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1976 J. Phys. A: Math. Gen. 9 1411

(http://iopscience.iop.org/0305-4470/9/9/004)

J. Phys. A: Math. Gen., Vol. 9, No. 9, 1976. Printed in Great Britain. © 1976

Evaluation of lattice sums using Poisson's summation formula. II

A N Chaba† and R K Pathria‡

† Universidade Federal da Paraíba, Departamento de Física, CCEN, João Pessoa, Paraíba, Brasil

‡ Department of Physics, University of Waterloo, Waterloo, Ontario, Canada

Received 21 April 1976

Abstract. Application of Poisson's summation formula for the analytic evaluation of a class of lattice sums in arbitrary dimensions is extended to a more generalized class of sums. The resulting formulae are applicable to a variety of problems such as electronic-structure studies of crystalline solids, the onset of Bose–Einstein condensation in finite systems, the analysis of stability of quantized vortex arrays in extreme type-II superconductors and in rotating superfluid helium, plasma oscillations in an array of filamentary conductors, etc. They also provide an alternative approach for the determination of Madelung constants and other related sums that appear in the theory of cubic lattices.

1. Introduction

In a recent paper (Chaba and Pathria 1975a, to be referred to as I, see also Hall 1976) we employed Poisson's summation formula for the analytic evaluation of m-dimensional sums:

$$\sum_{\{l_i\}=-\infty}^{\infty}{}' \exp[-a(l_1^2+l_2^2+\ldots+l_m^2)](l_1^2+l_2^2+\ldots+l_m^2)^{-s} \qquad (a>0) \tag{1}$$

where Σ' excludes the term with $l_1=l_2=\ldots=0$. In this paper we extend the use of the Poisson technique for evaluating more generalized sums such as

$$\sum_{\{l_i\}=-\infty}^{\infty}{}' \cos(2\pi\epsilon_1 l_1)\ldots\cos(2\pi\epsilon_m l_m)\exp[-a(l_1^2+\ldots+l_m^2)^s](l_1^2+\ldots+l_m^2)^{-s} \tag{2}$$

and

$$\sum_{\{l_i\}=-\infty}^{\infty} \exp\{-a[(l_1+\epsilon_1)^2+\ldots+(l_m+\epsilon_m)^2]^s\}[(l_1+\epsilon_1)^2+\ldots+(l_m+\epsilon_m)^2]^{-s}. \tag{3}$$

In (3), the vector $\boldsymbol{\epsilon}$ is generally non-zero and the sum includes the term with $l_1=l_2=\ldots=0$; however, if $\boldsymbol{\epsilon}=0$, then the term with $l_1=l_2=\ldots=0$ ought to be excluded. Some of these sums, especially of type (2), also appear in a recent paper by Hautot (1975) who has consistently used Poisson's summation formula of dimensionality lower than that of the sum itself. The reason for this, as pointed out by Hautot, is that because of the exclusion of the term with $l_1=l_2=\ldots=0$ in his sums Poisson's formula of the same dimensionality cannot be employed. At this stage it appears worthwhile to recall that, according to Poisson,

$$\sum_{\{l_i\}=-\infty}^{\infty} f(l_1, \ldots, l_m) = \sum_{\{q_i\}=-\infty}^{\infty} F(q_1, \ldots, q_m) \tag{4}$$

where

$$F(\boldsymbol{q}) = \int_{-\infty}^{\infty} \ldots \int_{-\infty}^{\infty} \mathrm{e}^{-2\pi\mathrm{i}(\boldsymbol{q}.\boldsymbol{l})} f(\boldsymbol{l})\, \mathrm{d}^m l. \tag{5}$$

It may be noted that

$$F(0) = \int_{-\infty}^{\infty} \ldots \int_{-\infty}^{\infty} f(\boldsymbol{l})\, \mathrm{d}^m l \tag{6}$$

which brings out the remarkable fact that the term with $\boldsymbol{q} = 0$ on the right-hand side of (4) is precisely equal to the asymptotic value of the sum on the left-hand side, as obtained by replacing the summation over $\boldsymbol{l}$ by an integration; the $\boldsymbol{q} \neq 0$ terms, therefore, arise from the discreteness of the sum. Under appropriate circumstances, the resulting sum over $\boldsymbol{q}$ may converge much faster than the original sum over $\boldsymbol{l}$.

