The Poisson equation and 'natural' Madelung constants

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Abstract: Remarkably, the Poisson equation of classical electrostatics has found recent applications in other fields, for example in graphics and image processing. It is of interest to revisit Poisson theory in regard to what actually happens in arbitrary dimensions. In either physic or graphics, one seeks solutions of $\nabla^2 P(\mathbf{r}) \;=\; -\rho(\mathbf{r})$, where $\mathbf{r}$ is an n-dimensional vector. The present treatment involves solutions $P$where ρ is the charge density of an infinite but n-dimensional crystal (NaCl-type). Because the potentials P being summed are only of the form $\pm 1/|r|$ for $n = 3$ dimensions, we have cause to define 'natural' Madelung constants on the basis of the true behavior $P \sim 1/r^{n-2}$ (or $\sim \log r$ in $n = 2$ dimensions). These new constants can sometimes be given closed forms; for example, we show that for $n = 2$ dimensions, the natural Madelung constant—essentially the binding energy density of a sheaf of line charges—is given by

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

Even when a closed form is not available, we do have for every $\mathcal{N}_n$ exponentially fast computational formulae. We also describe fast computational algorithms that achieve extreme precision for various relevant lattice sums.

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1 Poisson equation

The Poisson equation of classical physics reads

$$\nabla^2 P(\mathbf{r}) \;=\; -\rho(\mathbf{r}), \tag{1}$$

where P is electrostatic potential and ρ is spatial charge density.[1] We shall work in n dimensions, so that both P, ρ are functions of position $\mathbf{r} \in \mathbb{R}^n$. For *radial* charge densities ρ and potentials P—so that the only dependence is on the scalar radius $r := |\mathbf{r}|$—the Laplacian operator can be written

$$\nabla^2 \;\to\; \frac{1}{r^{n-1}}\frac{\partial}{\partial r}\left(r^{n-1}\frac{\partial}{\partial r}\right). \tag{2}$$

It is immediate that the choice of potential function

$$P \;=\; P_n(\mathbf{r}) \;:=\; \frac{1}{r^{n-2}}, \tag{3}$$

with the right-hand expression interpreted as $\log r$ in the special case of $n = 2$ dimensions, satisfies the homogeneous equation $\nabla^2 P_n = 0$, except—importantly—at the origin $\mathbf{r} = \mathbf{0}$.

1.1 Engineering connection

The Poisson equation, in giving rise to interesting lattice-sum problems, is interesting in its own abstract right. The present author, however, was reintroduced to this subject in recent years, when it became apparent that Poisson solutions actually have an important role in modern graphics engineering. For example, one may employ Dirichlet boundary conditions to meld images together [13], or Neumann boundary conditions to create interesting, gradient-dependent effects [1]. Incidentally, we are focusing in the present treatment on Dirichlet boundary conditions—as in the "Delord cube" scenario below.

1.2 Point-source solutions

The starting point of the present treatment is to establish particular point-source solutions Φ_n to[2]

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

that is, the source is a unit point charge concentrated at the origin, and we wish to establish a suitable Φ_n for every dimension $n \in \mathbb{Z}^+$. Here we use the physics nomenclature that for vector

[1] We have rendered the equation unitless—in physics settings the right-hand side is $-\rho/\epsilon_0$ in MKS units, or $-4\pi\rho$ in CGS units.

[2] We say "a particular" solution because, of course, any homogeneous solution $\bar{\phi}$, so $\nabla^2\bar{\phi} = 0$, can be added in.

$\mathbf{r} = (r_1, r_2, \ldots, r_n)$, the Dirac delta-function is $\delta^n(\mathbf{r}) := \delta(r_1)\cdots\delta(r_n)$, with the integral of this δ^n over $\mathbb{R}^n$ being unity.

It turns out that the following potentials Φ_n do solve the Poisson equation (4), and suffice to engender our forthcoming analysis of lattice sums. Consider, for $n \neq 2$ dimensions,

$$\begin{aligned} \Phi_n(\mathbf{r}) &:= \frac{C_n}{r^{n-2}}, \qquad n \neq 2, \\ \Phi_2(\mathbf{r}) &:= C_2 \log r, \end{aligned} \tag{5}$$

with

$$\begin{aligned} C_n &:= \frac{\Gamma(n/2-1)}{4\pi^{n/2}}, \qquad n \neq 2, \\ C_2 &:= -\frac{1}{2\pi}. \end{aligned} \tag{6}$$

It is evident that potentials P_n, Φ_n obey the simple scaling rule

$$\Phi_n = C_n P_n,$$

There are two distinct and interesting ways to establish that this explicit Φ_n collection satisfies (4) for each dimension n. First, writing a standard mathematica-physics rendition of the n-dimensional Dirac delta-function:

$$\delta^n(\mathbf{r}) = \frac{1}{(2\pi)^n} \int e^{i\mathbf{k}\cdot\mathbf{r}}\, d^n\mathbf{k},$$

we solve easily in $\mathbf{k}$-space to write (formally at least)

$$\Phi_n(\mathbf{r}) = \frac{1}{(2\pi)^n} \int \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{k^2}\, d^n\mathbf{k},$$

where it can be seen that the Laplacian operator ∇^2 inside the $\mathbf{k}$-integral annihilates the k^2 denominator. To lend rigor for all dimensions, one can consider, for infinitesimal positive reals ϵ, δ, integrals of the form

$$\Phi_n(\mathbf{r}) \approx \frac{1}{(2\pi)^n} \int \frac{e^{i\mathbf{k}\cdot\mathbf{r}} e^{-\sigma^2 k/2}}{k^2+\epsilon^2}\, d^n\mathbf{k} - c(\epsilon, \delta),$$

where the $\mathbf{k}$-integral always exists, and is in fact a solution to a so-called *screened Poisson equation*, with source term approaching a Dirac delta as parameter $\sigma \to 0$:

$$\nabla^2 F - \epsilon^2 F = \left(\frac{1}{2\pi\sigma^2}\right)^{n/2} e^{-\frac{r^2}{2\sigma^2}}.$$

The offset $c(\epsilon, \delta)$ would be a suitable correction—a constant solution to the homogeneous Poisson equation—that is subtracted off if necessary to cancel divergence as we take both $\epsilon, \delta \to 0^+$. One may employ hyperspherical coordinates $(k, \theta_1, \ldots, \theta_{n-1})$ for the $\mathbf{k}$-integral, then perform the rather laborious integrations, in this way achieving our intended list:of Φ_n potentials described via (5, 6). Specific values are:

$$\Phi_1(\mathbf{r}) \; := \; -\frac{1}{2}r, \tag{7}$$

$$\Phi_2(\mathbf{r}) \; := \; -\frac{1}{2\pi}\log r, \tag{8}$$

$$\Phi_3(\mathbf{r}) \; := \; \frac{1}{4\pi r}, \tag{9}$$

$$\Phi_4(\mathbf{r}) \; := \; \frac{1}{4\pi^2 r^2}, \tag{10}$$

$$\Phi_5(\mathbf{r}) \; := \; \frac{1}{8\pi^2 r^3}, \tag{11}$$

and so on. Note that for every dimension $n > 1$ the potential Φ_n is singular at the origin, and for $n = 1$ the shape of Φ_1 is that of a tent, since always $r := |\mathbf{r}|$.

