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Some new lattice sums including an exact result for the electrostatic potential within the NaCl lattice

P J Forrester and M L Glasser†

Department of Mathematics, University of Melbourne, Parkville, Victoria 3052, Australia

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Abstract. The electrostatic potential at point $(\frac{1}{6}, \frac{1}{6}, \frac{1}{6})$ in the unit cell of side length 2 of the NaCl lattice is found to be $\sqrt{3}$. An n-dimensional generalisation of a dipole sum, evaluated exactly by Glasser and Zucker in the case $n = 2$, is given.

1. Introduction

The problem of evaluating physically applicable lattice sums has a long history. In particular, the numerical evaluation of electrostatic lattice sums has its origin in the work of Madelung (1918) and Ewald (1921). However, the exact evaluation of these important sums has received little attention until comparatively recently (Glasser 1973). A recent review (Glasser and Zucker 1980) contains a very extensive listing of exact results, especially in two dimensions. In this review, it is pointed out that very few lattice sums in three dimensions of the form

$$\psi(\boldsymbol{r}, s) = \sum_{i=1}^{N} \sum_{l=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} q_i |(l, m, n) + (\boldsymbol{r}_i - \boldsymbol{r})|^{-2s} \tag{1}$$

have been evaluated exactly. In equation (1), $\psi(\boldsymbol{r}, \frac{1}{2})$ is the electrostatic potential at the point $\boldsymbol{r}$ within the unit cell of a simple cubic ionic crystal with charges q_i at $\boldsymbol{r}_i$, $i = 1, 2, \ldots, N$, $\Sigma_{i=1}^{N} q_i = 0$, and unit cell of side length 1. This note reports several new lattice sums including an exact result for the NaCl structure. Apart from its intrinsic interest, this result provides a useful test for checking the accuracy of numerical algorithms for computing the potential $\psi(\boldsymbol{r}, \frac{1}{2})$.

2. Calculation

Consider first an NaCl-type lattice with unit cell of side length 2 containing charges +1 at (0, 0, 0), (1, 1, 0), (1, 0, 1), (0, 1, 1) and charges −1 at (1, 0, 0), (0, 1, 0), (0, 0, 1), (1, 1, 1). The electrostatic potential at $\boldsymbol{r} \in [-\frac{1}{2}, \frac{3}{2}]^{\otimes 3}$ (this choice of unit cell avoids fractional charges) may be written

$$\phi(\boldsymbol{r}, \tfrac{1}{2}) = \sum_{l=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} (-1)^{l+m+n} |(l, m, n) - \boldsymbol{r}|^{-1}. \tag{2}$$

† Permanent address: Department of Mathematics and Computer Science, Clarkson College of Technology, Potsdam, New York, USA.

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Because the unit cell has zero dipole and quadrupole moments, this lattice sum is absolutely convergent (De Leeuw *et al* 1980). Equation (2) may be evaluated exactly for $\boldsymbol{r}=(-\frac{1}{6},-\frac{1}{6},-\frac{1}{6})$. Symmetry considerations then give the same value for $\boldsymbol{r}=(x,y,z)$ with x, y, z being any of $\pm\frac{1}{6},\frac{5}{6},\frac{7}{6}$.

Jacobi (1829) lists the identity

$$\left(\sum_{m=-\infty}^{\infty}(-1)^m q^{(3m^2+m)/2}\right)^3=\sum_{n=0}^{\infty}(-1)^n(2n+1)q^{(n^2+n)/2}. \tag{3}$$

