Fast evaluation of Epstein zeta functions

Richard E. Crandall
Center for Advanced Computation, Reed College, Portland OR

Abstract. Herein we explore means for numerical evaluation of the D-dimensional Epstein zeta function:

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

over a wide class of parameters (matrix A, complex s, vectors c, d); we exhibit a rapidly convergent algorithm valid over the entire s-plane. This is an old problem; the fundamental ideas for such efficient general expansion are long-known, dating back to Riemann. Yet, we address various computational issues of a more modern flavor. In particular there are means for transforming the parameters to advantage, and to optimize the required summations. We provide a collection of exact evaluations of Z_A for use in the testing of any numerical implementations.

Aug 1998

1. The computational problem

We consider a certain generalized (Epstein) zeta function of four parameters. Specifically, assume A is a D-by-D, real, positive definite matrix, s is a complex number, and c, d are real vectors. We adopt the definition

$$Z_A(s; c, d) = \sum_{n \in Z^D}{}' \frac{e^{2\pi i c \cdot An}}{|An - d|^s}, \tag{1.1}$$

where the vector n runs over the full, D-dimensional integer lattice and the notation $\sum'$ means any singularities are to be ignored in the course of summation. As to the very existence of the sum, there will generally be some real threshold σ for which the constraint $Re(s) > \sigma$ yields an absolutely convergent $\sum'$. Then we may infer the analytic continuation to $Re(s) \le \sigma$ by standard methods. We note that Z_A has a one-dimensional instance that coincides with the Riemann ζ function. For $A = 1$ (the identity matrix) we have

$$Z_1(s; 0, 0) = 2\zeta(s).$$

Just as with the Riemann zeta itself, there exist attractive closed-form evaluations of Z_A, in various dimensions D, as we present later.

Over the years, the sums Z_A have arisen in chemistry and physics research. Calculation of electrostatic energies of crystals use such sums in a natural way. In fact, in this context the matrix A is what characterizes the very structure of a periodic crystal, so that Z_A is related to physical energy. Interesting also is that the avoidance of the singularity in the Σ' is manifest in the physical scenario as avoidance of self-energy at an ionic center. There is a large and long-standing literature on such chemical application, grouped under such topical headings as "lattice sums," or "Madelung problem," and so on (see [Glasser and Zucker 1980][Crandall and Buhler 1986][Crandall and Delord 1987] and references therein). In theoretical physics, vacuum energy – or Casimir – calculations may also involve Epstein zeta functions [Amborn and Wolfram 1983]. The Epstein sums also figure into analytic number theory, for example in problems regarding sum-of-squares representations.

But quite beyond these practical scientific applications, the problem of evaluation of the Epstein zetas – to a great many decimal places, say – is interesting in its own right. There are some interesting optimizations we can state right off. First, it will turn out to be computationally efficient to handle matrices of unit determinant. To this end we observe a scaling property, valid for positive real γ:

$$Z_A(s; c, d) = \gamma^{-s} Z_{A/\gamma}(s; \gamma c, d/\gamma). \tag{1.2}$$

Now the choice

$$\gamma = (\det A)^{1/D}$$

allows us to carry out calculations for the right-hand side of (1.2), with its matrix A/γ having unit determinant. In the common case where A is a diagonal matrix, the γ parameter is simply the geometric mean of the diagonal elements.

A second initial optimization is this: we need not evaluate Z_A for unconstrained c, d vectors, because one can always reduce them according to the integer lattice Z^D. Define the inverse transpose:

$$B = A^{-T}$$

and reduce c, d with respect to the Z^D lattice by:

$$c' = B((B^{-1}c) \bmod 1),$$

$$d' = A((A^{-1}d) \bmod 1),$$

where it is intended that each component of a vector be reduced (mod 1); i.e., so that each component is in the interval $[0, 1)$. It turns out, then, that under such reduction to the lattice we have

$$Z_A(s; c, d) = e^{2\pi i c' \cdot (d - d')} Z_A(s; c', d'). \tag{1.3}$$

In this way the magnitudes of the c, d parameters can be controlled during computation. Accordingly, we shall heretofore assume c, d have been *a priori* reduced. In particular, a c or d parameter now belongs to the Z^D lattice if and only if it is the zero vector. .