We shall show that, by employing a technique developed by Fetter *et al* (1966), we can circumvent the difficulty mentioned by Hautot and make use of Poisson's summation formula of the same dimensionality as of the sum itself. Moreover, many of the desired results can be derived by taking Laplace transforms of appropriate formulae obtained by a prior, often simpler, application of the Poisson technique.

For illustration we shall start with one-dimensional sums and then proceed on to the more relevant sums in two and three dimensions. Some of the resulting formulae are applicable to the electronic-structure studies of crystalline solids (Harris and Monkhorst 1970), the investigation of Bose–Einstein condensation in finite systems (Greenspoon and Pathria 1974, Chaba and Pathria 1975b, 1976, Zasada and Pathria 1976), the analysis of stability of quantized vortex arrays in extreme type-II superconductors and in rotating superfluid helium (Fetter 1975), etc. They also provide an alternative approach for the determination of Madelung constants and other related sums that appear in the theory of cubic lattices (Hautot 1974, 1975, Zucker 1975, 1976).

Throughout this paper we shall use the following notation: $S(\epsilon_1, \ldots, \epsilon_m; a)$ and $U(\epsilon_1, \ldots, \epsilon_m; a)$ will denote sums (2) with $s = 1$ and $1/2$, respectively, while $T(\epsilon_1, \ldots, \epsilon_m; a)$ and $V(\epsilon_1, \ldots, \epsilon_m; a)$ will denote sums (3), again with $s = 1$ and $1/2$, respectively. Sometimes we shall use the symbols T' and V' to denote the exclusion of the term $l_1 = l_2 = \ldots = 0$ from the sums in question; in the case of S and U, such a term is already excluded.

2. Lattice sums in one dimension

We start with the Poisson identities

$$\sum_{l=-\infty}^{\infty} \cos(2\pi\epsilon l) \exp(-al^2) = (\pi/a)^{1/2} \sum_{q=-\infty}^{\infty} \exp[-\pi^2(q+\epsilon)^2/a] \tag{7}$$

and

$$\sum_{l=-\infty}^{\infty} \exp[-a(l+\epsilon)^2] = (\pi/a)^{1/2} \sum_{q=-\infty}^{\infty} \cos(2\pi\epsilon q) \exp(-\pi^2 q^2/a) \tag{8}$$

which hold for all $a>0$; for reasons of symmetry, it will be sufficient to consider $0\leqslant\epsilon\leqslant 1/2$. Separating the $(l=0)$-term from the left-hand side of (7) and integrating with respect to a, we obtain

$$S(\epsilon;a)=\sum_{l=-\infty}^{\infty}{}' \frac{\cos(2\pi\epsilon l)}{l^2}\exp(-al^2)$$

$$=\tfrac{1}{3}\pi^2(1-6\epsilon+6\epsilon^2)+a-(\pi a)^{1/2}\sum_{q=-\infty}^{\infty}E_{3/2}[\pi^2(q+\epsilon)^2/a] \qquad (9)$$

where the exponential integral is given by

$$E_n(z)=\int_1^{\infty} t^{-n}\exp(-zt)\,\mathrm{d}t \qquad (n\geqslant 0) \qquad (10)$$

so that, for $n>1$, $E_n(0)=1/(n-1)$. For $\epsilon=0$, we have

$$S(0;a)=\tfrac{1}{3}\pi^2-2(\pi a)^{1/2}+a-2(\pi a)^{1/2}\sum_{q=1}^{\infty}E_{3/2}(\pi^2q^2/a). \qquad (11)$$