1.3 Generalized Gauss law

A second way to derive our collection of potentials Φ_n is to employ an n-dimensional Gauss law, familiar from electrostatics in $n = 3$ dimensions, with potential $\Phi_3(\mathbf{r}) := 1/(4\pi r)$, and electric field $\mathbf{E} = -\nabla\Phi_3 = \hat{\mathbf{r}}/(4\pi r^2)$ where $\hat{\mathbf{r}}$ is the unit vector in the $\mathbf{r}$ direction. The generalized Gauss law is

$$\int \nabla^2 \Phi_n(\mathbf{r}) \; d^n\mathbf{r} \; = \; \int \nabla\Phi_n \cdot \hat{\mathbf{r}} \; d^{n-1}S, \tag{12}$$

in which law an n-dimensional volume integral at left coincides with a surface integral at right. One may simply insert the form (5) into (12), serving that the left integral is -1 due to the delta-function source. For the surface integral at right, we use the known formula for the surface area of an n-sphere to arrive at the C_n expressions (6). For example, the outlier case for $n = 2$ uses

$$-1 \; = \; C_2 \left(\frac{\partial}{\partial r} \log r \right) 2\pi r,$$

so that $C_2 \; = \; -1/(2\pi)$ as claimed.

1.4 Crystal structure and lattice sums

One generalization of the classical sodium-chloride (NaCl) crystal structure in three dimensions is afforded by contemplation of the n-dimensional Poisson equation

$$\nabla^2\phi_n(\mathbf{r}) \;=\; -\sum_{\mathbf{m}\,\in\,\mathbb{Z}^n}(-1)^{\mathbf{1}\cdot\mathbf{m}}\;\delta^n(\mathbf{r}-\mathbf{m}), \tag{13}$$

that is, unit charges are placed at lattice points, with a charge's sign being the parity, that is $\mathbf{1}\cdot\mathbf{m} := \sum_{k=1}^{n} m_k$. We shall presume the solution ϕ_n to be a superposition of Φ_n values, namely

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

For $n = 3$ dimensions, $\phi_3(\mathbf{r})$ is thus the electrostatic potential at any point $\mathbf{r}$ in the crystal, but due to an individual charge's potential being $\pm 1/(4\pi|\mathbf{r}-\mathbf{m}|)$, and *not* simply $\pm 1/|\mathbf{r}-\mathbf{m}|$. Such is the effect of a scaling factor $C_n \neq 1$.

2 Madelung definitions

To untangle the issues of scaling factors and varying radial-power dependence across dimensions for Poison solutions, let us establish nomenclature for certain lattice sums.

First, define the *Madelung potentials* of dimension n, complex variable s and spatial point $\mathbf{r} \in \mathbb{Z}^n$ to be

$$\mathcal{M}_n(s,\mathbf{r}) \;:=\; \sum_{\mathbf{p}\,\in\,\mathbb{Z}^n}\frac{(-1)^{\mathbf{1}\cdot\mathbf{p}}}{|\mathbf{p}-\mathbf{r}|^s}, \tag{14}$$

where n-vectors $\mathbf{p}$ have respective magnitudes p, Then, define the *Madelung energy* as a function of dimension and complex s:

$$\mathcal{M}_n(s) \;:=\; \lim_{\mathbf{r}\to\mathbf{0}}\left(\mathcal{M}_n(s,\mathbf{r}) - \frac{1}{r^s}\right) \tag{15}$$

$$\;=\; {\sum_{\mathbf{p}\,\in\,\mathbb{Z}^n}}'\frac{(-1)^{\mathbf{1}\cdot\mathbf{p}}}{p^s}, \tag{16}$$

where $\mathbf{1}$ is the vector of n 1's. In the original spirit of the Madelung energy of a crystal, the limit here yields the potential seen by a (missing) origin charge, when the bare-charge potential is hypothesized to behave in whatever model as $\pm 1/r^s$.

Here, and in all that follows, when a power s of radial magnitude appears, we assume analytic continuation. So for example, $\mathcal{M}_n(s)$ is absolutely convergent in the half-plane $\Re(s) > n$.

This brings us to the *Madelung constant*, namely

$$\mathcal{M}_n \ := \ \mathcal{M}_n(1). \tag{17}$$

which is an absolute constant amounting to the origin potential when the bare charge potentials are $\pm 1/r$. These $\mathcal{M}_n$ have been called Madelung constants in the past. The reason we have embarked on our circuitous route of definitions—with yet more defining below—is that potentials $1/r$ do not seem natural for any other than $n = 3$ dimensions, which we say on the basis of the Poisson equation.

2.1 'Natural' Madelung constants

We note that the dependence of Φ potentials C_n/r^{n-2} on dimension n has previously been exploited for the Helmholtz equation, with Madelung constants defined in a 'natural' sense, just as we presently shall [15]. Let us define, then, a *'natural' Madelung potential* for all dimensions $n \neq 2$,

$$\begin{aligned} \mathcal{N}_n(\mathbf{r}) \ &:= \phi_n(\mathbf{r}) & (18)\\ &= \ C_n \sum_{\mathbf{p}\,\in\,\mathbb{Z}^n} \frac{(-1)^{\mathbf{1}\cdot\mathbf{p}}}{|\mathbf{p}-\mathbf{r}|^{n-2}} & (19)\\ &= \ C_n\, \mathcal{M}_n(n-2,\mathbf{r}), & (20) \end{aligned}$$

said definition motivated by the fact of Poisson solutions being $\Phi(\mathbf{r}) \ = \ C_n/r^{n-2}$.[3] When $n = 2$ our formal definition for the 'natural' Madelung potential will be

$$\mathcal{N}_2(\mathbf{r}) \ := -\, C_2 \frac{\partial}{\partial s} \mathcal{M}_2(s, \mathbf{r})|_{s=0}. \tag{21}$$

One might cavalierly write this $\mathcal{N}_2(\mathbf{r})$ as

$$\mathcal{N}_2(\mathbf{r}) \ = -\frac{1}{2\pi} \sum_{\mathbf{p}\,\in\,\mathbb{Z}^2} (-1)^{\mathbf{1}\cdot\mathbf{p}} \log|\mathbf{p}-\mathbf{r}|,$$

a series with convergence issues—but once again, analytic continuation implied in (21) is the key. The intuitive point here is that the natural addling constant in $n = 2$ dimensions is a superposition of bare potentials that are *logarithmic*.

[3] By "natural" we mean "mathematically natural," not physically natural. After all, an NaCl (salt) crystal in 4 dimensions is unrealistic. We are defining natural Madelung constants $\mathcal{N}_n$ on the basis of the n-dependent radial power in Poisson solutions.