2. Riemann splitting

An analytic continuation method for Z_A, due in essence to Riemann, hinges upon a central, "theta-function" identity:

$$\sum_{n \in Z^D} e^{2\pi i c \cdot An - \pi t |An - d|^2} = t^{-D/2} \frac{e^{2\pi i c \cdot d}}{\det A} \sum_{k \in Z^D} e^{-2\pi i Bk \cdot d - \pi |Bk - c|^2 / t}, \tag{2.1}$$

This identity can be derived by standard means such as Poisson summation.

Riemann's idea is to cast a zeta function as a certain Mellin transform. Define a function δ on D-dimensional vectors by: $\delta(m) = 1$ if $m \in Z^D$, else $\delta(m) = 0$. Then the idea is to write

$$Z_A(s; c, d) = \frac{\pi^{s/2}}{\Gamma(s/2)} \int_0^\infty t^{s/2 - 1} dt (-\delta(d) + \sum_{n \in Z^D} e^{2\pi i c \cdot An - \pi t |An - d|^2}),$$

and furthermore to split the integral into a form $\int_0^1 + \int_1^\infty$. The integral over $(1, \infty)$ immediately yields a sum of evaluations of the incomplete gamma function

$$\Gamma(z, x) = \int_x^\infty t^{z-1} e^{-t} dt$$

whose rapid decay (in positive real x) will be advantageous. For the integral over $(0, 1)$ on the other hand, we use the theta-function identity (2.1), then change integration variables by $u := 1/t$, whence another series in incomplete gamma evaluations obtains. The full formula that leads readily to a practical algorithm works out, then, to be:

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

$$+e^{-\pi i c\cdot d}\sum_n{}' \frac{\Gamma(\frac{s}{2},\pi|An-d|^2)e^{2\pi i c\cdot An}}{(\pi|An-d|^2)^{s/2}} + \frac{e^{\pi i c\cdot d}}{\det A}\sum_k{}' \frac{\Gamma(\frac{D-s}{2},\pi|Bk-c|^2)e^{-2\pi i d\cdot Bk}}{(\pi|Bk-c|^2)^{\frac{D-s}{2}}}. \quad (2.2)$$

It is yet another tribute to Riemann's ingenuity that this expansion leads *either* to a theoretically important functional equation, or to an efficient computational scheme. As an aside, we note that for certain s, notably $s = 1$, other expansions can be obtained, via different theta-function definitions, where elementary functions sit in place of the incomplete gammas [Crandall and Buhler 1986]. Such elementary expansions are easier to implement, of course, but do not enjoy the evidently optimal convergence properties of the Riemann scheme (nor do they permit arbitrary s.)

The computational approach depends on the observation that, for real σ, τ and large real argument x we can estimate the incomplete gamma growth as:

$$\Gamma(\sigma + i\tau) = O(x^{\sigma-1}e^{-x}),$$

with the implied big-O constant independent of σ, τ, x, as is not hard to show directly from the integral definition of Γ. So, for a given limit L and complex t, a sum

$$\sum_{Q\le L^2}{}' \frac{|\Gamma(t,\pi Q)|}{(\pi Q)^t},$$

where Q is a positive definite quadratic form such as $(An-d)\cdot(An-d)$, leaves an error term whose damping factor is $e^{-\pi L^2}$. The sum is over an ellipsoidal lattice region, so given that $|d|$ is negligible, we can enclose such an ellipsoid in a sphere of radius $\sim L/\lambda$, where λ is the least eigenvalue of A. One simple strategy, then, is to sum over a D-cube of apothem L/λ, and check (during actual summation over said cube) the condition $Q \le L^2$. This strategy is explained in more detail in the next section.

