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Half-space electrostatic lattice sums

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Abstract. A new inversion formula analogous to the Jacobi theta function imaginary transformation for sums of the type $\Sigma_{l=0}^{\infty} \exp[-t(l+x)^2]$ is derived and used to find computable forms for the electrostatic energy of point charges and dipoles above the surface of an electrostatically neutral simple cubic lattice of charges and a simple cubic lattice of point dipoles.

1. Introduction

There is a large literature on the problem of calculating the electrostatic potential in an electrically neutral three-dimensionally infinite lattice of fixed point charges or dipoles (Ewald 1921, Born and Bradburn 1943, Glasser and Zucker 1977, Hoskins and Smith 1977). As written down, the lattice sums appear to diverge and some technique of forcing convergence must always be used. The cancellation of the divergences inherent in the problem is due to the electrical neutrality of the system. In order to investigate this cancellation (and to aid rapid computation of the sums) recourse is usually had to some inversion formula for turning slowly converging series into rapidly converging series. A typical case is the Jacobi theta function transformation

$$\sum_{l=-\infty}^{\infty} \exp[-t(l+x)^2] = \left(\frac{\pi}{t}\right)^{1/2} \sum_{l=-\infty}^{\infty} \exp[-(\pi^2 l^2/t) + 2l\pi \mathrm{i}x]. \tag{1.1}$$

We note that this sum runs from $-\infty$ to $+\infty$, reflecting the fact that the lattices for which these methods are used fill the whole of space.

The problem of the electrostatic potential above a half-space filled with an electrically neutral lattice of point charges or point dipoles is of considerable interest in many problems involving the interaction of charges and dipoles with surfaces. In this paper we develop a new method for handling these sums which is analogous to the methods of Born and Bradburn (1943), Zucker (1975) and Hoskins and Smith (1977). The lattices we study are simple cubic with unit spacing and with positive charges q at the lattice vertices and negative charges $-q$ placed at a vector $\boldsymbol{a} = (\alpha, \beta, \gamma)$ with respect to the vertices with α negative. The surface plane is the $(0, y, z)$ plane and a charge q_1 at $\boldsymbol{\rho} = (x, y, z)$ has a potential energy

$$\Phi_1(x, y, z) = \frac{qq_1}{4\pi\epsilon_0} \sum_{l=0}^{\infty} \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} (|\boldsymbol{R}_{lmn}(\boldsymbol{\rho})|^{-1} - |\boldsymbol{R}_{lmn}(\boldsymbol{\rho}+\boldsymbol{a})|^{-1}) \tag{1.2}$$

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where

$$\boldsymbol{R}_{lmn}(\boldsymbol{\rho}) = (l+x, m+y, n+z).$$

As we shall see, the sum in (1.2) is divergent, and convergence must be forced by some technique. A point dipole $\boldsymbol{\mu}$ at $\boldsymbol{\rho} = (x, y, z)$ has a potential energy

$$\Phi_2(x, y, z) = \frac{q\boldsymbol{\mu}}{4\pi\epsilon_0} \cdot \sum_{l=0}^{\infty} \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \left(\frac{\boldsymbol{R}_{lmn}(\boldsymbol{\rho})}{|\boldsymbol{R}_{lmn}(\boldsymbol{\rho})|^3} - \frac{\boldsymbol{R}_{lmn}(\boldsymbol{\rho}+\boldsymbol{a})}{|\boldsymbol{R}_{lmn}(\boldsymbol{\rho}+\boldsymbol{a})|^3} \right). \tag{1.3}$$

Above the surface of a cubic lattice of point dipoles $\boldsymbol{\mu}$, a charge q_1 at $\boldsymbol{\rho} = (x, y, z)$ has potential energy

$$\Phi_3(x, y, z) = \frac{q_1\boldsymbol{\mu}}{4\pi\epsilon_0} \cdot \left(\sum_{l=0}^{\infty} \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \frac{\boldsymbol{R}_{lmn}(\boldsymbol{\rho})}{|\boldsymbol{R}_{lmn}(\boldsymbol{\rho})|^3} \right) \tag{1.4}$$

and a dipole $\boldsymbol{\nu}$ at $\boldsymbol{\rho} = (x, y, z)$ has potential energy

$$\Phi_4(x, y, z) = \frac{\boldsymbol{\nu}}{4\pi\epsilon_0} \cdot \sum_{l=0}^{\infty} \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \left(\frac{\boldsymbol{\mu}}{|\boldsymbol{R}_{lmn}(\boldsymbol{\rho})|^3} - \frac{(\boldsymbol{R}_{lmn}(\boldsymbol{\rho}))(\boldsymbol{\mu} \cdot \boldsymbol{R}_{lmn}(\boldsymbol{\rho}))}{|R_{lmn}(\boldsymbol{\rho})|^5} \right). \tag{1.5}$$