Finally we define our *'natural Madelung constants* in keeping with the limiting procedure (15) for classical Madelung entities; namely, the 'natural' constants will be

$$\mathcal{N}_n \;=\; \lim_{\mathbf{r}\to\mathbf{0}} \left(\phi_n(\mathbf{r}) \;-\; \Phi_n(\mathbf{r})\right) \tag{22}$$

$$=\; C_n \sum_{\mathbf{p}\,\in\,\mathbb{Z}^n}{}' \frac{(-1)^{\mathbf{1}\cdot\mathbf{p}}}{p^{n-2}} \tag{23}$$

$$=\; C_n \mathcal{M}_n(n-2), \tag{24}$$

where now, as desired, we are defining an origin potential of the (missing) origin charge when bare potentials are the Poisson solutions Φ_n.

2.2 An important exponential sum over odd tuples

We shall make good use of an exponentially convergent a lattice sum (here, $\mathbb{O}^{+(n)}$ denotes the positive-odd-integer n-tuples, e.g. $(3,7,5) \in \mathbb{O}^{+(3)}$)

$$\mathcal{Y}_n \;:=\; \frac{2^n}{\pi} \sum_{\mathbf{d}\,\in\,\mathbb{O}^{+(n)}} \frac{1}{d(1+e^{\pi d})}, \tag{25}$$

where now each $\mathbf{d}$ has odd integer coordinates and so no prime is needed on the sum.

2.3 Examples of the nomenclature

To exemplify the nomenclature: The classical NaCl Madelung constant for $n = 3$ dimensions—where potentials *do* decay as $1/r$—can be written

$$\mathcal{M}_3 \;=\; \mathcal{M}_3(1) \;=\; \sum_{m_1,m_2,m_3\in\mathbb{Z}} \frac{(-1)^{m_1+m_2+m_3}}{\sqrt{m_1^2+m_2^2+m_3^2}} \;=\; -1.74756459\ldots, \tag{26}$$

with the corresponding *natural* Madelung constant—due to actual Poisson-solution potential being C_3/r—having the value

$$\mathcal{N}_3 \;=\; \frac{1}{4\pi}\mathcal{M}_3 \;=\; -0.139067\ldots$$

For $n = 4$ dimensions our natural constant is known to be [7]

$$\mathcal{N}_4 \;=\; C_4\,\mathcal{M}_4(2) \;=\; \frac{1}{4\pi^2} \sum_{m_1,m_2,m_3,m_4\in\mathbb{Z}} \frac{(-1)^{m_1+m_2+m_3+m_4}}{m_1^2+m_2^2+m_3^2+m_4^2} \;=\; -\frac{\log 2}{\pi^2},$$

where the closed-form evaluation here follows from the more general known evaluation

$$\mathcal{M}_4(s) \;=\; -8\,\eta(s/2)\,\eta(s/2-1),$$

where the Dirichlet sums here are

$$\eta(s) \;:=\; \sum_{k\in\mathbb{Z}^+} \frac{(-1)^{k-1}}{k^s},$$

$$\beta(s) \;:=\; \sum_{k\in\mathbb{O}^+} \frac{(-1)^{(k-1)/2}}{k^s},$$

One caution is that some meaningful, physical problems cannot be handled immediately within this Poisson formalism. For example, it is a celebrated result that for potential $V(\mathbf{r}) := 1/r$, and a *plane* of alternating charges—said plane importantly being embedded in three dimensions—the so-called two-dimensional Madelung constant at said plane's origin is, formally, the primed lattice sum

$$\mathcal{M}_2 \;:=\; {\sum_{m,p\,\in\,\mathbb{Z}}}' \frac{(-1)^{m+p}}{\sqrt{m^2+p^2}} \;=\; -4\,\eta(1/2)\,\beta(1/2), \tag{27}$$

The next section sheds somewhat more light on the stark difference between this two-dimensional classical constant $\mathcal{M}_2$ for a charge plane, and our natural Madelung constant $\mathcal{N}_2$, described analytically by (21).

2.4 "Wire-sheaf" model for $n = 2$ dimensions

Imagine a sheaf of line charges—essentially a bundle of wires—embedded in 3 dimensions. Let each wire have (positive or negative) linear charge density but not carrying current per se. Consider a plane to be end-on to these wires, so that in looking down on said plane, the wires appear as an alternating signed array of points, like a 2-dimensional NaCl crystal. Then the operative Poisson equation is, in physical reality, the $(n = 2)$-dimensional form of (13) on this end-on plane.

As we have seen, the Poisson-solution potential a distance r from a line charge is logarithmic in r, and our natural Madelung constant is the potential seen by a (missing) line charge at the origin, so we are asking for a continuation value of (21). Because this scenario is very much unlike that of a plane of charge embedded in three dimensions, the classical $\mathcal{M}_2$ defined in (27) cannot be expected to be anything algebraically like $\mathcal{N}_2$.

Even for $(n = 1)$ dimension there is conceptual dichotomy. The classical, one-dimensional Madelung constant is often given as an elementary exercise, in that

$$\mathcal{M}_1 \;:=\; {\sum_{m\in\mathbb{Z}}}' \frac{(-1)^m}{m} \;=\; -2\log 2,$$

which is the potential seen from the (missing) origin charge, but for an alternating line of charges again embedded in three dimensions, so potentials are proportional to $1/r$. But our natural Madelung constant involves potentials for the 1-dimensional Poisson scenario, and $\Phi_1(\mathbf{r}) = -r/2$, so that we expect formally

$$\mathcal{N}_1 \;=\; -\frac{1}{2}\sum_{m\in\mathbb{Z}}(-1)^m m,$$

whose interpretation as a continuation value should rightfully be[4]

$$\mathcal{N}_1 = \eta(-1) \;= 1/4.$$

Having interpreted the natural constant $\mathcal{N}_1$, we shall need more analysis to resolve $\mathcal{N}_2$ and higher-dimensional constants in closed form; or barring that, at least we can develop rapidly converging series. But first, to the detailed analysis of the Poisson solutions.

3 Boundary conditions: The Delord cube

When one has an n-dimensional charge lattice—as represented by an array of Dirac delta functions on the right-hand side of (13)—it is evident, as observed by Crandall and Delord [9]—that

Principle [Delord cube symmetry]: *The potential ϕ_n—a solution to (13)—can be assumed to vanish on all faces of the Delord cube, whose 2^n vertices are* $(\pm 1/2, \pm 1/2, \ldots, \pm 1/2)$.

This remarkable fact is a consequence of the charge symmetry of the crystal lattice. So we consider the Delord cube as having potential $\phi_n = 0$ on all cube faces, and so observe

Principle [Madelung equivalence]: *The natural Madelung constant $\mathcal{N}_n$ is precisely the potential of a single charge residing at the origin inside a grounded Delord cube, where the bare potential of a solitary charge is our solution Φ_n to the Poisson equation with source (4).*

One instructive way to visualize the Delord-cube boundary conditions is to imagine—say in 3 dimensions, for physical clarity—a positive charge (that would be the origin charge) residing at the cube's center. Then the grounded (potential zero) Delord cube is a conductor on which is built up over the faces a negative charge density, whose surface integral is is in turn exactly one negative charge to balance the positive origin charge. The potential energy of this configuration is the relevant Madelung constant.

