^{81} \dots) \\ &= \frac{1}{2} \left\{ \frac{(1 - \theta_4)}{2} - \frac{3[1 - \theta_4(q^9)]}{2} \right\}. \end{aligned} \quad (\text{C.8})$$

It is then found that

$$\mathcal{W}_2(1/6, 1/6, s) = M_s \frac{1}{4} \{ \theta_4^2 - 1 - 6 [\theta_4 \theta_4(q^9) - 1] + 9 [\theta_4^2(q^9) - 1] \} \quad (\text{C.9})$$

$$= \frac{1}{2} [(1 - 2^{1-s})(1 - 3^{2-2s}) \zeta(s) L_{-4}(s) + 3(1 + 2^{1-s}) L_{-3}(s) L_{12}(s)]. \quad (\text{C.10})$$

When $s=1$

$$\mathcal{W}_2(1/6, 1/6, 1) = \frac{\pi \log(2 + \sqrt{3})}{3}$$