Some logarithmic lattice sums

1995 J. Phys. A: Math. Gen. 28 6999

(http://iopscience.iop.org/0305-4470/28/23/037)

J. Phys. A: Math. Gen. 28 (1995) 6999–7009. Printed in the UK

Some logarithmic lattice sums

R Shail

Department of Mathematical and Computing Sciences, University of Surrey, Guildford, Surrey GU2 5XH, UK

Received 16 February 1995

Abstract. In this paper we consider certain lattice sums which arise when a system of line charges set in a compensating jelly of opposite charge interact via the two-dimensional logarithmic potential. A lattice-limit discontinuity phenomenon, similar to that discovered by Borwein *et al* in the three-dimensional case, is explored and a high-precision asymptotic method is described for the numerical computation of two-dimensional lattice limits.

1. Introduction

In two recent papers (Borwein *et al* 1988, 1989), hereafter referred to as A and B, some problems involving the calculation of certain limits of lattice sums were considered. These 'lattice limits' arose originally from the Wigner (1934) model of a metal in which an electron gas is bathed in a compensating 'jelly' of positive charge, the whole being electrically neutral. For a given infinitely extended lattice of electrons a quantity of interest is the energy of one electron in the electrostatic field of the others and the jelly.

Suppose that the electrons are placed at the lattice points (m, n, p). The interaction energy of the electron at the origin is (in suitable units)

$$U = \Sigma'(m^2+n^2+p^2)^{-\frac{1}{2}} - \int (x^2+y^2+z^2)^{-\frac{1}{2}}\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z \tag{1}$$

where the summation is over all integer triples (m, n, p), the prime denoting the omission of (0,0,0), and the integral is taken over all space. Unfortunately, the evaluation of U is made difficult by the fact that both the sum and the integral are divergent!

The 'classical' method of evaluation of U (Coldwell-Horsfall and Maradudin 1960, Bonsall and Maradudin 1977) uses mathematically dubious transformations, but in the spirit of renormalization, it yields finite results. The rigorous approach of Borwein *et al* in A and B arose from the observation that the multiple series

$$F(s) = \Sigma'(m^2+n^2+p^2)^{-s}$$

is convergent for $\operatorname{Re} s > \frac{1}{2}$ and that the value of (1) is obtained from the analytic continuation of $F(s)$ into the region $\operatorname{Re} s \leqslant \frac{1}{2}$. Thus not only were the results of Coldwell-Horsfall and Maradudin reproduced in a relatively simple manner, but also an intriguing discontinuity was discovered, namely that U and

$$\lim_{s\to\frac{1}{2}+}\left(\Sigma'(m^2+n^2+p^2)^{-s} - \int (x^2+y^2+z^2)^{-s}\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\right) \tag{2}$$

were unequal. Physically, two different limiting processes are involved. In (1) the law of electrostatic interaction is the Coulomb inverse square law, and the limiting process is that of extending a finite lattice to infinity in all directions. However, (2) uses an inverse sth power law and an interaction energy is derived in the limiting case of this law becoming the Coulomb law, i.e. $s \to \frac{1}{2}$. It was pointed out in B that, despite this type of discontinuity, the relative stability of lattices of different geometries remains the same whichever limiting process is used, but energy separations differ.

The two-dimensional version of (1),

$$V = \Sigma'(m^2+n^2)^{-1/2} - \int (x^2+y^2)^{-1/2}\,\mathrm{d}x\,\mathrm{d}y \tag{3}$$

has been used by Bonsall and Maradudin (1977) in energy calculations for two-dimensional crystals. However, as shown in A, the quantity

$$V(s) = \Sigma'(m^2+n^2)^{-s} - \int (x^2+y^2)^{-s}\,\mathrm{d}x\,\mathrm{d}y \tag{4}$$

is continuous at $s = \frac{1}{2}$. An interesting question, therefore, is whether there is a two-dimensional lattice sum with the discontinuity property noted for (2). In this paper we answer this question in the affirmative and give some further calculations of lattice limits. Briefly, the discontinuity is found if account is taken of the fact for a two-dimensional lattice of *line charges*, the correct potential to use is the logarithmic potential rather than the inverse-distance potential, i.e. we need to use the appropriate Green function for the two-dimensional Laplace equation.