3.1 Formal solution for the Delord-cube boundary conditions

Consider the trigonometric sum

$$\sum_{\mathbf{p}\,\in\,\mathbb{O}^n}\prod_{k=1}^{n}\cos(\pi p_k r_k),$$

[4] The fact of this natural Madelung constant being uniquely positive is testimony to the instability of the Poisson charge-or-wire assemblies in lower dimensions. We shall see that $\mathcal{N}_2$ is barely negative; moreover one can show that—at least in $n = 3$ dimensions—the origin charge sits at *unstable* quartic equilibrium [9].

where $\mathbf{r} = (r_1, \ldots, r_n)$ is a given point in $\mathbb{R}^n$. This kind of sum is no stranger to mathematical physicists, for it is—in the spirit of delta-function theory, the crystal-lattice delta-function array already encountered, namely this function of $\mathbf{r}$:

$$\sum_{\mathbf{m} \in \mathbb{Z}^n} (-1)^{\mathbf{1}\cdot\mathbf{m}} \; \delta^n(\mathbf{r} - \mathbf{m})$$

as appears in (13). Such can be established via Poisson transformation of either the delta-function array or the cosine series. But this leads immediately to a series representation for the solution $\Phi_n$equation, in the form

$$\phi_n(\mathbf{r}) \;=\; \frac{1}{\pi^2} \sum_{\mathbf{p} \in \mathbb{O}^n} \frac{\cos(\pi p_1 r_1) \cdots \cos(\pi p_n r_n)}{p^2}, \tag{28}$$

valid when each $r_n \in [-1/2./2]^n$, i e. for $\mathbf{r}$ in the Delord cube. We first note that for $n = 1$ dimension, the series (28) boils down to

$$\phi_1(r) \;=\; \frac{2}{\pi^2} \sum_{m \in \mathbb{O}^+} \frac{\cos(\pi m r)}{m^2}$$

$$= \; \frac{1}{4} \;-\; \frac{1}{2}|r|,$$

for $r \in (-1/2, 1/2)$. This solves for the 1-dimensional Delord-cube boundary conditions; sure enough, ϕ_1 does vanish at the boundary points $r = \pm 1/2$.

3.2 Series acceleration and evaluation

The series formulation (28) enjoys that rather uncommon double attribute of being both elegant and practical. As such, this Φ-series is ripe for experimental mathematics. To enhance convergence for all dimensions $n \geq 2$, we may employ another Poisson identity, for positive real a:

$$\sum_{m \in \mathbb{O}} \frac{\cos \pi m x}{m^2 + a^2} \;=\; \frac{\pi}{2a} \frac{\sinh\left(\pi a \left(\frac{1}{2} - |x|\right)\right)}{\cosh\left(\frac{\pi a}{2}\right)}. \tag{29}$$

Summing over just one odd index in (28)), say p_1, then gives

$$\phi_n(\mathbf{r}) \;=\; \frac{1}{2\pi} \sum_{\mathbf{R} \in \mathbb{O}^{n-1}} \frac{\sinh\left(\pi R \left(\frac{1}{2} - |r_1|\right)\right) \prod_{k=1}^{n-1} \cos(\pi R_k r_{k+1})}{R \cosh(\pi R/2)}. \tag{30}$$

Importantly, the summation vector R of odd-integer elements is now reduced to being $(n-1)$ dimensional. Observe that (30) does vanish on all faces of the Delord cube. What is not so obvious is that this $(n-1)$-dimensional summation is *symmetric* under any permutations or sign-flips of $r_1, r_2 \ldots r_n$; for example, $\phi_3(x, y, z) = \phi_3(-z, y, -z)$ and so on. Thus r_1 in the argument of sinh can be taken to be the largest in magnitude of the elements of r, with a view to optimal convergence.

The series (30) can be used to plot Poisson solutions ϕ_n to (13), as exemplified in Figure 1, where we have pictorialized the scenario for $n = 2$ dimensions.