Following the method of Glasser (1973) we substitute $q=\mathrm{e}^{-\frac{2}{3}t}$ in (3). By multiplying both sides by a suitable function $F(t)$ and integrating over t from 0 to ∞ we obtain the reduction formula

$$\sum_{l=-\infty}^{\infty}\sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}(-1)^{l+m+n}\Phi[(l+\tfrac{1}{6})^2+(m+\tfrac{1}{6})^2+(n+\tfrac{1}{6})^2]$$
$$=\sum_{n=0}^{\infty}(-1)^n(2n+1)\Phi(\tfrac{1}{3}(n+\tfrac{1}{2})^2) \tag{4}$$

where $\Phi(p)$ denotes the Laplace transform of F. In particular for $\Phi(p)=p^{\nu}\,\mathrm{e}^{-ap^{1/2}}$ we obtain

$$\sum_{l=-\infty}^{\infty}\sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}[(l+\tfrac{1}{6})^2+(m+\tfrac{1}{6})^2+(n+\tfrac{1}{6})^2]^{\nu}\exp\{-a[(l+\tfrac{1}{6})^2+(m+\tfrac{1}{6})^2+(n+\tfrac{1}{6})^2]^{1/2}\}$$
$$=12^{-\nu}\sum_{n=0}^{\infty}(-1)^n(2n+1)^{2\nu+1}\exp[-\tfrac{1}{2}a3^{-1/2}(2n+1)]. \tag{5}$$

The sum on the right-hand side can be evaluated in closed form whenever ν is integral or half integral. For example $\nu=-\frac{1}{2}$ gives

$$\sum_{l=-\infty}^{\infty}\sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}(-1)^{l+m+n}\frac{\exp\{-a[(l+\frac{1}{6})^2+(m+\frac{1}{6})^2+(n+\frac{1}{6})^2]^{1/2}\}}{[(l+\frac{1}{6})^2+(m+\frac{1}{6})^2+(n+\frac{1}{6})^2]^{1/2}}=\frac{\sqrt{3}}{\cosh\frac{1}{2}3^{-1/2}a} \tag{6}$$

for which $a=0$ shows

$$\phi((-\tfrac{1}{6},-\tfrac{1}{6},-\tfrac{1}{6}),\tfrac{1}{2})=\sqrt{3}. \tag{7}$$

A second example of physical interest may be obtained by taking $\Phi(p)=(p+a^2)^{-\nu}$ which gives

$$\sum_{l=-\infty}^{\infty}\sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}\frac{(-1)^{l+m+n}}{[(l+\frac{1}{6})^2+(m+\frac{1}{6})^2+(n+\frac{1}{6})^2+a^2]^{\nu}}=12^{\nu}\sum_{n=0}^{\infty}\frac{(-1)^n(2n+1)}{[(2n+1)^2+12a^2]^{\nu}} \tag{8}$$

The sum on the RHS can be evaluated when $a\neq 0$, $\nu=$ integer, in terms of the digamma function, and when $a=0$, $\nu>\frac{1}{2}$, in terms of

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

(and thus for all ν with $|\arg\nu|<\pi$ by analytic continuation).

One other curious result, which arises by setting $\Phi(p)=p^{-\nu}\operatorname{sech} ap^{1/2}$, is

$$\sum_{l=-\infty}^{\infty}\sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}\frac{(-1)^{l+m+n}\operatorname{sech}\pi\mu[(l+\frac{1}{6})^2+(m+\frac{1}{6})^2+(n+\frac{1}{6})^2]^{1/2}}{[(l+\frac{1}{6})^2+(m+\frac{1}{6})^2+(n+\frac{1}{6})^2]^{\nu}}=0 \tag{9}$$

whenever $\mu=\sqrt{3}$, $\nu=1-2q$ or $\mu=3$, $\nu=1-3q$ $(q=1,2,3,\ldots)$.