2. The logarithmic lattice limit

An essential ingredient in the evaluation of (2) is the interpretation of U as a suitable limit. Preserving electrical neutrality at all stages, a possible definition of the interaction energy is

$$U = \lim_{N\to\infty} \sigma_N(1/2)$$

where

$$\sigma_N(1/2) = \sum_{m=-N}^{N}\sum_{n=-N}^{N}\sum_{p=-N}^{N}{}' (m^2+n^2+p^2)^{-1/2} - \int_{-(N+1/2)}^{N+1/2}\int_{-(N+1/2)}^{N+1/2}\int_{-(N+1/2)}^{N+1/2} (x^2+y^2+z^2)^{-1/2}\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z.$$

In the two-dimensional case define, for $\operatorname{Re} s > 0$,

$$\sigma_N(s) = \frac{1}{s}\left\{ \sum_{m=-N}^{N}\sum_{n=-N}^{N}{}' ((am^2+2bmn+cn^2)^{-s}-1) - \int_{-(N+1/2)}^{N+1/2}\int_{-(N+1/2)}^{N+1/2} ((ax^2+2bxy+cy^2)^{-s}-1)\,\mathrm{d}x\,\mathrm{d}y \right\} \tag{5}$$

$$= \frac{1}{s}\left\{ \sum_{m=-N}^{N}\sum_{n=-N}^{N}{}' (am^2+2bmn+cn^2)^{-s} - \int_{-(N+1/2)}^{N+1/2}\int_{-(N+1/2)}^{N+1/2} (ax^2+2bxy+cy^2)^{-s}\,\mathrm{d}x\,\mathrm{d}y + 1 \right\} \tag{6}$$

where $a > 0$ and $b^2 - ac < 0$, to ensure the positive definiteness of the quadratic denominators. Then both the double series and integral in (5) and (6) are divergent as $N \to \infty$ for $0 < \operatorname{Re} s < 1$. Also,

$$\sigma_N(0) \equiv \lim_{s\to 0+} \sigma_N(s) = -\sum_{m=-N}^{N}\sum_{n=-N}^{N}{}' \ln(am^2 + 2bmn + cn^2) + \int_{-(N+1/2)}^{N+1/2}\int_{-(N+1/2)}^{N+1/2} \ln(ax^2 + 2bxy + cy^2)\,\mathrm{d}x\,\mathrm{d}y \tag{7}$$

and when $a = 1, b = 0, c = 1$ we recover the physical line-charge interaction energy as $N \to \infty$.

Consider first the existence and evaluation of $\lim_{N\to\infty} \sigma_N(s)$ for $0 < \operatorname{Re} s < 1$; we subsequently relate $\lim_{s\to 0+} \lim_{N\to\infty} \sigma_N(s)$ to $\lim_{N\to\infty} \sigma_N(0)$. Following the procedures used in A and B, define

$$\delta_N(s) = \sigma_N(s) - \sigma_{N-1}(s) \tag{8}$$

an elementary calculation then shows that

$$\delta_N(s) = \frac{1}{s}\left\{2\sum_{n=-N}^{N}((an^2 + 2bnN + cN^2)^{-s} + (aN^2 + 2bNn + cn^2)^{-s}) - \frac{2}{N^{2s}}((a + 2b + c)^{-s} + (a - 2b + c)^{-s}) - \Delta_N\right\} \tag{9}$$

where

$$\Delta_N = \left(\int_{-(N+1/2)}^{N+1/2}\int_{-(N+1/2)}^{N+1/2} - \int_{-(N-1/2)}^{N-1/2}\int_{-(N-1/2)}^{N-1/2}\right)(ax^2 + 2bxy + cy^2)^{-s}\,\mathrm{d}x\,\mathrm{d}y. \tag{10}$$

The double integrals in (10) may be transformed by the substitutions $x = (N \pm 1/2)X$ and $y = (N \pm 1/2)Y$ as appropriate, and the resulting integrals over the unit square converted to polar coordinates (r, θ). The radial integration can be carried out, and the substitution $t = \tan\theta$ then shows that

$$\Delta_N = \frac{1}{(1-s)}\{(N + 1/2)^{2(1-s)} - (N - 1/2)^{2(1-s)}\} - C(s) \tag{11}$$

where

$$C(s) = \int_{-1}^{1}\{(a + 2bt + ct^2)^{-s} + (at^2 + 2bt + c)^{-s}\}\,\mathrm{d}t. \tag{12}$$

Observe that, whilst for fixed N the integrals in (10) are convergent only for $0 < \operatorname{Re} s < 1$, $C(s)$ is an everywhere analytic function of s.