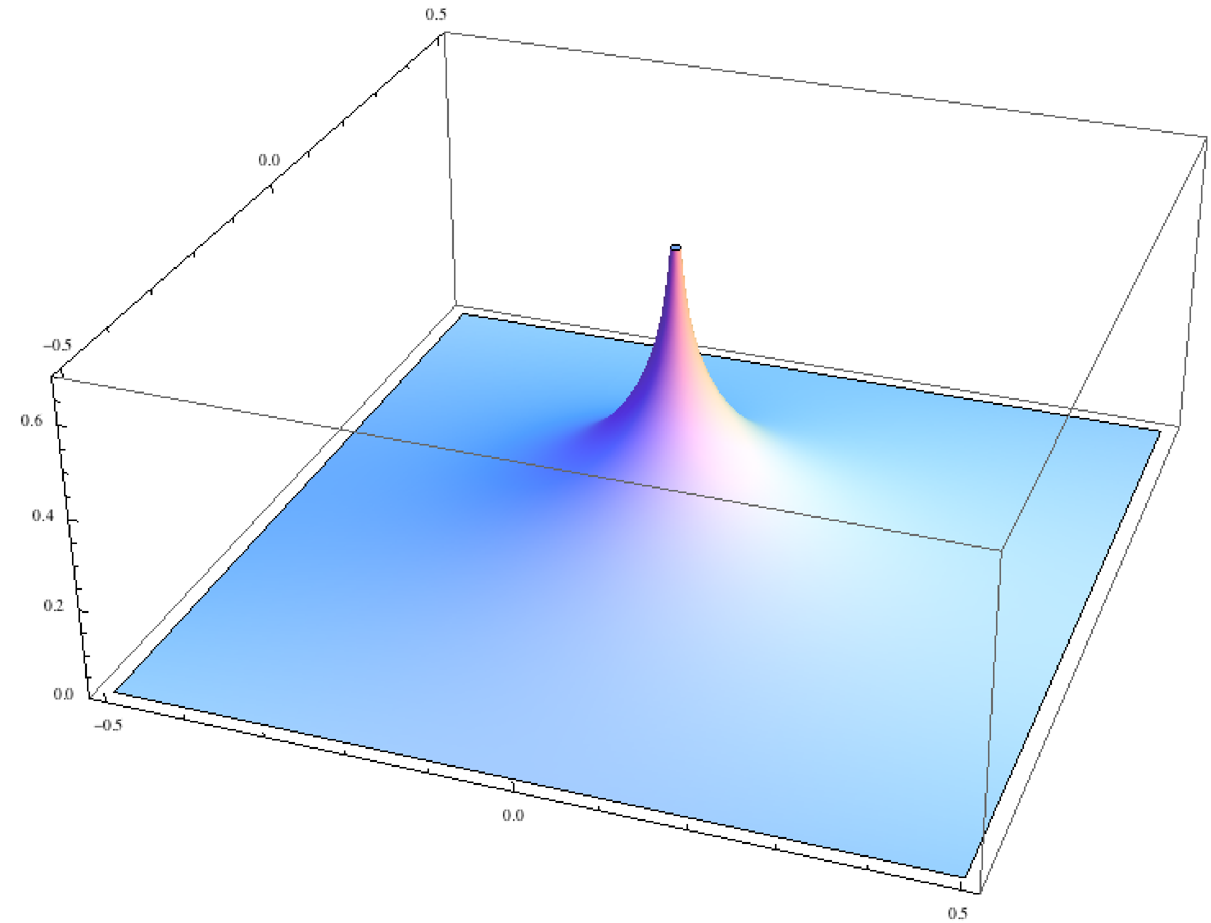

Figure 1: Plot of the $(n = 2)$-dimensional crystal potential—the solution $\phi_2(\mathbf{r})$ of Poisson equation (13)—with the boundary conditions of vanishing on the sides of the Delord square (vertices at $(\pm 1/2, \pm 1/2)$). Such a plot can be generated efficiently from series (32). The natural Madelung constant is the energy of this configuration, meaning $\lim_{\mathbf{r}\to\mathbf{0}} (\phi_2(\mathbf{r}) - \Phi_2(\mathbf{r}))$. Thus, removing the Coulomb singularity at the origin is an important analytic step.

3.3 Handling the Coulomb singularity

Looking at the limiting form (22) for the 'natural' Madelung constants, one is compelled to remove the origin singularity—called the Coulomb singularity in the classical scenario. To this end, we rewrite (30) as

$$\phi_n(\mathbf{r}) \;=\; \frac{1}{\pi}\sum_{\mathbf{R}\,\in\,\mathbb{O}^{n-1}} \frac{e^{-\pi R|r_1|}\prod_{k=2}^{n}\cos(\pi R_k r_k)}{R} \;-\frac{1}{\pi}\sum_{\mathbf{R}\,\in\,\mathbb{O}^{n-1}} \frac{\prod_{k=2}^{n}\cos(\pi R_k r_k)}{R(1+e^{\pi R})}, \tag{31}$$

in which we have siphoned off the r_1 dependence as the first sum.

The instance $n = 2$ is interesting and somewhat tractable. We can actually evaluate the first sum in (31) to achieve

$$\phi_2(x,y) \;=\; \frac{1}{4\pi}\log\frac{\cosh(\pi x)+\cos(\pi y)}{\cosh(\pi x)-\cos(\pi y)} - \frac{2}{\pi}\sum_{\mathbf{m}\,\in\,\mathbb{O}^{+}} \frac{\cosh(\pi m x)\cos(\pi m y)}{m(1+e^{\pi m})}. \tag{32}$$

For dimension $n > 2$ it is difficult to evaluate the r_1-dependent sum in (31) in any convenient analytic form.

Letting $x = r_1 \to 0^+$ with all other $r_k = 0$, we arrive at

$$\mathcal{N}_n \;=\; \lim_{x\to 0^+}\left(\frac{1}{\pi}\sum_{\mathbf{R}\,\in\,\mathbb{O}^{n-1}} \frac{e^{-\pi R_1 x}}{R} \;-\Phi_n(x,0,0,\ldots,0)\right) \;-\; \frac{1}{\pi}\sum_{\mathbf{R}\,\in\,\mathbb{O}^{n-1}} \frac{1}{R(1+e^{\pi R})}, \tag{33}$$

Now Poisson-transforming the $(n-1)$-dimensional sum in the limit, and performing, say hyperspherical integration, we arrive at

$$\mathcal{N}_n \;=\; C_n \sideset{}{'}\sum_{\mathbf{m}\,\in\,\mathbb{Z}^{(n-1)}} \frac{(-1)^{\mathbf{1}\cdot\mathbf{m}}}{m^{n-2}} \;-\; \frac{2^{n-1}}{\pi}\sum_{\mathbf{R}\,\in\,\mathbb{O}^{+(n-1)}} \frac{1}{R(1+e^{\pi R})}, \qquad \text{if } n \neq 2, \tag{34}$$

or the special case for $n = 2$, using the singularity-removal procedure involving (22) and (32):

$$\mathcal{N}_2 \;=\frac{1}{4\pi}\log\left(\frac{4}{\pi^2}\right) \;-\; \frac{2}{\pi}\sum_{\mathbf{m}\,\in\,\mathbb{O}^{+}} \frac{1}{m(1+e^{\pi m})}. \tag{35}$$

Thus we have a nseries resolution of the 'natural' Madelung constant $\mathcal{N}_2$.

As for $n = 1$ dimension: It is immediate from $\phi_1(x) = 1/4 - |x|/2, \Phi_1(x) = -|x|/2$ that $\mathcal{N}_1 = 1/4)$.

For $n > 2$ we have the dimensional reduction (34), which can also be cast as a dimensional-reduction formula

$$\mathcal{N}_n \;=\; C_n\mathcal{M}_{n-1}(n-2) \;-\; \mathcal{Y}_{n-1}, \qquad \text{if } n \neq 2 \tag{36}$$

which for $n = 3$ involves the classical Madelung constant $\mathcal{M}_2(1)$ which is known; thus

$$\mathcal{N}_3 \;=\; -\frac{1}{\pi}\eta(1/2)\,\beta(1/2) \;-\; \frac{4}{\pi}\sum_{\mathbf{R}\,\in\,\mathbb{O}^{+(2)}} \frac{1}{R(1+e^{\pi R})}$$

$$=\; -\frac{1}{\pi}\eta(1/2)\,\beta(1/2) \;-\; \mathcal{Y}_2,$$

an expansion essentially known to Hautot [12] (for the classical Madeung constant $\mathcal{M}_3$).

In the above series developments, one can see the recurrence of the exponential series (25). In some scenarios, one can think of $\mathcal{Y}_n$ as a 1-dimensional sum. For example,

$$\mathcal{Y}_2 \;=\; \frac{4}{\pi}\sum_{0\,<\,N\,\equiv\,2 (\mathrm{mod}\ 8)} \frac{r_2(N)}{\sqrt{N}\left(1+e^{\pi\sqrt{N}}\right)}\,,$$

where $r_2(N) \;=\; 4\sum_{\mathrm{odd}\ d|N}(-1)^{(d-1)/2}$ is the number of representations of N as a sum of two squares. Such observations can sometimes allow for highly efficient computation.