A similar sequence of results can be obtained by manipulating the LHS of (3), so that the q series becomes

$$\sum_{n=0}^{\infty}(-1)^n(2n+1)q^{\frac{1}{8}(2n+1)^2}$$

$$=\left(\sum_{n=-\infty}^{\infty}(-1)^n q^{n^2}\right)\left(\sum_{n=-\infty}^{\infty}(-1)^n q^{3(n+\frac{1}{6})^2}\right)\left(\sum_{n=-\infty}^{\infty}(-1)^n q^{\frac{3}{2}(n+\frac{1}{6})^2}\right). \tag{10}$$

By carrying out the analysis which led to equation (7) we find

$$\sum_{l=-\infty}^{\infty}\sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}(-1)^{l+m+n}[l^2+\tfrac{3}{2}(m+\tfrac{1}{6})^2+3(n+\tfrac{1}{6})^2]^{-1/2}=\sqrt{2}. \tag{11}$$

Equation (11) is the electrostatic potential within a crystal of rectangular unit cells, with alternating positive and negative point charges along the three orthogonal axes.

We conclude this note with the n-dimensional generalisation of the sum (5.7) in Glasser and Zucker (1980) (the case $n=2$ arises when calculating the dielectric constant in a cubic crystal):

$$S_n=\sum_{l_1,l_2,\ldots,l_n=1}^{\infty}\frac{(-1)^{l_1+l_2+\ldots+l_n}(l_1^2+l_2^2+\ldots+l_n^2)^{1/2}}{\sinh\pi(l_1^2+l_2^2+\ldots+l_n^2)^{1/2}}=\frac{(-\frac{1}{2})^n}{(n+1)\pi}. \tag{12}$$

To demonstrate this, we use the elementary summation formula

$$\sum_{l_1=-\infty}^{\infty}(-1)^{l_1}\frac{1}{l_1^2+a^2}=\frac{\pi}{a\sinh\pi a}. \tag{13a}$$

It follows that

$$\sum_{l_1=-\infty}^{\infty}(-1)^{l_1}\frac{\exp[-\mu(l_1^2+a^2)]}{l_1^2+a^2}=\frac{\pi}{a\sinh\pi a}F(\mu,a) \tag{13b}$$

where $F(0,a)=1$ and F is continuous for $\mu\geqslant 0$. Take $a^2=l_2^2+l_3^2+\ldots+l_{n+1}^2$, multiply both sides by $a^2(-1)^{l_2+l_3+\ldots+l_{n+1}}$, and sum over $l_2, l_3, \ldots, l_{n+1}$ from 1 to ∞ to get

$$2\sum_{l_1,l_2,\ldots,l_{n+1}=1}^{\infty}\frac{(-1)^{l_1+l_2+\ldots+l_{n+1}}(l_2^2+l_3^2+\ldots+l_{n+1}^2)\exp[-\mu(l_1^2+l_2^2+\ldots+l_{n+1}^2)]}{l_1^2+l_2^2+\ldots+l_{n+1}^2}$$

$$+\left(\sum_{l=1}^{\infty}(-1)^l e^{-\mu l^2}\right)^n$$

$$=\pi\sum_{l_1,l_2,\ldots,l_n=1}^{\infty}\frac{(-1)^{l_1+l_2+\ldots+l_n}(l_1^2+l_2^2+\ldots+l_n^2)^{1/2}}{\sinh\pi(l_1^2+l_2^2+\ldots+l_n^2)^{1/2}}F(\mu,a). \tag{13c}$$

Cyclically interchange summation labels $n+1$ times, then add the resulting $n+1$ equations. This gives

$$2n\left(\sum_{l=1}^{\infty}(-1)^l e^{-\mu l^2}\right)^{n+1}+(n+1)\left(\sum_{l=1}^{\infty}(-1)^l e^{-\mu l^2}\right)^n$$

$$=\pi(n+1)\sum_{l_1,l_2,\ldots,l_n=1}^{\infty}\frac{(-1)^{l_1+l_2+\ldots+l_n}(l_1^2+l_2^2+\ldots+l_n^2)^{1/2}}{\sinh\pi(l_1^2+l_2^2+\ldots+l_n^2)^{1/2}}F(\mu,a). \tag{13d}$$

Taking the limit $\mu\to 0$ in (13d) gives the required result (12).

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