3. General computational algorithm

As for computation, we remind ourselves that one can use (1.2) always to force $\det A = \det B = 1$, rendering formula (2.2) simpler. But there is another reason for normalizing the determinants: the two sums of incomplete gamma function terms then converge with roughly the same speed. In addition, there are some immediate evaluations (such as for $s = 0$ and $s = D$) that should be checked. An overall computational strategy, valid for all complex s, can be outlined as follows.

Algorithm for evaluation of Epstein zeta

Given a real, positive-definite D-by-D matrix A, complex s, real vectors c, d, this algorithm evaluates $Z_A(s; c, d)$ to desired precision.

1) Invoke the reduction formulae (1.2), (1.3) as necessary, so that new parameters A, c, d have these properties: that $\det A = 1$ and for $B = A^{-T}$, all components of $B^{-1}c, A^{-1}d$ lie in $[0, 1)$ via (mod 1) reduction to the integer lattice.

2) Next we handle the two possibilities $s = 0, D$. First check for the known evaluation at $s = 0$: If $s = 0$ return either -1 (in the case d vanishes), or return zero (in the case $d \neq 0$). Then check for possible singularity at $s = D$: If both $s = D$ and $c = 0$, return with indication of singularity, otherwise continue to step (3).

3) Choose a summation limit L (so that computational error will be, roughly speaking, $e^{-\pi L^2}$). Find also the least and greatest eigenvalues, respectively λ, μ, of A.

4) Sum the first series of (2.2), over each component $n_i \in [-L/\lambda, +L/\lambda]$, evaluating only those summands having $|An - d| \leq L$. Then sum the second series of (2.2) similarly, but using instead $k_i \in [-\mu L, +\mu L]$, resolving only those summands with $|Bk - c| \leq L$.

5) Using the rest of the terms in (2.2), and any reduction formulae that were invoked in step(1), return an evaluation of the original Z_A.

Let us give an indication of how the control of summation indices works in step(4). Say $D = 3$ dimensions, $d = c = (0, 0, 0)$, and assume a diagonal A with diagonal elements a_1, a_2, a_3. Then in step (1), we obtain new elements $a'_i = a_i/(a_1 a_2 a_3)^{1/3}$, so that the modified matrix A' has $\det A' = 1$. After choosing some limit L in step (3), we are to perform the first incomplete-gamma sum over the 3-dimensional cube $|n_i| \leq L/\lambda$ where $\lambda = min\{a'_i\}$, evaluating summands only for $|A'n| \leq L$, which condition in fact signifies an ellipsoidal region. The number of lattice points thus involved in non-trivial summation is about equal to the ellipsoidal volume, or $O((L/a'_1)(L/a'_2)(L/a'_3)) = O(L^3)$. The idea here is that the ellipsoid in question is always contained in a cube of apothem L/λ. But this computational effort is the same for the second incomplete-gamma sum, if we take the domain to be $|k_i| \leq L/\mu$, and use only terms having $|Bk| \leq L$. So the sums take about the same time, and furthermore the accuracies are comparable.

There is an important point concerning highly symmetrical cases. When A is diagonal and a parameter d or c is 0, for example, any summation index n_i or k_i in the appropriate gamma sum contributes equally upon sign reversal. In such cases, one may use the evident symmetry to cast a relevant $\sum'$ into a sum over the fully nonnegative D-tant. Specifically, if $G(n) = G(n_1, ..., n_D)$ enjoys invariance under any reversal $n_i \to -n_i$, then we can write

$$\sum_{n \in Z^D} {}' G(n) = \sum_{n_i \in [0,\infty]} F(n) G(n),$$

where $F(0, ..., 0) = 0$, otherwise $F(n) = 2^{D-Z}$ whenever n has exactly Z vanishing components. Such symmetry techniques can speed up the evaluation of Z_A by as much as a factor of 2^D, which is considerable for large dimension D.