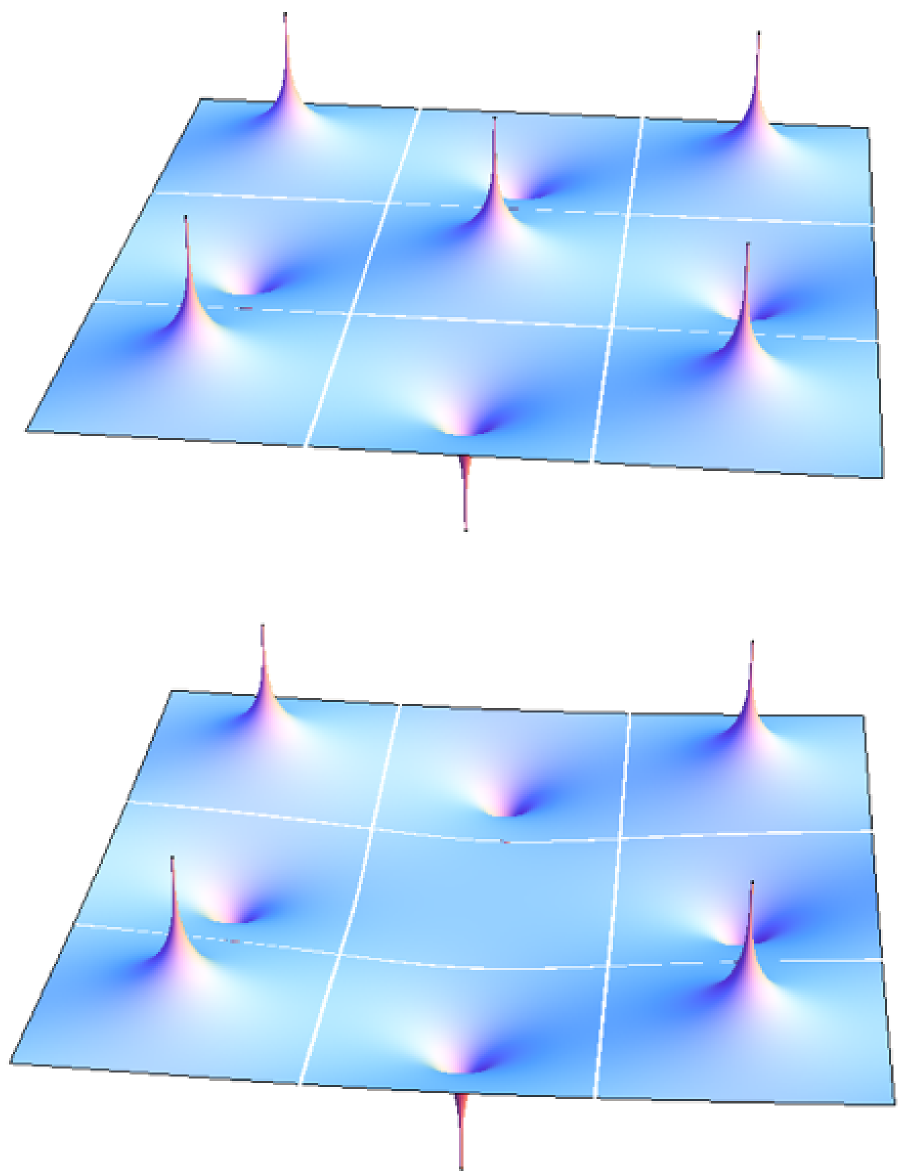

Figure 2: Upper plot: A wider view of Figure 1, in which one can see the vanishing (white scored lines) on Delord 2-cubes (squares). The lower plot is the potential seen by the origin charge; such plot if efficiently generated by removing the origin singularity, i.e. subtracting $\Phi_2(\mathbf{r}) = -(1/2\pi) \log r$ from the form (32). Note that the plot has a slight negative depression at the origin. This negative value ≈ -0.09826 is our natural Madelung constant $\mathcal{N}_2$. We eventually achieve a closed form for this constant

3.4 Riemann-splitting algorithm

Whenever one encounters lattice sums of the types herein, it is often possible to invoke another fast technique that applies to Epstein zeta functions quite generally. Even when one has already embarked on our previous series acceleration, one may still contemplate handling, say,such as the $\mathcal{M}_{n-1}(n-2)$ term in (36) via the following approach to Epstein entities.

In [6] it is established that for

$$Z_A(s;c,d) \ := \ \sum_{n\in Z^n}{}' \frac{e^{2\pi i c\cdot An}}{|An-d|^s}, \tag{37}$$

with A being a matrix, c, d vectors, there is always a fast, Riemann-splitting series for computational (or analytic) applications. In the present case of Poisson-equation solutions, we may consider

$$\mathcal{M}_n(s) \ = \ Z_I\left(s, \frac{\mathbf{1}}{\mathbf{2}}, \mathbf{0}\right),$$

i.e $A = I$ the identity matrix, c consists of all (1/2)'s, and d is the zero vector. The rapidly convergent series at hand involves incomplete-gamma evaluations:

$$\begin{aligned} \Gamma(s/2)\mathcal{M}_n(s) \quad &= \quad -\frac{2}{s}\pi^{s/2} + \sum_{\mathbf{m}\,\in\,\mathbb{Z}^n}{}' \frac{\Gamma(\frac{s}{2}, \pi m^2)(-1)^{\mathbf{1}\cdot\mathbf{m}}}{m^s} \ + \\ & \qquad \pi^{s-n/2} \sum_{\mathbf{k}\,\in\,\mathbb{Z}^n} \frac{\Gamma(\frac{n-s}{2}, \pi|\mathbf{k}-\mathbf{1/2}|^2)}{|\mathbf{k}-\mathbf{1/2}|^{n-s}}, \end{aligned}$$

and allows for general analytic values—any complex s. Note that the second sum on the right is essentially over odd-integer vectors. This is one way to see why Madelung-type alternating sums are so intimately connected with odd-integer sums.

There is also a general functional equation that allows rapid transformation of sums with alternating signs $(-1)^{\mathbf{a}\cdot\mathbf{m}}$ to sums over odd-integer vectors and vice-versa. The entity

$$\Lambda_A(s;c,d) = \sqrt{\det A}e^{-\pi i c\cdot d}\frac{\Gamma(s/2)}{\pi^{s/2}}Z_A(s;c,d)$$

is invariant under a specific parametric transformation:

$$\Lambda_A(s;c,d) = \Lambda_B(n-s;-d,c).$$

3.5 Riemann splitting for the solutions $\phi_n(\mathbf{r})$

For ϕ_n given by the cosine series (28), the relevant splitting form can be derived for *all* $\mathbf{r}$ and any $n \neq 2$ as

$$\bar{\phi}_n(\mathbf{r}) = \frac{\delta_{\mathbf{r}}}{4\pi(1-n/2)} + \frac{1}{4\pi^2}\sum_{\mathbf{m}\in\mathbb{Z}^n} \frac{\Gamma\left(1, \pi|\mathbf{m}-\mathbf{1/2}|^2\right)}{|\mathbf{m}-\mathbf{1/2}|^2} e^{i\pi(2\mathbf{m}-\mathbf{1})\cdot\mathbf{r}} + \frac{1}{4\pi^{n/2}}\sum_{\mathbf{k}\in\mathbb{Z}^n}{}' \frac{\Gamma\left(n/2-1, \pi|\mathbf{k}-\mathbf{r}|^2\right)}{|\mathbf{k}-\mathbf{r}|^{n-2}}(-1)^{\mathbf{1}\cdot\mathbf{k}}, \tag{38}$$

where the Kronecker delta $\delta_{\mathbf{r}}$ vanishes if and only if $\mathbf{r} = \mathbf{0}$. This expedient—of detecting a vanishing radius—mean that $\bar{\phi}_n$ agrees with our Poisson solution ϕ_n, except that when $\mathbf{r} = \mathbf{0}$, we actually get the natural Madelung constant, i.e. $\bar{\phi}_n(\mathbf{0}) = \mathcal{N}_n$ for all $n \neq 2$ (which outlying case being perhaps best handled by the series (32)).