We next estimate $\delta_N(s)$ for large N; applying the Euler–Maclaurin expansion to the summation in (9) (using a suitable computer algebra program written in MAPLE), combined with an asymptotic expansion of (11), shows that for $0 < \operatorname{Re} s < 1$

$$\delta_N(s) = \frac{1}{6N^{2s+1}}\{(1 - 2s)C(s) - 2((a + 2b + c)^{-s} + (a - 2b + c)^{-s})\} + W_N(s) \tag{13}$$

where $W_N(s) = O(N^{-2s-3})$ as $N \to \infty$. Hence,

$$\sigma_p(s) = \sum_{N=1}^{p} \delta_N(s) + \sigma_0(s) = \tfrac{1}{6}\{(1 - 2s)C(s) - 2((a + 2b + c)^{-s} + (a - 2b + c)^{-s})\}$$

$$\times \sum_{N=1}^{p} N^{-2s-1} + \sigma_0(s) + \sum_{N=1}^{p} W_N(s) \tag{14}$$

and for $0 < \mathrm{Re}\, s < 1$,

$$U(a,b,c;s) \equiv \lim_{p\to\infty} \sigma_p(s) = \frac{1}{6}\{(1-2s)C(s) - 2((a+2b+c)^{-s} + (a-2b+c)^{-s})\} \times \zeta(2s+1) + \sigma_0(s) + W(s) \tag{15}$$

where $W(s)$ is an analytic function of s and, from (5) $\sigma_0(s)$ is found as

$$\sigma_0(s) = \frac{1}{s}\left\{1 - \frac{2^{2s-2}}{1-s}C(s)\right\}. \tag{16}$$

The existence of the lattice limit $U(a,b,c;s)$ has now been established for $0 < \mathrm{Re}\, s < 1$. Further, arguments identical to those in A and B show that the value of $U(a,b,c;s)$ in (15) is found for $0 < \mathrm{Re}\, s < 1$ as

$$U(a,b,c;s) = \frac{1}{s}\,(S(a,b,c;s) + 1) \tag{17}$$

where the function $S(a,b,c;s)$ is defined for $\mathrm{Re}\, s > 1$ by the convergent double sum

$$\sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty}{}' (am^2 + 2bmn + cn^2)^{-s} \tag{18}$$

and for $0 < \mathrm{Re}\, s < 1$ by the appropriate analytic continuation of (18).

We next examine $\lim_{s\to 0+} U(s)$, where for brevity we omit the arguments (a,b,c). An elementary but somewhat lengthy calculation shows that

$$U(s) = \tfrac{1}{6} s\, \zeta(2s+1)\left\{ -8 - \int_{-1}^{1} (\ln(a+2bt+ct^2) + \ln(at^2+2bt+c))\,\mathrm{d}t \right.$$
$$\left. +2(\ln(a+2b+c) + \ln(a-2b+c) + \mathrm{O}(s) \right\} + \sigma_0(s) + W(s)$$
$$\text{as } s \to 0+. \tag{19}$$

From (16), $\lim_{s\to 0+} \sigma_0(s) = \alpha$, say, exists and is finite; thus using the result that $\lim_{s\to 0+} s\,\zeta(2s+1) = \frac{1}{2}$, it follows that the double limit

$$U(0+) \equiv \lim_{s\to 0+} U(s) = \lim_{s\to 0+} \lim_{p\to\infty} \sigma_p(s)$$
$$= -\tfrac{2}{3} - \tfrac{1}{12}\int_{-1}^{1} (\ln(a+2bt+ct^2) + \ln(at^2+2bt+c))\,\mathrm{d}t$$
$$+\tfrac{1}{6}(\ln(a+2b+c) + \ln(a-2b+c)) + W(0) + \alpha. \tag{20}$$

In order to calculate the double limit of (20) in the reverse order, we return to (12) and (13) from which it is immediately apparent that $\delta_N(0) = W_N(0)$. Thus

$$U(0) \equiv \lim_{p\to\infty} \lim_{s\to 0+} \sigma_p(s) = \sum_{p=1}^{\infty} W_p(0) + \sigma_0(0)$$
$$= W(0) + \alpha. \tag{21}$$

The required discontinuity result is now obtained directly from (20) and (21) as

$$U(0+) - U(0) = \lim_{s\to 0+} \lim_{p\to\infty} \sigma_p(s) - \lim_{p\to\infty} \lim_{s\to 0+} \sigma_p(s)$$
$$= -\tfrac{2}{3} - \tfrac{1}{12}\int_{-1}^{1} (\ln(a+2bt+ct^2) + \ln(at^2+2bt+c))\,\mathrm{d}t$$
$$+\tfrac{1}{6}\,(\ln(a+2b+c) + \ln(a-2b+c))\,. \tag{22}$$

