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On the convergence problem for lattice sums

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Dedicated to physicist and Professor Jean F Delord on the occasion of his retirement

Abstract. Three-dimensional lattice sums $\Sigma \pm r^{-s}$, where r is the distance to a $\pm$ charged lattice point, arise in classical lattice point problems ($s = 0$) and the Madelung problem of physics and chemistry ($s = 1$). In the latter case the sum over an infinite lattice is purely formal and the value of the Madelung constant must be defined precisely, e.g., via related convergent sums or analytic continuation in s. Indeed, the partial sum over the sphere $r < R$ does not converge as R becomes large. Here we verify a conjecture of J F Delord that convergence can be obtained by neutralising each sphere with an appropriate surface charge. Specifically, if $L_R(s)$ is the sum over the lattice points in the sphere $r < R$ then, for neutrally charged lattices, we show that as R goes to infinity the difference $L_R(s) - R^{-s}L_R(0)$ approaches $L(s)$, where $L(s)$ is defined by analytic continuation. When $s = 1$ the term $L(1)$ is the Madelung constant and $L_R(0)/R$ is the Coulombic correction term.

1. The convergence problem

The familiar Madelung constant for the NaCl crystal is defined, formally, to be the infinite sum

$$M = \sum_{(x_1,x_2,x_3)\neq(0,0,0)} (-1)^{x_1+x_2+x_3}(x_1^2+x_2^2+x_3^2)^{-1/2} \tag{1.1}$$

over all non-zero integer triples $(x_1, x_2, x_3) \in Z^3$. Since the sum does not converge absolutely it must be defined in some unambiguous fashion; this convergence problem is especially difficult when 'natural' orderings of the terms do not give convergent sums.

One reasonable idea is to sum the terms in a sphere of radius R and then let R go to infinity. Unfortunately this procedure is not convergent (Borwein *et al* 1985). However, summation over larger and larger cubes does converge (Evjen 1932, Calara and Miller 1976, Borwein and Borwein 1986). A clue to the failure of the spherical method is that the charge in the interior of the sphere

$$Q(R) = \sum_{|x|<R} (-1)^{x_1+x_2+x_3} \tag{1.2}$$

fluctuates radically even though the infinite crystal has neutral symmetry. This fluctuation can be traced to the fact that if a sphere is cut out of a crystal then the detailed structure of the spherical surface is extremely complicated, favouring positive or negative charges alternately as the radius R changes. It was conjectured to us by Delord (1988) that summing over spheres should work if one were to somehow 'add back' the missing charge $-Q(R)$. Specifically, he conjectured that if M_R is the

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Madelung sum over the region $0<|x|<R$ then the limit

$$\lim_{R\to\infty}\left(M_R-\frac{Q(R)}{R}\right) \tag{1.3}$$

should exist and be equal to the traditional Madelung constant M as obtained via analytic continuation or other convergence procedures. The physical motivation is that if one placed a charge of $-Q(R)$ on the surface of the sphere then the (finite) crystal would be neutral and the approximation to the Madelung constant should be more accurate.

The purpose of this paper is to give a surprisingly straightforward proof using contour integration techniques; there is no additional effort involved in proving this for more general lattice sums constructed as follows. Define a lattice sum over integer 3-tuples by

$$L_R(s)=\sum_{v\in Z^3,0<|v|<R} e^{2\pi i d\cdot v}|v|^{-s} \tag{1.4}$$

where $x\in C$ is a complex number and $d\in[0,1)^3$ is a 3-tuple. For $\mathrm{Re}(s)>3$ it is a standard fact that this sum converges absolutely as $R\to\infty$ and that the resulting function of s has an meromorphic continuation to the entire complex s-plane (Terras 1985, Glasser and Zucker 1980, Crandall and Buhler 1987). Let $L(s)$ denote this continuation and let δ be 1 if $d=(0,0,0)$ and let δ be 0 if d is non-zero.

Theorem. For all s with $\mathrm{Re}(s)>0$,

$$\lim_{R\to\infty}\left(L_R(s)-R^{-s}L_R(0)-\frac{4\pi sR^{3-s}\delta}{3(3-s)}\right)=L(s). \tag{1.5}$$

Remarks. (i) This result can be extended to more general three-dimensional lattice sums; for instance, to lattices not centred at the origin. The ideas can be modified to apply to higher-dimensional lattice sums, but the result is more elegant in the three-dimensional case.