Implementation of the scheme (38) results in such higher-dimensional values as

$$\mathcal{N}_4 = \frac{1}{4\pi^2}\sum_{a,b,c,d\in\mathbb{Z}} \frac{(-1)^{a+b+c+d}}{a^2+b^2+c^2+d^2}$$
$$= -0.07023049277268287640893859949699 7\ldots$$

It turns out this constant is known from the theory of sums of four squares, or from Jacobi theta-function identities, as[5]

$$\mathcal{N}_4 = -\frac{2}{\pi^2}\,\eta(1)\eta(0) = -\frac{\log 2}{\pi^2},$$

so the numerical value given here is a sharp check on a Riemann-splitting implementation. Incidentially we shall have more to say about $n = 4$ dimensions below.

Much more nontrivial is the problem of the fifth-dimensional natural Madelung constant $\mathcal{N}_5$, whose value can be given to reasonable precision via (38), as

$$\mathcal{N}_5 = \frac{1}{8\pi^2}\sum_{\mathbf{m}\in\mathbb{Z}^5}{}' \frac{(-1)^{\mathbf{1}\cdot\mathbf{m}}}{m^3}$$
$$= -0.05175805614526386395600369546224480906 80\ldots$$

This constant, like $\mathcal{N}_3$, is not known in closed form.

[5]Indeed, in even dimensions $n = 2, 4, 6, 8, \ldots$, lattice sums tend to be radically simpler than for odd dimensions. One way to understand this is to note that formulae for the number of representations of an integer N as a sum of k squares—call it $r_k(N)$—are radically more tractable for even k.

4 Status of the $(n=3)$-dimensional Madelung constant

The celebrated, classical Madelung constant $\mathcal{M}_3$—and per force our natural $\mathcal{N}_3$—remains unresolved in closed form. A treatment by Borwein and Crandall [3] discusses the metamathematics, philosophy, and culture of "closed forms," speculating for example on what it means that constants such as $\mathcal{M}_3$ remain elusive. (One explanation is that "rings of hyperclosure"—algebraic constructs generated by hypergeometric evaluations—are countable, leaving much room for outlying constants.)

In spite of the historical failure to resolve $\mathcal{M}_3$, fast series have been known for decades, exemplified by the Benson–Mackenzie series [11]

$$\mathcal{M}_3 \ = \ 4\pi\mathcal{N}_3 \ = \ -12\pi \sum_{m,n\geq 0} \operatorname{sech}^2\left(\frac{\pi}{2}\sqrt{(2m+1)^2+(2n+1)^2}\right), \tag{39}$$

In modern times—meaning over the last decade—the work of S. Tyagi, J. Zucker, J. Buhler and R. Crandall has resulted in the extraction of "much of" the Madelung constant. For example, a 13-digit-accurate assemblage of fundamental constants is evident in

$$\mathcal{M}_3 \ \approx \ -\frac{1}{8} - \frac{\log 2}{4\pi} - \frac{4\pi}{3} + \frac{1}{\sqrt{8}} + \frac{\Gamma(1/8)\Gamma(3/8)}{\pi^{3/2}\sqrt{2}} \ + \ \frac{12}{e^{8\pi}-1} \ - \ 2 \sum_{\mathbf{m}\,\in\,\mathbb{Z}^3,\, m>1}{}' \frac{(-1)^{\mathbf{1}\cdot\mathbf{m}}}{m\,(e^{8\pi m}-1)}$$

$$= \ -1.7475645946331(7)\ldots \ - \ 2\sum{}' \ .$$

One may further strip off 1-dimensional subsums to obtain additional (elliptic-integral-class) constants, to yield yet more good digits of $\mathcal{M}_3$ prior to the lattice summation.

Generally, these newest Madelung representations involve an error term in the form of a rapidly converging exponential series. As another example, one may insider the sum

$$S(x) \ := \ \sum_{\mathbf{u}\,\in\,\mathbb{O}^3} \frac{\operatorname{cosech}(\pi x u)}{u}.$$

It has been shown by Buhler and Crandall [7] that

$$\mathcal{M}_3 \ = \ -\lambda \ + \ \sum_{\mathbf{v}\,\in\,\mathbb{Z}^3}{}' \frac{(-1)^{\mathbf{1}\cdot\mathbf{v}}}{v}(1-\tanh(\lambda v)) \ + \ \frac{2\pi}{\lambda} S\left(\frac{\pi}{2\lambda}\right),$$

for *any* positive real parameter λ. From this free-parameter expansion we infer

$$\mathcal{M}_3 \ = \ \lim_{\lambda\to\infty}\left(-\lambda + \frac{2\pi}{\lambda} S\left(\frac{\pi}{2\lambda}\right)\right).$$

Through the efforts of Buhler, Crandall, Tyagi and Zucker, S values are known exactly for certain arguments. The deepest known such result is Zucker's $S(1/\sqrt{24})$, which gives a fine approximation

$$\mathcal{M}_3 \;\approx\; -\pi\sqrt{6} \;+\; \frac{\sqrt{\frac{1}{6}\left(3\sqrt{2}-6\sqrt{3}+6\sqrt{6}\right)}\;\Gamma\left(\frac{1}{8}\right)^2}{\pi\;\Gamma\left(\frac{1}{4}\right)} \;=\; -1.74756\ldots,$$

which we exhibit just to indicate what kinds of algebraic machinations might be relevant to $\mathcal{M}_3$.

To underscore once again the importance of number theory in lattice-sum analyses: Crandall [8] applied a θ-cubed identity of G. Andrews to establish some new representations, including the following finite-domain (unit disk) integral:

$$\mathcal{M}_3 \;=\; \frac{1}{2\pi}\int_0^1 dr \int_0^{2\pi} d\theta \frac{-6+4(1+r^{-(\cos\theta-\sin\theta)^2})^{-1}}{(1+r^{\cos^2\theta})(1+r^{\sin^2\theta})}.$$

It would be interesting to attempt further transformation of such an entity; after all, just as with the Delord-cube argument, one here works entirely within a finite domain regardless of the infinite extent of the crystal lattice.