Incidentally, there is at least one method for "dynamical looping;" i.e., casting a D-dimensional loop, where D itself is an input parameter, over a cube of constant apothem L; i.e., each $|n_i| \le L$ for $i = 1, ..., D$. The method is to do a *single* loop over all integers $j \in [-((2L+1)^D - 1)/2, -((2L+1)^D - 1)/2]$, expressing each such j in balanced-digit representation. Thus for $D = 2$ we represent all integers in balanced-base 5, in the form $j = 5n_1 + n_2$, where each $n_i \in [-2, 2]$. One loops through the stated interval for j, and can recover at any moment the digits n_i. In this way, lattice sums can be implemented with D treated as input parameter.

As for overall computational complexity of D-dimensional Epstein zeta evaluation, we evidently need to sum over volumes $O(L^D)$ to achieve rough error $O(e^{-\pi L^2})$. Roughly speaking we can expect

$$O(\Delta^{D/2})$$

summands to be required to resolve Δ good digits of Z_A. As for the incomplete gamma terms, there are various algorithms for rapid evaluation of $\Gamma(z, x)$; namely, continued fraction, asymptotic series, ascending series, Poisson formulae, and so on. In any given region of the complex z-plane there is a suitably convergent scheme [Crandall 1994].

4. Exact theoretical evaluations

There exist a host of closed-form results and known evaluations of the Epstein zetas. These results extremely useful – if not indispensable – for proper testing of any computational engine that is supposed to be evaluating Z_A. Happily, there are known evaluations for different classes of parameters; e.g., d or c or both $\neq 0$, and so on). In what follows, we remind ourselves that c, d parameters are assumed reduced to the Z^D lattice, as was explained for reduction relation (1.3).

First there is the functional equation, which we can infer from the Riemann strategy. From (2.2) it is evident that 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. Indeed,

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

This functional equation is of course a higher-dimensional analogue of the celebrated relation for $\zeta(s)$.

An exact evaluation at $s = 0$ also follows from (2.2); namely:

$$Z_A(0; c, d) = -\delta(d),$$

from which the well known evaluation $\zeta(0) = -1/2$ follows in the one-dimensional setting. Likewise, the fact of a pole at $s = D$ depends, as we see in (2.2), on whether c vanishes: there is a pole at $s = D$ if and only if $c = 0$, and the residue is easy to infer as $2\pi^{D/2}(\det B)/\Gamma(D/2)$.

A beautiful class of closed-form evaluations has arisen over the years in the art of applying Z_A in the sciences. Many such relations arise in the theory of Jacobi theta-functions; often combinatrics and number theory are involved in fascinating ways. Here and elsewhere, 1_D means either the D-dimensional identity matrix, or a D-vector consisting of all 1's as appropriate by context; while α_D denotes a D-vector $\{\alpha, \alpha, ..., \alpha\}$. In addition, we define some specific L-series which figure into some of the closed-form evaluations:

$$\beta(s) = 1^{-s} - 3^{-s} + 5^{-s} - ...,$$
$$\eta(s) = (1 - 2^{1-s})\zeta(s) = 1^{-s} - 2^{-s} + 3^{-s} - ...,$$
$$\lambda(s) = (1 - 2^{-s})\zeta(s) = 1 + 3^{-s} + 5^{-s} + ...,$$
$$L_{-3}(s) = 1^{-s} - 2^{-s} + 4^{-s} - 5^{-s} + 7^{-s} - ...,$$
$$L_{-8}(s) = 1^{-s} + 3^{-s} - 5^{-s} - 7^{-s} + 9^{-s} + 11^{-s} - ...$$
$$L_{+8}(s) = 1^{-s} - 3^{-s} - 5^{-s} + 7^{-s} + 9^{-s} - 11^{-s} - ...$$

Some of these series themselves enjoy exact evaluation, such as $\beta(1) = \pi/4$ and the analytic continuation evaluation $\beta(0) = 1/2$.