Writing $\Delta U = \Delta U(a, b, c)$ for the discontinuity defined by (22), the integration can be effected with the result that

$$\Delta U = \frac{b}{12}\left(\frac{1}{a}+\frac{1}{c}\right)\ln\left(\frac{a-2b+c}{a+2b+c}\right) - \frac{D}{6a}\left\{\tan^{-1}\left(\frac{a+b}{D}\right)+\tan^{-1}\left(\frac{a-b}{D}\right)\right\}$$
$$-\frac{D}{6c}\left\{\tan^{-1}\left(\frac{c+b}{D}\right)+\tan^{-1}\left(\frac{c-b}{D}\right)\right\} \qquad (23)$$

where $D = \sqrt{ac-b^2}$. In the special case $a = c = 1$, $b = 0$, (23) reduces to $-\pi/6$, which *coincidentally is the value of the discontinuity in the three-dimensional Coulomb potential* case!

3. Some numerical results

Consider first the evaluation for $0 < \mathrm{Re}\, s < 1$ of $U(s)$, which is expressed in (17) in terms of the function $S(a, b, c; s)$, defined for $\mathrm{Re}\, s > 1$ by (18). Double sums of the form (18) have been extensively studied by, for example, Glasser (1973), Zucker and Robertson (1975, 1976a, b, 1984), with the object of determining which sums can be expressed as sums of products of Dirichlet L-functions. When this is possible, these authors say that the double series can be solved. For example, when $a = c = 1$, $b = 0$, we have that

$$S(1, 0, 1; s) = 4\zeta(s)L_{-4}(s) \qquad (24)$$

where for $\mathrm{Re}\, s > 1$

$$\zeta(s) = \sum_{n=0}^{\infty}(n+1)^{-s}$$

and for $\mathrm{Re}\, s > 0$.

$$L_{-4}(s) = \sum_{n=0}^{\infty}(-1)^n(2n+1)^{-s}.$$

Thus, for $0 < \mathrm{Re}\, s < 1$,

$$U(1, 0, 1; s) = \frac{1}{s}(4\zeta(s)L_{-4}(s) + 1) \qquad (25)$$

wherein the appropriate analytic continuation of $\zeta(s)$ into $0 < \mathrm{Re}\, s < 1$ must be used. The limit of (25) as $s \to 0+$, $U(1, 0, 1; 0+)$, can be determined and the discontinuity formula (23) used to evaluate $U(1, 0, 1; 0)$, which from (7) is the physical two-dimensional line-charge interaction energy. However, before doing this we set our computations in a somewhat wider context and note some definitions and properties of the L-functions.

The Dirichlet L-functions $L_{\pm k}(s)$ are defined by

$$L_{\pm k}(s) = \sum_{n=1}^{\infty}\chi_k(n)n^{-s} \qquad (26)$$

where for a positive integer k, $\chi_k(n)$ is a number theoretic character modulo k, with the defining properties

$$\chi_k(1) = 1 \qquad \chi_k(n) = \chi_k(n+k)$$
$$\chi_k(m)\chi_k(n) = \chi_k(mn) \qquad \text{for all } m, n$$
$$\chi_k(n) = 0 \qquad \text{if } (k, n) \neq 1.$$

Thus non-zero characters take only the values ± 1 and the subscript $\pm k$ is used in (26) accordingly as $\chi_k(k-1) = \mp 1$ (Zucker and Robertson 1976a). All the series for $L_{\pm k}(s)$ converge for $\mathrm{Re}\, s > 0$ except $L_1(s)$, the Riemann zeta function, which converges for $\mathrm{Re}\, s > 1$. The Dirichlet functions also satisfy the functional equations (Landau 1909)

$$L_{-k}(s) = 2^s \pi^{s-1} k^{-s+\frac{1}{2}} \cos(s\pi/2) L_{-k}(1-s)\Gamma(1-s) \tag{27}$$

$$L_{+k}(s) = 2^s \pi^{s-1} k^{-s+\frac{1}{2}} \sin(s\pi/2) L_{+k}(1-s)\Gamma(1-s) \tag{28}$$

which can be used for analytic continuation into $\mathrm{Re}\, s \leqslant 0$. We also record here a useful integral representation for the Dirichlet functions (Zucker and Robertson 1976a), namely that for $\mathrm{Re}\, s > 0$,

$$L_{\pm k}(s)\Gamma(s) = \int_0^\infty \frac{u^{s-1}}{1-\mathrm{e}^{-ku}} \left(\sum_{n=1}^{k} \chi_k(n) \mathrm{e}^{-nu} \right) \mathrm{d}u. \tag{29}$$