(ii) The proof in the next section uses various estimates of contour integrals common in the study of Dirichlet series in analytic number theory. It is possible to give another proof using Green's theorem by thinking of $L_R(s)$ as a potential; the analytical details are substantially more complicated, but this proof has the advantage of applying to more general regions by showing that the lattice sum converges when summed over any sequence of increasing regions with zero net charge.

(iii) The function $L_R(s)$ is related to many well studied lattice sums. For example, the number of lattice points within a sphere of radius R is $L_R(0)$ (for $d=0$). The problem of evaluating the order of growth of this (and related sums) has engaged number theorists for many years (Walfisz 1924, Grosswald 1985). For non-zero d it is known that $L_R(0)/R^{3/2}$ is bounded and that $L_R(0)/R$ is unbounded as R becomes large (Landau 1962). The determination of the true order of growth—i.e. the smallest a such that $L_R(0)=O(R^{a+\varepsilon})$ for all positive ε—is an outstanding open problem that is the three-dimensional version of the Gauss circle problem.

(iv) The Madelung problem itself is to evaluate $L(1)$ (for various d). To this day no closed form evaluation of this sum is known for any physically meaningful crystal lattice. Much work has been done on this evaluation problem (Glasser and Zucker 1980, Crandall and Buhler 1987 and references therein), typically leading to summations with exponentially decaying summands.

(v) Note that when $d \neq 0$ the theorem, together with fact that $L_R(0)/R$ is unbounded, immediately implies the known fact that the $L_R(1)$ does not converge as R becomes large. Indeed, the difference between $L_R(1)$ and the fluctuating term $L_R(0)/R$ converges to $L(1)$ so $L_R(1)$ does not converge at all. The theorem also implies the standard result that if $L_R(0) = \mathrm{O}(R^c)$ then

$$\lim_{R\to\infty} L_R(s) = L(s) \qquad \text{for } \mathrm{Re}(s) > c. \tag{1.6}$$

Of course, as mentioned above, the determination of the smallest possible value of c is an open problem.

2. The contour integral method

We start by recalling the well known analytic continuation of $L(s)$. Define

$$L(s) = \sum_{v\in \boldsymbol{Z}^3, v\neq 0} \mathrm{e}^{2\pi i d\cdot v}|v|^{-s} \qquad \text{and} \qquad \bar{L}(s) = \sum_{v\in \boldsymbol{Z}^3, v\neq d} |v-d|^{-s} \tag{2.1}$$

for a fixed $d \in [0, 1)^3$. These sums converge absolutely for $\mathrm{Re}(s) > 3$ and have meromorphic continuations to the complex plane that satisfy a functional equation: if

$$\Lambda(s) = \pi^{-s/2}\Gamma(s/2)L(s) \qquad \text{and} \qquad \bar{\Lambda}(s) = \pi^{-s/2}\Gamma(s/2)\bar{L}(s) \tag{2.2}$$

then

$$\Lambda(s) = \bar{\Lambda}(3-s). \tag{2.3}$$

Moreover, $\Lambda(s)$ is analytic everywhere unless d is an integral 3-tuple, in which case it is analytic except for a simple pole with residue 4π at $s = 3$.

Let $H(x)$ be the function

$$H(x) = \begin{cases} 0 & \text{if } x < 1 \\ \frac{1}{2} & \text{if } x = 1 \\ 1 & \text{if } x > 1. \end{cases} \tag{2.4}$$

Perron's formula states that if c is positive then

$$\frac{1}{2\pi \mathrm{i}} \int_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty} x^s \frac{\mathrm{d}s}{s} = H(x). \tag{2.5}$$

For positive real x define the truncated series $L_x(s)$ by

$$L_x(s) = \sum_{v\in \boldsymbol{Z}^3, v\neq 0} H\left(\frac{x}{|v|}\right) \mathrm{e}^{2\pi i d\cdot v}|v|^{-s}. \tag{2.6}$$

(This differs slightly from notation of the previous section since terms on the boundary are treated differently if x is exactly equal to $|v|$ for some v; this notational discrepancy is unimportant since the left-hand side of (1.5) in the theorem is easily seen to be a continuous function of R. Thus it suffices to prove the theorem for R not a square root of an integer, so $R \neq |v|$ for any v, and thus the treatment of the terms on the boundary is ultimately unimportant.)