The method introduced by Born and Bradburn (1943) and used later by others (e.g. Zucker 1975) for whole-space series is to consider sums of the form

$$\sum_{l=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} |\boldsymbol{R}_{lmn}(\boldsymbol{\rho})|^{-2S} \tag{1.6}$$

as an analytic function of S for $\mathrm{Re}(S) > 3/2$. Charge neutrality and other effects (Smith and Perram 1975) then allow analytic continuation to the required value of S. In this paper we shall concern ourselves solely with this process. As a result we obtain formulae for the potential energies which can be calculated by machine. We do not concern ourselves much with the properties of the part of the potential energy analytic in S.

For the lattices the method we use is to write

$$\sum_{l=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} [(l+x)^2+(m+y)^2+(n+z)^2]^{-S}$$

$$= \frac{1}{\Gamma(S)} \int_0^{\infty} t^{S-1}\,\mathrm{d}t \sum_{l=-\infty}^{\infty} \mathrm{e}^{-t(l+x)^2} \sum_{m=-\infty}^{\infty} \mathrm{e}^{-t(m+y)^2} \sum_{n=-\infty}^{\infty} \mathrm{e}^{-t(n+z)^2}. \tag{1.7}$$

The integral is split in two, from 0 to π and from π to ∞. On $[\pi, \infty]$ the integrand is left unchanged and on $[0, \pi]$ the sums are inverted using Jacobi's imaginary transformation. The divergence at $S = 3/2$ can then be found as a simple pole. For the sum in (1.2) we would use the same method, but to find the singularities we need an inversion transformation for $\Sigma_{l=0}^{\infty} \exp[-t(l+x)^2]$. In § 2 of this paper we develop the necessary inversion formula and in § 3 we develop formulae for the lattice sums (1.2), (1.3), (1.4) and (1.5). We conclude the paper with a discussion section.

2. Inversion transformations

We write the sum

$$\Psi^*(\boldsymbol{\rho}; S) = \sum_{l=0}^{\infty} \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} [(l+x)^2+(m+y)^2+(n+z)^2]^{-S} \tag{2.1}$$

in the form

$$\Psi^*(\rho; S) = \frac{1}{\Gamma(S)} \int_{\pi}^{\infty} \mathrm{d}t\, t^{S-1} \sum_{l=0}^{\infty} \mathrm{e}^{-t(l+x)^2} \sum_{m=-\infty}^{\infty} \mathrm{e}^{-t(m+y)^2} \sum_{n=-\infty}^{\infty} \mathrm{e}^{-t(n+z)^2}$$

$$+ \frac{1}{\Gamma(S)} \int_{0}^{\pi} \mathrm{d}t\, t^{S-1} \sum_{l=0}^{\infty} \mathrm{e}^{-t(l+x)^2} \sum_{m=-\infty}^{\infty} \mathrm{e}^{-t(m+y)^2} \sum_{n=-\infty}^{\infty} \mathrm{e}^{-t(n+z)^2}. \tag{2.2}$$

We leave the integrand in the first integral unchanged. This integral is analytic for $\mathrm{Re}(S) > 0$. We can approximate it fairly accurately by taking the largest few terms in each sum and expressing the integrals as incomplete gamma functions. For the case $S = 1/2$, these integrals are error functions, which may be evaluated very rapidly.

For the second integral, we replace the two doubly infinite sums using the Jacobi transformation (1.1). This method has been used before, but has then relied on being able to do the remaining integral as a sum of Riemann zeta functions whose analytic continuation is fairly well understood. The reliance on doing the integrals exactly makes this method unsuitable for general use. In this work we develop an inversion transformation for the semi-infinite sum on l.

We use the identity

$$\mathrm{e}^{-ta^2} = \frac{1}{2\sqrt{(\pi t)}} \int_{-\infty}^{\infty} \exp\left(-\frac{u^2}{4t} - \mathrm{i}ua\right) \mathrm{d}u \tag{2.3}$$

on the elements of the semi-infinite sum to obtain

$$\sum_{l=0}^{\infty} \exp[-t(l+x)^2] = \frac{1}{2\sqrt{(\pi t)}} \int_{-\infty}^{\infty} \exp\left(-\frac{u^2}{4t} + \mathrm{i}ux\right)\left(\sum_{l=0}^{\infty} \mathrm{e}^{-\mathrm{i}ul}\right) \mathrm{d}u. \tag{2.4}$$