Zucker and Robertson (1976a) deduce from (29) a further representation for $L_{\pm k}(s)$, valid for all s:

$$L_{\pm k}(s) = \frac{\Gamma(1-s)}{2\pi i} \int_C \frac{(-w)^{s-1}}{1-\mathrm{e}^{-kw}} \left(\sum_{n=1}^{k} \chi_k(n) \mathrm{e}^{-nw} \right) \mathrm{d}w \tag{30}$$

where C is a contour in the complex w-plane which starts from $+\infty$, encircles the origin once in the counter-clockwise direction and returns to $-\infty$ without enclosing any of the poles $2\pi n i/k$, $n = \pm 1, \pm 2, \ldots$ of the integrand. A particularly simple formula for $L_{\pm k}(0)$ follows from (30); with $s = 0$ direct evaluation of the contour integral in terms of the residue at the pole $w = 0$ gives

$$L_{\pm k}(0) = \sum_{n=1}^{k} \chi_k(n) \left(\frac{1}{2} - \frac{n}{k} \right). \tag{31}$$

We now return to (25) and determine $U(1, 0, 1; 0+)$ and $U(1, 0, 1; 0)$. From (25),

$$\begin{aligned} U(1,0,1;0+) &= \lim_{s \to 0+} \frac{1}{s} \{4\zeta(s) L_{-4}(s) + 1\} \\ &= 4 \lim_{s \to 0+} \frac{d}{ds} \zeta(s) L_{-4}(s) \\ &= 4\zeta'(0) L_{-4}(0) + 4\zeta(0) L'_{-4}(0). \end{aligned} \tag{32}$$

It is well known that $\zeta(0) = -\frac{1}{2}$ and $\zeta'(0) = -\ln(2\pi)/2$. Further, $L_{-4}(0) = \frac{1}{2}$ follows from (31) and it only remains to calculate $L'_{-4}(0)$. In terms of the generalized zeta function $\zeta(s, a)$, where

$$\zeta(s, a) = \sum_{n=0}^{\infty} \frac{1}{(a+n)^s} \qquad \mathrm{Re}(s) > 1$$

$L_{-4}(s)$ can be expressed as

$$L_{-4}(s) = \frac{1}{4^s} (\zeta(s, 1/4) - \zeta(s, 3/4)). \tag{33}$$

It follows that

$$\begin{aligned} L'_{-4}(0) &= -\ln 4(\zeta(0, 1/4) - \zeta(0, 3/4)) + \ln\Gamma(1/4) - \ln\Gamma(3/4) \\ &= \ln(\Gamma(1/4)/2\Gamma(3/4)) \end{aligned} \tag{34}$$

using the results (Gradshteyn and Ryzhik 1980)

$$\zeta(0, a) = \tfrac{1}{2} - a \qquad \zeta'(0, a) = \ln\Gamma(a) - \tfrac{1}{2}\ln 2\pi.$$

Equations (32) and (34) now provide the closed-form result that

$$U(1,0,1\colon 0+) = -\ln 2\pi - 2\ln(\Gamma(1/4)/2\Gamma(3/4)) = -2.621\,065\,851\,823\,019\,036\,50. \tag{35}$$

Further, using the discontinuity formula (23), the physical two-dimensional line-charge interaction energy is

$$U(1,0,1;0) = U(1,0,1;0+) + \tfrac{1}{6}\pi = -2.097\,467\,076\,224\,720\,163\,43. \tag{36}$$

An entertaining by-product of this analysis provides the sum in closed form of a very slowly convergent series. Suppose that $L'_{-4}(0)$ is evaluated by differentiating (28) with respect to s and setting $s = 0$. Then using the value (34) for $L'_{-4}(0)$, we find that

$$\ln\left(\frac{\Gamma(1/4)}{2\Gamma(3/4)}\right) = \frac{2}{\pi}L_{-4}(1)\Gamma(1) - \frac{2}{\pi}(\Gamma'(1)L_{-4}(1) + \Gamma(1)L'_{-4}(1)). \tag{37}$$

Now $\Gamma'(1) = -\gamma$, where γ is Euler's constant, $L_{-4}(1) = \pi/4$ and a form for $L'_{-4}(1)$ follows by differentiating the defining infinite series with respect to s and setting $s = 1$. After some manipulation we obtain the sum

$$\sum_{n=0}^{\infty}(-1)^{n+1}\frac{\ln(2n+1)}{2n+1} = \frac{\pi\gamma}{4} + \frac{\pi}{4}\ln\left(\frac{\pi}{2}\right) - \frac{\pi}{2}\ln\left(\frac{\Gamma(1/4)}{2\Gamma(3/4)}\right) = 0.192\,901\,316\,796\,912\,429\,36 \tag{38}$$

correct to 20 decimal places. The sum of the series can be estimated numerically by other methods; for example, repeated Shanks transformations on the first 20 partial sums produces the sum correct to 15 decimal places, but increasing the number of partial sums fails to improve on this.