Various exact evaluations are known for $D = 2$ dimensions, for example

$$Z_{1_2}(s; 0_2, 0_2) = \sum_{m,n \in Z}{}' \frac{1}{(m^2 + n^2)^{s/2}} = 4\zeta(s/2)\beta(s/2),$$

$$Z_{1_2}(s; (\frac{1}{2})_2, 0_2) = \sum_{m,n \in Z}{}' \frac{(-1)^{m+n}}{(m^2 + n^2)^{s/2}} = -4\eta(s/2)\beta(s/2).$$

Note that the second zeta above is a "Madelung constant" for $D = 2$, i.e. the potential energy of the origin charge in a certain 2-dimensional charge lattice. About the physically genuine, 3-dimensional Madelung constant we shall have more to say later. For the moment, we note that 2-dimensional zeta eveluations have been taken yet further, for example the Madelung problem on an hexagonal lattice has been solved, in the sense of exact evaluation. The relevant hexagonal sum is taken to be:

$$H(s) = \sum_{m,n \in Z}{}' \frac{(\frac{n-m+1}{3})}{((n + m/2)^2 + 3(m/2)^2)^{s/2}},$$

where $(\frac{x}{3})$ is the Legendre symbol, which runs $1, -1, 0, 1, -1, 0, ...$ as x runs $1, 2, 3, 4, 5, 6, ...$. Now $H(x)$ can be written as a superposition of four complex Epstein zetas. However, it is argued in [Borwein and Borwein 1987, p. 292] that one can instead eveluate just two (real) zetas:

$$H(s) = \frac{1 - 3^{1-s/2}}{2}(2Z_A(s; 0_2, 0_2) - Z_A(s; (\frac{1}{2})_2, 0_2)),$$

with matrix

$$A = \begin{bmatrix} 1 & \frac{1}{2} \\ 0 & \frac{\sqrt{3}}{2} \end{bmatrix},$$

and by such means arrive at the exact value

$$H(s) = 3(1 - 3^{1-s/2})\zeta(s/2)L_{-3}(s/2),$$

so that the "Madelung" value is $H(1)$, while the case $s = 2$ comes down to the attractive result $H(2) = \pi \ln 3\sqrt{3}$. Beyond this, but still in two dimensions, sums with denominators $(m^2 + |d|n^2)^{s/2}$ have been evaluated, through adroit application of number theoretic and transform techniques, for certain classes of discriminant d [Glasser and Zucker 1980]. An example of the beauty of some of the known two-dimensional Epstein zeta evaluations is Zucker's sum:

$$\sum{}' \frac{(-1)^{m+n}}{(4m-1)^2 + 13(4n-1)^2} = \frac{\pi}{16\sqrt{13}} \log \frac{(1+\sqrt{2})^3}{5+\sqrt{26}}.$$

Further dimensional generalizations include the following collection for $D = 4$, starting with an attractive chain of evaluations [Zucker 1984][Glasser and Zucker 1980][Crandall and Buhler 1986]:

$$\begin{aligned}
\log 2 = -\frac{1}{4} Z_{1_4}(2, (\frac{1}{2})_4, 0_4) &= -\frac{1}{4} \sum_{\{a,b,c,d\} \in Z^4} \frac{(-1)^{a+b+c+d}}{a^2+b^2+c^2+d^2} \\
&= -\frac{\pi}{2} - Z_{1_4}(2; ((\frac{1}{2})_3, 0), 0_4) \\
&= -\frac{1}{2} Z_{1_4}(2; ((\frac{1}{2})_2, 0_2), 0_4) \\
&= \frac{\pi}{2} - Z_{1_4}(2; (\frac{1}{2}, 0_3), 0_4) \\
&= -\frac{1}{8} Z_{1_4}(2; 0_4, 0_4).
\end{aligned}$$