In the limit $a\to 0$, we obtain the asymptotic behaviour

$$S(\epsilon;a)=\begin{cases}\tfrac{1}{3}\pi^2(1-6\epsilon+6\epsilon^2)+a-\mathrm{O}(a^{3/2}\,\mathrm{e}^{-\pi^2/a}) & (\epsilon\neq 0)\\ \tfrac{1}{3}\pi^2-2(\pi a)^{1/2}+a-\mathrm{O}(a^{3/2}\,\mathrm{e}^{-\pi^2/a}) & (\epsilon=0).\end{cases}$$

It is obvious that equation (9) can also be used for determining the asymptotic behaviour of the sum $\Sigma_q E_{3/2}[a(q+\epsilon)^2]$.

Carrying out a similar operation with (8), we obtain

$$T(\epsilon;a)=\sum_{l=-\infty}^{\infty}\frac{1}{(l+\epsilon)^2}\exp[-a(l+\epsilon)^2]$$

$$=\zeta(2,\epsilon)+\zeta(2,1-\epsilon)-2(\pi a)^{1/2}-2(\pi a)^{1/2}\sum_{q=1}^{\infty}\cos(2\pi\epsilon q)E_{3/2}(\pi^2q^2/a) \qquad (12)$$

where

$$\zeta(n,\epsilon)=\sum_{l=0}^{\infty}(l+\epsilon)^{-n} \qquad (n>1), \qquad (13)$$

so that $\zeta(n,1)=\zeta(n)$, the Riemann zeta function, whereas $\zeta(n,\epsilon\to 0)=\epsilon^{-n}+\zeta(n)$. The special case of $\epsilon=1/2$ is worth noting:

$$\sum_{l=0}^{\infty}\frac{1}{(l+\frac{1}{2})^2}\exp[-a(l+\tfrac{1}{2})^2]$$

$$=\tfrac{1}{2}\pi^2-(\pi a)^{1/2}-(\pi a)^{1/2}\sum_{q=1}^{\infty}(-1)^qE_{3/2}(\pi^2q^2/a). \qquad (14)$$

Again, one can obtain asymptotic behaviour of either of the two sums involved here.

We now consider the sum

$$U(\epsilon;a)=\sum_{l=-\infty}^{\infty}{}'\frac{\cos(2\pi\epsilon l)}{|l|}\exp(-a|l|), \qquad (15)$$

which may be evaluated by integrating the Poisson identity

$$\sum_{l=-\infty}^{\infty} \cos(2\pi\epsilon l) \exp(-a|l|) = 2a \sum_{q=-\infty}^{\infty} \frac{1}{a^2+4\pi^2(q+\epsilon)^2}. \tag{16}$$

We obtain

$$U(\epsilon; a) = -2 \ln[2 \sin(\pi\epsilon)] + a - \sum_{q=-\infty}^{\infty} \ln\left(1+\frac{a^2}{4\pi^2(q+\epsilon)^2}\right). \tag{17}$$

The sum (15) can, however, be evaluated by elementary means, with the result

$$U(\epsilon; a) = -\ln[1-2\cos(2\pi\epsilon)\, e^{-a} + e^{-2a}]. \tag{18}$$

Comparing (17) and (18) we obtain the remarkable result

$$\prod_{q=-\infty}^{\infty} \left(1+\frac{a^2}{4\pi^2(q+\epsilon)^2}\right) = \frac{\cosh a - \cos(2\pi\epsilon)}{2\sin^2(\pi\epsilon)}, \tag{19}$$

which holds for all a and ϵ. Special cases $\epsilon \to 0$ and $\epsilon = 1/2$ are rather well known; the case $\epsilon = 1/4$ is not so well known but is clearly interesting.