As a second example involving a solvable sum, consider the case $a = 2$, $b = \frac{1}{2}$, $c = 7$. According to Zucker and Robertson (1984), for $\operatorname{Re} s > 1$

$$S(2,1/2,7;s) = \tfrac{1}{2}(\zeta(s)L_{-55}(s) - L_5(s)L_{-11}(s)). \tag{39}$$

Thus, for $0 < \operatorname{Re} s < 1$,

$$U(2,1/2,7;s) = \frac{1}{2s}(\zeta(s)L_{-55}(s) - L_{-5}(s)L_{-11}(s) + 2) \tag{40}$$

and

$$U(2,1/2,7;0+) = \lim_{s\to 0+} U(2,1/2,7;s) = \tfrac{1}{2}(\zeta'(0)L_{-55}(0) + \zeta(0)L'_{-55}(0) - L'_5(0)L_{-11}(0) - L_5(0)L'_{-11}(0)). \tag{41}$$

The values of $L_5(0)$, $L_{-11}(0)$ and $L_{-55}(0)$ follow from (31) as 0, 1 and 4. Further, $L'_5(0)$ is found as $\ln((1+\sqrt{5})/2)$ by differentiating (28) with respect to s and putting $s = 0$. In principle $L'_{-55}(0)$ can be evaluated in closed form as in the previous example by expressing $L_{-55}(s)$ in terms of generalized zeta functions and carrying out the differentiation. However, the high value of k ($= 55$) makes this a daunting task, and a numerical value is generated more rapidly by using (27). Thus from (27),

$$L'_{-55}(0) = 4\ln(2\pi/55) - \frac{\sqrt{55}}{\pi}\frac{\mathrm{d}}{\mathrm{d}s}(\Gamma(s)L_{-55}(s))\bigg|_{s=1}$$

and the final term can be found from (29) by differentiation with respect to s and numerical integration. (The calculation of the character sum and simplification of the integrand are conveniently performed using the number-theoretic capabilities of MAPLE; the numerator and denominator of the integrand feature polynomials in e^{-x} of degrees 38 and 40 respectively!) The final result is that

$$U(2, 1/2, 7; 0+) = -1.041\,050\,728\,996\,859\,008\,3 \tag{42}$$

to 20 significant figures. The discontinuity formula (23) then gives

$$U(2, 1/2, 7; 0) = -0.541\,933\,195\,368\,360\,426\,20. \tag{43}$$

As a final solvable example we mention the case $a = 1$, $b = \frac{1}{2}$, $c = 1$; in the physical line-charge situation this corresponds to the configuration in which the line charges are placed at the vertices of an equilateral triangular lattice with unit spacing between the lattice points. Here

$$S(1, 1/2, 1; s) = 6\zeta(s)L_{-3}(s)$$

and for $0 < \operatorname{Re} s < 1$

$$U(1.1/2.1; s) = \frac{1}{s}(6\zeta(s)L_{-3}(s) + 1).$$

The computations now follow closely the derivations of (35) and (36), with the results for the interaction energy that

$$\begin{aligned} U(1, 1/2, 1; 0+) &= -\ln 2\pi - 3\ln\left(\Gamma(1/3)/3^{\frac{1}{3}}\Gamma(2/3)\right) \\ &= -2.786\,075\,893\,081\,966\,293\,7 \end{aligned} \tag{44}$$

and

$$U(1, 1/2, 1; 0) = -2.241\,075\,027\,967\,736\,023\,5. \tag{45}$$

It is possible to generate many other examples using the results of Zucker and Robertson (1984), but it is of interest to consider the problem of determining $U(a, b, c; 0+)$ and $U(a, b, c; 0)$ when the double sum $S(a, b, c; s)$, $\operatorname{Re} s > 1$, is *not* solvable. In the absence of a sum in terms of products of Dirichlet series, the analytic continuation technique can no longer be used. One approach to the evaluation of $U(a, b, c; s)$, $0 < \operatorname{Re} s < 1$, is to use the Euler–Maclaurin sum formula as outlined in section 2; however, this is not a viable method of determining $U(a, b, c; 0+)$ and hence we concentrate on $U(a, b, c; 0)$. We show how to evaluate this to high accuracy by the Euler–Maclaurin method, and $U(a, b, c; 0+)$ then follows from the discontinuity formula (23).