Now use Perron's formula to evaluate $L_x(w)$ for a complex number w with real part $u = \mathrm{Re}(w)$:

$$\frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} L(s)x^s \frac{ds}{s-w} = \frac{1}{2\pi i}\int_{c-u-i\infty}^{c-u+i\infty} L(s+w)x^{s+w}\frac{ds}{s}$$
$$= x^w \sum e^{2\pi i d\cdot v}|v|^{-w} \frac{1}{2\pi i}\int_{c-u-i\infty}^{c-u+i\infty} \left(\frac{x}{|v|}\right)^s \frac{ds}{s}$$
$$= x^w \sum e^{2\pi i d\cdot v}|v|^{-w} H\left(\frac{x}{|v|}\right) = x^w L_x(w) \tag{2.7}$$

where $3 < c$ (so that the first contour integral is in the region of absolute convergence of $L(s)$), and $0 \leqslant u < c$.

Now use this formula, together with a little algebra and the same formula for $w = 0$, to get

$$L_x(w) - x^{-w}L_x(0) = wx^{-w}\frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} L(s)x^s \frac{ds}{s(s-w)}. \tag{2.8}$$

Replace the integral over the vertical line by the integral over the contour α in figure 1. The difference is an integral over a rectangle that can be easily evaluated by Cauchy's residue theorem; there are simple poles at $s = 0$, $s = w$, and (if $d = 0$) $s = 3$. The result is

$$L_x(w) - x^{-w}L_x(0) = -x^{-w}L(0) + L(w) + \frac{4\pi\delta w x^{3-w}}{3(3-w)} + wx^{-w}\frac{1}{2\pi i}\int_\alpha L(s)x^s \frac{ds}{s(s-w)} \tag{2.9}$$

where δ is as in the statement of the theorem. The crux of the theorem is that the contour integral can be sharply bounded.

Lemma. For any positive ε

$$\frac{1}{2\pi i}\int_\alpha L(s)x^s \frac{ds}{s(s-w)} = O(x^\varepsilon). \tag{2.10}$$

In fact, the proof will show that the integral is bounded by a constant times $\log(x)$.

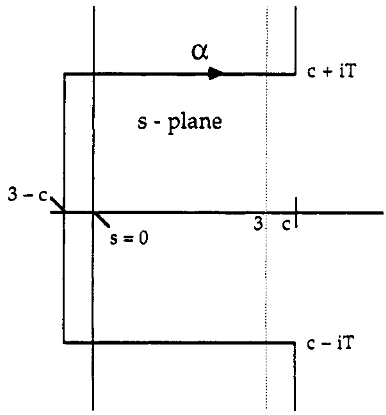

Figure 1. The convergence problem can be reduced to an analysis of the integral of the L function along a certain contour.

Now let x go to ∞ in (2.9). Since $\mathrm{Re}(w)>0$ and $L(0)$ is a constant it follows from the lemma that

$$\lim_{x\to\infty}\left(L_x(w)-x^{-w}L_x(0)-\frac{4\pi w x^{3-w}\delta}{3(3-w)}\right)=L(w). \tag{2.11}$$

Since this is our main result the proof of the theorem has been reduced to the proof of the lemma. The proof of the lemma relies on standard techniques in analytic number theory; we sketch the ideas.

The integrals along the upper and lower infinite vertical segments of α are easily bounded by noting that $|L(s)|\leqslant|L(c)|$ and $(s(s-w))^{-1}=\mathrm{O}(t^{-2})$; the contributions from these segments are $\mathrm{O}(x^cT^{-1})$.