Some of which being instances of the following:

$$Z_{1_4}(s; (\frac{1}{2}, 0_3), 0_4) = 4\beta(s/2)\beta(s/2-1) - 2^{3-s}\eta(s/2)\eta(s/2-1),$$

$$Z_{1_4}(s; ((\frac{1}{2})_3, 0), 0_4) = -4\beta(s/2)\beta(s/2-1) - 2^{3-s}\eta(s/2)\eta(s/2-1),$$

$$Z_{1_4}(s; 0_4, ((\frac{1}{2})_3, 0)) = 2^s(\lambda(s/2)\lambda(s/2-1) - \beta(s/2)\beta(s/2-1)),$$

$$Z_{1_4}(s; 0_4, (\frac{1}{2}, 0_3)) = 2^s(\lambda(s/2)\lambda(s/2-1) + \beta(s/2)\beta(s/2-1)),$$

$$Z_{1_4}(s; ((\frac{1}{2})_3, 0), (0_3, \frac{1}{2})) = 2^s(L_{-8}(s/2)L_{-8}(s/2-1) + L_{+8}(s/2)L_{+8}(s/2-1)),$$

$$Z_{1_4}(s; (\frac{1}{2}, 0_3), (0, (\frac{1}{2})_3)) = 2^s(L_{-8}(s/2)L_{-8}(s/2-1) - L_{+8}(s/2)L_{+8}(s/2-1)),$$

Then there are some isolated evaluations in even higher dimension, such as the beautiful 6-dimensional result of Zucker:

$$\sum{}' \frac{(-1)^{a+b+c+d+e+f}}{(a^2+3b^2+3c^2+3d^2+3e^2+3f^2)^{3/2}} = -\frac{2\pi\zeta(3)}{3\sqrt{3}} - \frac{4\pi^3\log 2}{81\sqrt{3}},$$

and an 8-dimensional result:

$$Z_{1_8}(8;(\frac{1}{2})_8, 0_8) = \sum_{n\in Z^8}{}' \frac{(-1)^{n_1+\ldots+n_8}}{(n_1^2+\ldots+n_8^2)^4} = -\frac{8\pi^4\log 2}{45}.$$

For the remainder of this section we focus on $D = 3$, which cases include evaluations applicable in the physical sciences.

The celebrated Madelung constant of chemistry and physics is a 3-dimensional construct

$$M = Z_{1_3}(1;(\frac{1}{2})_3, 0_3) = \sum_{(x,y,z)\in Z^3}{}' \frac{(-1)^{x+y+z}}{\sqrt{x^2+y^2+z^2}},$$

which has never been cast into any convenient closed form. It is of interest that this 3-dimensional setting is in many ways more difficult than any of the 2,4,8-dimensional settings previous. This discrepancy could be thought of as a relative paucity of relations for odd powers of Jacobi theta functions. It should be remarked, however, that literally dozens of three-dimensional Epstein zetas admit of closed-form evaluation, as in [[Zucker 1987, 1990], yet none of these is precisely the Madelung M. Nevertheless, using the method of the present treatment – which amounts to a long-known "Ewald expansion" for such a crystal energy – one is able to obtain numerical values such as

$$M \sim -1.74756459463318219063621203554439740348516143662474175815282535076...$$

in a short time, and, in practice, carry out such numerics to thousands of decimal places. Incidentally one reason for attaining such precision would be somewhat more than recreational: the PSLQ methods of Bailey, et. al. just might yield finally a representation of M in terms of other celebrated constants, and to effect a PSLQ approach one should have access to hundreds of digits at least. The Madelung constant enjoys relations with other Z_A evaluations, for example the following nontrivial connections are known [Zucker 1979][Crandall and Delord 1987] :

$$M = \frac{3}{\pi} Z_{1_3}(2;((\frac{1}{2})_2, 0), 0_3) = \frac{3}{\pi}\sum_{(x,y,z)\in Z^3}{}' \frac{(-1)^{x+y}}{x^2+y^2+z^2}$$

$$= \frac{3}{\pi}\sum_{(x,y,z)\in Z^3}{}' \frac{(-1)^{x+y+z}}{x^2+2y^2+2z^2}$$

$$= \frac{1}{\pi} Z_{1_3}(2; 0_3, (\frac{1}{2})_3) = \frac{4}{\pi} \sum_{(x,y,z)\in(2Z+1)^3} \frac{1}{x^2+y^2+z^2},$$

this last form defined over all odd triples (and, as always, as an analytic continuation since the literal sum does not converge). There is also the attractive relation:

$$\sum{}' \frac{3(-1)^x + 3(-1)^{x+y} + (-1)^{x+y+z}}{(x^2+y^2+z^2)^{3/2}} = -4\pi \log 2,$$

which can be cast as an identity involving $Z_{1_3}(3, b/2, 0_3)$ for a certain three binary vectors b.