To compute $U(a, b, c; 0)$ we return to (9) and consider

$$\delta_N(0) \equiv \lim_{s\to 0+} \delta_N(s)$$

the limiting process produces the sums

$$\sum_{n=-N}^{N} \ln(an^2 + 2bnN + cN^2)$$

and

$$\sum_{n=-N}^{N} \ln(aN^2 + 2bNn + cn^2)$$

both of which can be expanded asymptotically for large N (using MAPLE) by the Euler–Maclaurin sum formula. After considerable reduction (including the cancellation of integrals arising from (10)) it is found that

$$\delta_N(0) = \sum_{k=1}^{5} \frac{p_{2k+1}(a,b,c)}{(a-2b+c)^{2k}(a+2b+c)^{2k}N^{2k+1}} + \mathrm{O}(N^{-13}) \tag{46}$$

where, for example,

$$p_3(a,b,c) = -\frac{1}{180}(7a^4 + 112b^4 + 7c^4 + 4a^3c + 4ac^3 - 8a^2b^2 \\ -8b^2c^2 - 6c^2a^2 - 112ab^2c). \tag{47}$$

The remaining polynomial p-functions are too long to quote, but it has been observed that $p_{2k+1}(a,b,c)$ contains $(2k+1)^2$ terms, each of total degree $4k$ in a, b, c!

Using (8) and (21),

$$\begin{aligned} U(0) &\equiv \lim_{p\to\infty} \sigma_p(0) \\ &= \sigma_j(0) + \sum_{N=j+1}^{\infty} \delta_N(0). \end{aligned} \tag{48}$$

By choosing j to be sufficiently large, the sum in (48) can be estimated very accurately using (46) and

$$\sum_{N=j+1}^{\infty} N^{-2k-1} = \zeta(2k+1) - \sum_{N=1}^{j} N^{-2k-1}.$$

Further, $\sigma_j(0)$ is given by (7), and carrying out the integration we find that

$$\sigma_j(0) = 2\sum_{n=0}^{j}\sum_{m=0}^{j}{}' \ln\{(an^2+cm^2)^2 - 4b^2m^2n^2\} \\ -2j\ln(ac) - 8\sum_{n=1}^{j}\ln n - 8(j+\tfrac{1}{2})^2\ln(j+\tfrac{1}{2}) - (j+\tfrac{1}{2})^2 Q \tag{49}$$

where

$$Q = \frac{1}{ac}\left\{2D\left(a\tan^{-1}\left(\frac{c+b}{D}\right) + a\tan^{-1}\left(\frac{c-b}{D}\right) + c\tan^{-1}\left(\frac{a+b}{D}\right)\right.\right. \\ \left. +c\tan^{-1}\left(\frac{a-b}{D}\right)\right) + (bc+2ca+ab)\ln(a+2b+c) \\ \left. -(bc-2ca+ab)\ln(a-2b+c) - 12ac\right\}. \tag{50}$$

All the elements for the evaluation of $U(0)$ in (48) are now available.

As an initial test of the effectiveness of this approach, $U(1,0,1;0)$ and $U(2,1/2,7;0)$ were re-evaluated. With $j = 22$, (36) was reproduced to all the 20 decimal places shown, and (43) was found correct to 18 decimal places. Thus one has considerable confidence that the asymptotic expansion (46) contains sufficient terms (more of course can be computer-generated if necessary). We now give some illustrative results which cannot be found from the analytic continuation of a solvable double sum. The parameters used are chosen somewhat arbitrarily and no claim is made of any physical significance.

For $a = 1$, $b = 1/2$, $c = \sqrt{3}$ with $j = 20$

$$U(1, 1/2, \sqrt{3}; 0) = -1.874\,676\,749\,791\,522\,382\,6$$

$$U(1, 1/2, \sqrt{3}; 0+) = -2.402\,805\,468\,097\,055\,706\,3.$$

For $a = \sqrt{3}$, $b = \sqrt{5}$, $c = \sqrt{11}$ with $j = 30$

$$U(\sqrt{3}, \sqrt{5}, \sqrt{11}; 0) = -2.030\,638\,221\,974\,750$$
$$U(\sqrt{3}, \sqrt{5}, \sqrt{11}; 0+) = -2.658\,940\,830\,267\,172.$$

For $a = 1$, $b = 2$, $c = 70$ with $j = 26$

$$U(1, 2, 70; 0) = 5.220\,217\,001$$
$$U(1, 2, 70; 0+) = 4.831\,718\,984.$$

For $a = 1.1$, $b = 1$, $c = 1$ with $j = 30$

$$U(1.1, 1, 1; 0) = -1.918\,715\,326\,216\,7$$
$$U(1.1, 1, 1; 0+) = -2.666\,809\,794\,483\,8.$$

All these results are correct to the last figure shown, but the same accuracy is not attainable in every case from the asymptotic expansion (46).