5 Closed forms for some potentials

Recall that our solution to the Poisson equation (13) is

$$\phi_2(x,y) \;=\; \frac{1}{\pi^2}\sum_{m,p\in\mathbb{O}} \frac{\cos(\pi m x)\cos(\pi p y)}{m^2+p^2},$$

which form for various x, y becomes an interesting and often difficult lattice sum.

5.1 Evaluations of ϕ_2 at specific points

Some closed forms for the Poisson solution $\phi_2(x,y)$ are known, thanks to recent observations of J. Zucker. and J. Borwein [5]; for example,

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

Lest one start believing we always have logarithms of quadratic surds, there is the more fearsome evaluation

$$\phi_2(0,1/4) \;=\; \frac{1}{8\pi}\log\left(5+\sqrt{2}\left(4+2(1+\sqrt{2})^{3/2}\right)\right)$$

involving a quartic algebraic. (See the related treatment by J. Borwein et al. [4] for a more thorough survey of closed forms.)

A separate research effort is underway to establish more such evaluations, and to explore the algebraic character of the logarithmic arguments.

5.2 Resolution of $\mathcal{N}_2$

In regard to the natural Madelung constant $\mathcal{N}_2$, it has been pointed out to the author by Zucker and Borwein [17] [2, Sec. 3.2, Ex. 11] that we know the odd-tuple lattice sum (25)

$$\mathcal{Y}_1 := \frac{1}{\pi}\sum_{\mathbf{m}\,\in\,\mathbb{O}^+}\frac{1}{m(1+e^{\pi m})} \;=\; \frac{1}{2\pi}\log\frac{\pi^{1/4}}{\Gamma(3/4)}.$$

This gives, via (35), the closed form

$$\mathcal{N}_2 \;=\; \frac{1}{4\,\pi}\log\frac{4\,\Gamma^3(3/4)}{\pi^3}. \tag{40}$$

There is an interesting way to verify this result. From the supposition (21) we infer

$$\begin{aligned}\mathcal{N}_2 \;&=\; \frac{1}{2\pi}\frac{\partial}{\partial s}(-4\eta(s/2)\,\beta(s/2))|_{s=0}\\ &= -\frac{1}{\pi}\left(\eta'(0)\beta(0)+\eta(0)\beta'(0)\right)\end{aligned}$$

which resolves to the same constant (40).

5.3 Evaluating ϕ_3

Observe that for $n = 3$ dimensions, the Madelung potential (14) and our ϕ_3 coincide up to the normalizer C_3:

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

The one closed-form evaluation of $\mathcal{M}_3(1,\mathbf{r})$ of which the present author is aware is

$$\begin{aligned}\mathcal{M}_3\left(1,\frac{\mathbf{1}}{\mathbf{6}}\right) \;&=\; \sum_{m,n,p\,\in\,\mathbb{Z}}\frac{(-1)^{m+n+p}}{\sqrt{(m-1/6)^2+(n-1/6)^2+(p-1/6)^2}}\\ &=\; \sqrt{3}.\end{aligned}$$

Certainly not the best way to calculate the square root of 3! This marvelous evaluation by Forrester and Glasser [10] has the fascinating feature that it can be used in an attractive heuristic argument to estimate the Madelung constant $\mathcal{M}_1$ to be $-\sqrt{3}$, with an error of only about 1% [9].

We cannot resist mentioning a vey new connection between lattice sums, Mahler measures, and elliptic curves; an example of which, while not a direct consequence of Poisson theory, being this marvelous closed form, due to M. Rogers and W. Zudilin [14]:

$$\mathcal{M}_4\left(4,\frac{\mathbf{1}}{\mathbf{6}}\right) \;=\; \sum_{m,n,p,q\,\in\,\mathbb{Z}}\frac{(-1)^{m+n+p+q}}{((m-1/6)^2+(n-1/6)^2+(p-1/6)^2+(q-1/6)^2)^2}$$

$$
\begin{aligned}
&= 27\,\pi \int_0^1 \sqrt{\frac{t}{1-t^3}}\,\log(1+2t)\,dt \\
&= 2\pi^2\log(54) - \frac{2}{9}\pi^2\,{}_4F_3\left(1,1,\frac{4}{3},\frac{5}{3};2,2,2;\frac{1}{2}\right) \\
&= 76.1410535984462883012\ldots
\end{aligned}
$$

It is interesting that again, the Madelung potential in question is tractable in hypergeometric form when all coordinates equal 1/6. This particular Rogers–Zudilin number can be thought of as the potential at said position within a 4-dimensional NaCL lattice, with bare potentials being $\pm 1/r^4$.

6 What is known about the 'natural' Madelung constants

Here we list what is now known about the $\mathcal{N}_n$:

- For $n = 1$ dimension,

$$
\begin{aligned}
\mathcal{N}_1 &= \frac{1}{4} \\
&= 0.250000\ldots
\end{aligned}
$$

- For $n = 2$,

$$
\begin{aligned}
\mathcal{N}_2 &= \frac{1}{4\,\pi}\log\frac{4\,\Gamma^3(3/4)}{\pi^3} \\
&= -0.098259993167175586985985920078 6\ldots
\end{aligned}
$$

- For $n = 3$, a direct relationship to the (still unresolved) classical Madelung constant,

$$
\begin{aligned}
\mathcal{N}_3 &= \frac{1}{4\pi}\mathcal{M}_3 \\
&= -\frac{1}{\pi}\eta(1/2)\,\beta(1/2) \; - \; \mathcal{Y}_2 \\
&= -0.1390667718041276263\ldots
\end{aligned}
$$

  where we refer to the odd-tuple exponential sums (25).

- For $n = 4$, another closed form:

$$
\begin{aligned}
\mathcal{N}_4 &= -\frac{\log 2}{\pi^2} \\
&= -0.070230492772682876408938599496997\ldots
\end{aligned}
$$

- For $n = 5$,

$$\mathcal{N}_5 = -\frac{1}{\pi^2}\eta(3/2)\eta(1/2) - \mathcal{Y}_4$$
$$= -0.05175805614526386395600369546206\ldots$$

- For $n = 6$,

$$\mathcal{N}_6 = \frac{1}{24\pi} - \frac{2G}{\pi^3}$$
$$= -0.04581967987614060588104028295 50\ldots,$$

  where G is the Catalan constant $\beta(2)$.

One can carry these procedures further, generally resolving $\mathcal{N}_{\mathrm{even}}$ in closed form, while evidently being forced to invoke the $\mathcal{Y}_{n-1}$ exponential sums—or some other eeries expedient such as the Riemann-splitting formalism—for $\mathcal{N}_{\mathrm{odd}}$.

The numerical trend of these 'natural' Madelung constants prompts us to posit

Conjecture 1 *The 'natural' Madelung constant $\mathcal{N}_n$ is most negative for the physical instance $n = 3$ dimensions, and for $n \geq 3$ the $\mathcal{N}_n$ form a monotonic increasing sequence with a limit of 0^-.*

In regard to this conjecture, a beckoning challenge is to develop an asymptotic description of $\mathcal{N}_n$ as $n \to \infty$.

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