In any test suite for numerical evaluation, all the above are useful checking relations. We have seen – for the hexagonal lattice sum $H(s)$–a nontrivial A matrix. Another case of nontrivial A, in fact for the matrix $A = diag(\{2, \sqrt{2}, \sqrt{2}\})$, is:

$$Z_A(s, (\frac{1}{4}, 0_2), (\frac{1}{2}, 0_2)) = \sum_{(x,y,z)\in Z^3} \frac{(-1)^m}{((2x-\frac{1}{2})^2 + 2y^2 + 2z^2)^{s/2}} = 2^s L_{-8}(s-1).$$

One may also test further some nontrivial instances of c, d parameters such as:

$$Z_{1_3}(s, (\frac{1}{2}, 0_2), (0_2, \frac{1}{2})) = \sum_{(x,y,z)\in Z^3} \frac{(-1)^x}{(x^2+y^2+(z-\frac{1}{2})^2)^{s/2}} = 2^{s+1}\beta(s-1).$$

In particular, setting $s = 2$ yields the Catalan constant $G = \beta(2) = 1 - 1/3^2 + 1/5^2 - 1/7^2 + ...$ as:

$$G = \frac{1}{16} Z_{1_3}(3, (\frac{1}{2}, 0_2), (0_2, \frac{1}{2})),$$

while for $s = 1$ we would obtain the exact potential energy at a certain point within a peculiar, alternating charge-plane crystal. Another example of nontrivial – but physically meaningful – parameters is the following attractive evaluation of [Forrester and Glasser 1982], which can be thought of as the potential energy at the point $(x, y, z) = (\frac{1}{6}, \frac{1}{6}, \frac{1}{6})$ within the (sodium chloride) lattice of the basic Madelung problem:

$$Z_{1_3}(1, (\frac{1}{2})_3, (\frac{1}{6})_3) = \sum_{(x,y,z)\in Z^3} \frac{(-1)^{x+y+z}}{\sqrt{(x-\frac{1}{6})^2 + (y-\frac{1}{6})^2 + (z-\frac{1}{6})^2}} = \sqrt{3}.$$

Of course, the present algorithm is not the most efficient way to calculate the square root of three.

5. Acknowledgments

The author would like to thank Scott Koranda, Michael Trott, and Stephen Wolfram for drawing recent attention to this computational problem. J. Borwein provided insight. I. J. Zucker provided detailed theoretical evaluations.

6. References

Amborn J and Wolfram S 1983, "Properties of the Vacuum I. Mechanical and Thermodynamic," Annals of Physics, 147, 1

Borwein J and Borwein P 1987, *Pi and the AGM*, John Wiley & Sons, New York

Crandall R 1994, *Projects in Scientific Computation*, TELOS/Springer-Verlag, New York

Crandall R and Buhler J 1986, "Elementary function expansions for Madelung constants," J. Phys. A.: Math. Gen, 5497-5510

Crandall R and Delord J 1987, "The potential within a crystal lattice," J. Phys. A.: Math. Gen, 20, 2279-2292

Forrester P and Glasser M 1982, J. Phys. A.: Math. Gen. 15, 911-914

Glasser M and Zucker I 1980, "Lattice Sums," Theor. Chem.: Adv. Persp., 5, 67-139

Zucker I 1979, J. Phys. A.:Math. Gen., 9, 499-505

Zucker I 1984, "Some Infinite Series of Exponential and Hyperbolic Functions," SIAM J. Math., 15, 2, 406-413

Zucker I 1987, "A systematic way of converting infinite series into infinite products," J. Phys. A.:Math. Gen., 20, L13-L17

Zucker I 1990, "Further relations amongst infinite series and products:II. The evaluation of three-dimensional lattice sums," J. Phys. A.:Math. Gen., 23, 117-132