4. Conclusion

In this paper we have examined a further example of a lattice-limit discontinuity, a phenomenon first discussed in A. The calculations of this paper pertain to a two-dimensional lattice system of negative line charges set in a jelly of positive line charges. The interaction energy of the line charge at the origin is calculated directly in the limit of an infinite extension of a system of line charges, each producing a logarithmic potential (in fact a generalization of this is considered in (20)), and also by considering the 'energy' function of a suitable infinitely extended system with the logarithmic potential obtained by a limiting process applied to this 'energy' function. The results are shown to be different, and the magnitude of the consequent discontinuity is calculated in a general setting. Thus we have found in two dimensions the analogue of results for three dimensions given in B.

The basic discontinuity result can in fact be extended to d dimensions, $d \geqslant 3$; although the most general case is still to be discussed and the appropriate discontinuity calculated, the following result is conjectured. Let

$$\sigma_N(s) = \sum{}'(n_1^2 + n_2^2 + \cdots + n_d^2)^{-s} - \int (x_1^2 + x_2^2 + \cdots + x_d^2)^{-s}\,\mathrm{d}x_1\,\mathrm{d}x_2 \ldots \mathrm{d}x_d$$

where each summation is from $-N$ to N and each integration is from $-N - \frac{1}{2}$ to $N + \frac{1}{2}$. Then $\lim_{N\to\infty} \sigma_N(s)$ exists for $s = \frac{1}{2}d - 1$ and for $\frac{1}{2}d - 1 < \operatorname{Re} s < \frac{1}{2}d$ but

$$\lim_{N\to\infty} \sigma_N(\tfrac{1}{2}d - 1) \neq \lim_{s\to\frac{1}{2}d-1} \lim_{N\to\infty} \sigma_N(s). \tag{51}$$

This discontinuity has been verified in the case $d = 4$.

Finally should we really be surprised at the existence of these lattice-limit discontinuities? It seems that the answer to this question is no since it happens in a simple *one-dimensional* situation! Define $\gamma_N(s)$ for $s \neq 1$ by

$$\begin{aligned}\gamma_N(s) &= \sum_{n=1}^{N} n^{-s} - \int_1^N t^{-s}\mathrm{d}t \\ &= \left(\sum_{n=1}^{N} n^{-s} - \frac{N^{1-s}}{1-s}\right) + \frac{1}{1-s}.\end{aligned}$$

Then for $0 < s < 1$,

$$\lim_{N\to\infty} \gamma_N(s) = \zeta(s) + \frac{1}{1-s}$$

and

$$\lim_{s\to 0+} \lim_{N\to\infty} \gamma_N(s) = \zeta(0) + 1 = \tfrac{1}{2}.$$

However,

$$\gamma_N(0) = N - (N-1) = 1$$

and

$$\lim_{N\to\infty} \gamma_N(0) = 1.$$

Thus

$$\lim_{N\to\infty} \lim_{s\to 0+} \gamma_N(s) \neq \lim_{s\to 0+} \lim_{N\to\infty} \gamma_N(s)$$

giving a discontinuity of magnitude $\frac{1}{2}$.

Acknowledgments

Some of the results described in this paper were presented at a conference held in Dublin in December 1991 to mark the retirement of Professor Peter Chadwick FRS. This paper is dedicated to him in appreciation of a friendship going back many years. I also thank a referee for a suggestion which materially improved some results.

References

Bonsall L and Maradudin A A 1977 *Phys. Rev.* B **15** 1959–73
Borwein D, Borwein J M, Shail R and Zucker I J 1988 *J. Phys. A: Math. Gen.* **21** 1519–31
Borwein D, Borwein J M and Shail R 1989 *J. Math. Anal. Applics* **143** 126–37
Coldwell-Horsfall R A and Maradudin A A 1960 *J. Math. Phys.* **1** 395–404
Glasser M L 1973 *J. Math. Phys.* **14** 409–13
Gradshteyn I S and Ryzhik M 1980 *Table of Integrals, Series, and Products* (New York: Academic)
Landau E 1909 *Handbuch der Lehre von der Verteilung der Primzahlen* (Stuttgart: Teubner)
Wigner E P 1934 *Phys. Rev.* **46** 1002–11
Zucker I J and Robertson M M 1975 *J. Phys. A: Math. Gen.* **8** 874–61
——1976a *J. Phys. A: Math. Gen.* **9** 1207–14
——1976b *J. Phys. A: Math. Gen.* **9** 1215–25
——1984 *Proc Camb. Phil. Soc.* **95** 5–13