Shifting the contour of integration down (to $(-\infty - \mathrm{i}c, +\infty - \mathrm{i}c)$ with $c > 0$) enables us to calculate the sum as a geometric series. If we then return the contour to its original line we obtain

$$\sum_{l=0}^{\infty} \exp[-t(l+x)^2] = \frac{1}{2\sqrt{(\pi t)}} \int_{-\infty}^{\infty} \exp\left(-\frac{u^2}{4t} + \mathrm{i}ux\right)\left(\frac{1}{1-\mathrm{e}^{-\mathrm{i}u}}\right) \mathrm{d}u. \tag{2.5}$$

Of course, the contour cannot return entirely to the real axis: it must go around the poles at $u = 2\pi n$ in the lower half-plane. We are left with a sum of half-residues from poles and a Cauchy principal part integral. The sum of half-residues gives a contribution

$$T_1(t, x) = \frac{1}{2}\left(\frac{\pi}{t}\right)^{1/2} \sum_{l=-\infty}^{\infty} \exp(-\pi^2 l^2/t) \cos(2\pi l x), \tag{2.6}$$

exactly half the doubly infinite sum (cf equation (1.1)). In the Cauchy principal part integral, the imaginary part of the integrand is odd in u and we find

$$\sum_{l=0}^{\infty} \exp[-t(l+x)^2] = T_1(t, x) + T_2(t, x)$$

where

$$T_2(t, x) = \frac{1}{4\sqrt{(\pi t)}} \int_{-\infty}^{\infty} \exp\left(-\frac{u^2}{4t}\right) \frac{\sin[u(x+\frac{1}{2})]}{\sin(\frac{1}{2}u)} \mathrm{d}u. \tag{2.7}$$

We may write $T_2(t,x)$ as a sum of integrals on $[2(l-\frac{1}{2})\pi, 2(l+\frac{1}{2})\pi]$ to obtain

$$T_2(t,x)=\tfrac{1}{2}(\pi t)^{-1/2}\sum_{l=-\infty}^{\infty} e^{-\pi^2 l^2/t}\int_0^{\pi} du\,\frac{e^{-u^2/4t}}{\sin(\frac{1}{2}u)}\Big[\cos(2l\pi x)\sin[(\tfrac{1}{2}+x)u]\cosh\Big(\frac{l\pi u}{t}\Big)$$
$$+\sin(2l\pi x)\cos[(\tfrac{1}{2}+x)u]\sinh\Big(\frac{l\pi u}{t}\Big)\Big]$$
$$\equiv\tfrac{1}{2}(\pi t)^{-1/2}\sum_{l=-\infty}^{\infty} e^{-\pi^2 l^2/t} b_l(t,x). \tag{2.8}$$

Asymptotic expansion of $T_2(t,x)$ for small t yields

$$T_2(t,x)\sim(\tfrac{1}{2}+x)\Big(1-\frac{2}{\sqrt{\pi}}e^{-\pi^2/4t}\Big). \tag{2.9}$$

Thus for t very small we obtain

$$\sum_{l=0}^{\infty}\exp[-t(l+x)^2]\sim\tfrac{1}{2}(\pi/t)^{1/2}+(\tfrac{1}{2}+x). \tag{2.10}$$

We have, for the semi-infinite sum

$$\sum_{l=0}^{\infty}\exp[-t(l+x)^2]=\frac{1}{2}\Big(\frac{\pi}{t}\Big)^{1/2}\sum_{l=-\infty}^{\infty} e^{-\pi^2 l^2/t}\Big(\cos(2\pi l x)+\frac{1}{\pi}b_l(t,x)\Big) \tag{2.11}$$

which we use as an inversion formula in the place of the formula (1.1) for doubly infinite sums.

If we use (2.11), (2.10) and (1.1) in equation (2.2), we can subtract the diverging part from the second integral in (2.2) and add it on separately. We find

$$\Psi^*(\boldsymbol{\rho};S)=\Psi(\boldsymbol{\rho};S)+\frac{\pi^S}{2\Gamma(S)(S-\frac{3}{2})}+\frac{\pi^S(\frac{1}{2}-x)}{\Gamma(S)(S-1)} \tag{2.12}$$