The integral along the upper and lower horizontal segments can be bounded by using Stirling's formula and the Phragmén-Lindelöf theorem to derive (see, e.g., Ivic 1985, p 25)

$$|L(\sigma+\mathrm{i}t)|=\mathrm{O}(t^{c-3/2}) \qquad 3-c<\sigma<c. \tag{2.12}$$

It is then easy to show that the integral along these segments is $\mathrm{O}(x^cT^{c-7/2})$.

In order for all of the error terms to be small it is necessary to take c to satisfy $3<c<7/2$ and $T=x^{7/(7-2c)}$.

The integral along the finite vertical segment of α is more interesting. Change variables by replacing s by $3-s$ in the integral on the upper part of that segment; use the functional equation to get (a non-zero constant times):

$$\int_c^{c+\mathrm{i}T}\frac{\pi^{-s}\Gamma(s/2)\bar{L}(s)x^{3-s}}{\Gamma[(3-s)/2](s-3)(s+w-3)}\,\mathrm{d}s. \tag{2.13}$$

By using the absolute convergence of the series for $\bar{L}(s)$ on the line $\mathrm{Re}(s)=c>3$, and using Stirling's formula to show that higher-order terms can be ignored, one finds that it suffices to bound

$$I=x^{3-c}\sum_{v\in \boldsymbol{Z}^3, v\neq d}|v-d|^{-c}\int_{t_0}^{T}t^{c-7/2}\,\mathrm{e}^{\mathrm{i}f(t)}\,\mathrm{d}t \tag{2.14}$$

where

$$f(t)=t\log(t)-t+t\log(2\pi x|v-d|) \tag{2.15}$$

and where t_0 is an arbitrary constant.

This oscillatory integral can be bounded by the method of stationary phase (or 'saddle point') method. To make this rigorous we need two elementary estimates on exponential integrals (see Titschmarsh 1951, ch IV, or Ivic 1985, p 56). Suppose that $g(x)$ is a positive monotonic function such that $|g(x)|\leqslant G$ for $x\in[a,b]$. Let

$$I(f,g)=\int_a^b g(x)\,\mathrm{e}^{\mathrm{i}f(x)}\,\mathrm{d}x. \tag{2.16}$$

The two results in question are as follows.

(*A*) If f' is monotonic and $|f'(x)|>m$ then $|I(f,g)|<4G/m$.

(*B*) If f is twice differentiable and $|f''(x)|>m$ then $|I(f,g)|<8G/\sqrt{m}$. We will apply these facts to bound the integral in each term in the sum for I in (2.14). Note that $f'(t)=\log(t)-\log(2\pi x|v-d|)$ and $f''(t)=1/t$; the unique critical point of f is at $t_1=2\pi x|v-d|$.

If $T < t_1/2$, i.e. v is large enough so that $|v-d| \geq T/\pi x$, then result (A) says that the integral is bounded by a constant that is independent of v and x.

On the other hand for v small, i.e $|v-d| < T/\pi x$, the integral is bounded outside the interval $[t_1/2, 2t_1]$ as above by result (A), and bounded inside the interval by the inequality

$$\left|\int_{t_{1/2}}^{2t_1} t^{c-7/2}\,\mathrm{e}^{\mathrm{i}f(t)}\,\mathrm{d}t\right| \leq 8(\pi x|v-d|)^{c-7/2}\sqrt{4\pi x|v-d|} = \mathrm{O}(x^{c-3}|v-d|^{c-3}) \qquad (2.17)$$

which is a consequence of result (B).

All in all we find that the expression I in (2.14) is bounded by a constant times

$$\sum_{|v-d|<T/(\pi x)} |v-d|^{-3} + \text{a bounded function of } x. \qquad (2.18)$$

It is a standard fact that this sum, which is analogous to the sum $\Sigma_{n<x} n^{-1}$, is bounded by a constant times $\log(T/x) = \mathrm{O}(\log(x))$, so that the contour integral in question is clearly $\mathrm{O}(x^{\varepsilon})$ for all positive ε. (Alternatively, replacing summation over a sphere with summation over a larger cube leads to an elementary estimate that shows that the sum is $\mathrm{O}(x^{\varepsilon})$.) This finishes the estimation of all of the terms in the contour integral (2.10) and, by earlier remarks, finishes the proof of the lemma and the theorem.

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