where

$$\Psi(\boldsymbol{\rho};S)=\frac{1}{\Gamma(S)}\int_{\pi}^{\infty} t^{S-1}\,dt\sum_{l=0}^{\infty} e^{-t(l+x)^2}\sum_{m=-\infty}^{\infty} e^{-t(m+y)^2}\sum_{n=-\infty}^{\infty} e^{-t(n+z)^2}$$
$$+\frac{\pi^{3/2}}{2\Gamma(S)}\int_0^{\pi} t^{S-\frac{5}{2}}\,dt\Big\{\Big[\sum_{l=-\infty}^{\infty} e^{-\pi^2 l^2/t}\Big(\cos(2\pi l x)+\frac{1}{\pi}b_l(t,x)\Big)\Big]$$
$$\times\Big(\sum_{m=-\infty}^{\infty} e^{-\pi^2 m^2/t}\cos(2\pi m y)\Big)\Big(\sum_{n=-\infty}^{\infty} e^{-\pi^2 n^2/t}\cos(2\pi n z)\Big)$$
$$-\Big[1+2\Big(\frac{t}{\pi}\Big)^{1/2}(\tfrac{1}{2}-x)\Big]\Big\} \tag{2.13}$$

is an analytic function of S for $\mathrm{Re}(S)>0$. Equation (2.12) now allows us to compute the lattice sums introduced in § 1.

3. Evaluation of lattice sums

For the potential $\Phi_1(x, y, z)$ in equation (2.1) we find

$$\Phi_1(x, y, z) = \frac{qq_1}{4\pi\epsilon_0}(\Psi(\boldsymbol{\rho}; \tfrac{1}{2}) - \Psi(\boldsymbol{\rho} + \boldsymbol{a}; \tfrac{1}{2})) - \frac{2q_1(q\alpha)}{4\pi\epsilon_0}. \tag{3.1}$$

The contribution from the pole at $S = 3/2$ is zero by the charge neutrality of the semi-infinite lattice. The term $-2q_1(q\alpha)/4\pi\epsilon_0$ is from the pole at $S = 1$ so that our analytic continuation to $S = \frac{1}{2}$ must go through complex values of S. This divergence does not depend on $\boldsymbol{\rho}$ and is caused by the fact that the system of a neutral lattice with a charge near its surface is not electrostatically neutral. The layers of positive and negative charges at fixed values of l give layers of dipoles in the x direction of strength $|q\alpha|$. The charge above the surface must have a cancelling charge at infinite distance from the lattice with potential energy $2q_1(q\alpha)/4\pi\epsilon_0$ so that the correct form for the potential in equation (1.2) is in fact

$$\Phi_1^*(x, y, z) = \frac{qq_1}{4\pi\epsilon_0}(\Psi(\boldsymbol{\rho}; \tfrac{1}{2}) - \Psi(\boldsymbol{\rho} + \boldsymbol{a}; \tfrac{1}{2})). \tag{3.2}$$

This result may now be computed without worrying about the divergences in the original sum.

We may evaluate the other potential energies in § 1 by considering the denominators in the sums to be of the form $|\boldsymbol{R}_{lmn}(\boldsymbol{\rho})|^{2S}$ and taking gradients of the function $\Psi(\boldsymbol{\rho}; S)$ at $\mathrm{Re}(S) > 3/2$. The results may then be continued to the correct value of S. We find, for the potential energy of a dipole $\boldsymbol{\mu}$ above a neutral lattice of charges,

$$\Phi_2(x, y, z) = -\frac{q}{4\pi\epsilon_0}(\nabla\Psi(\boldsymbol{\rho}; \tfrac{1}{2}) - \nabla\Psi(\boldsymbol{\rho} + \boldsymbol{a}; \tfrac{1}{2})) \tag{3.3}$$

and for a charge q, above the surface of a simple cubic lattice of dipoles $\boldsymbol{\mu}$,

$$\Phi_3(x, y, z) = -\frac{q_1}{4\pi\epsilon_0}\nabla\Psi(\boldsymbol{\rho}; \tfrac{1}{2}) \tag{3.4}$$

where we have left out a term from the pole at $S = 1$ since it must be cancelled by a charge $-q_1$ at large distance from the surface.

The potential energy of a dipole $\boldsymbol{\nu}$ above the surface of a simple cubic lattice of dipole $\boldsymbol{\mu}$ is a triple sum of two parts. The poles at $S = 3/2$ from the two parts cancel, but not to zero, and give a term equal to half the corresponding term for the whole-space sums (Smith and Perram 1975). The contribution from the pole at $S = 1$ is zero and we find

$$\Phi_4(x, y, z) = \frac{1}{4\pi\epsilon_0}[\tfrac{2}{3}\pi(\boldsymbol{\mu} \cdot \boldsymbol{\nu}) - (\boldsymbol{\mu} \cdot \nabla)(\boldsymbol{\nu} \cdot \nabla)\Psi(\boldsymbol{\rho}; \tfrac{1}{2})]. \tag{3.5}$$

We have now developed convergent and 'computable' forms for the lattice sum potential energies introduced in § 1.

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