Finally we note that the sum

$$\begin{aligned} V(\epsilon; a) &= \sum_{l=-\infty}^{\infty} \frac{1}{|l+\epsilon|} \exp(-a|l+\epsilon|) \\ &= \frac{e^{-a\epsilon}}{\epsilon} F(\epsilon, 1, 1+\epsilon; e^{-a}) + \frac{e^{-a(1-\epsilon)}}{1-\epsilon} F(1-\epsilon, 1, 2-\epsilon; e^{-a}) \end{aligned} \tag{20}$$

where $F(a, b, c; z)$ is the hypergeometric function. In the limit $a \to 0$,

$$F(\epsilon, 1, 1+\epsilon; e^{-a}) \simeq \epsilon[\ln(1/a) + \psi(1) - \psi(\epsilon)],$$

where $\psi(z)$ is the digamma function $d[\ln \Gamma(z)]/dz$. Accordingly,

$$V(\epsilon; a) \simeq [2\ln(1/a) + 2\psi(1) - \psi(\epsilon) - \psi(1-\epsilon)]. \tag{21}$$

Since $\psi(1) - \psi(1/2) = 2\ln 2$,

$$V(\tfrac{1}{2}; a) \simeq 2\ln(4/a), \tag{22}$$

which is consistent with the exact result, namely

$$V(\tfrac{1}{2}; a) = 2\ln[\coth(\tfrac{1}{4}a)]. \tag{23}$$

3. Lattice sums in two dimensions

Starting with the two-dimensional version of (7), we obtain

$$\begin{aligned} S(\epsilon_1, \epsilon_2; a) &= \sum_{l_{1,2}=-\infty}^{\infty}{}' \frac{\cos(2\pi\epsilon_1 l_1)\cos(2\pi\epsilon_2 l_2)}{l_1^2+l_2^2} \exp[-a(l_1^2+l_2^2)] \\ &= S(\epsilon_1, \epsilon_2; 0) + a - \pi \sum_{q_{1,2}=-\infty}^{\infty} E_1\left(\frac{\pi^2}{a}[(q_1+\epsilon_1)^2+(q_2+\epsilon_2)^2]\right). \end{aligned} \tag{24}$$

The limiting case $\epsilon \to 0$ has already appeared in I:

$$S(0,0;a) = -\pi \ln a + C_2 + a - \pi \sum_{q_{1,2}=-\infty}^{\infty}{}' E_1\left(\frac{\pi^2}{a}(q_1^2+q_2^2)\right) \tag{25}$$

where

$$C_2 = \lim_{a\to 0} [S(0,0;a) - \pi \ln(1/a)] = \pi\left(\gamma - \ln \frac{[\Gamma(\frac{1}{4})]^4}{4\pi^3}\right) = 0{\cdot}771605. \tag{26}$$

Comparing (24) and (25), one obtains the asymptotic behaviour of the sum $S(\epsilon_1, \epsilon_2; 0)$:

$$\lim_{\epsilon\to 0} S(\epsilon_1,\epsilon_2;0) = -2\pi \ln(\pi\epsilon) + C_2 - \pi\gamma \tag{27}$$

where $\epsilon = (\epsilon_1^2+\epsilon_2^2)^{1/2}$. The following special values of $S(\epsilon_1, \epsilon_2; 0)$ may also be noted (Glasser 1973, Zucker 1974, Zucker and Robertson 1975):

$$S(0,\tfrac{1}{2};0) = -\tfrac{1}{2}\pi \ln 2; \qquad S(\tfrac{1}{2},\tfrac{1}{2};0) = -\pi \ln 2. \tag{28}$$

The asymptotic behaviour of $S(\epsilon_1, \epsilon_2; a)$, as $a \to 0$, is readily obtained from (24).

Next, we obtain from the two-dimensional version of (8)

$$\begin{aligned} T(\epsilon_1,\epsilon_2;a) &= \sum_{l_{1,2}=-\infty}^{\infty} \frac{1}{(l_1+\epsilon_1)^2+(l_2+\epsilon_2)^2} \exp\{-a[(l_1+\epsilon_1)^2+(l_2+\epsilon_2)^2]\} \\ &= -\pi \ln a + B(\epsilon_1,\epsilon_2) - \pi \sum_{q_{1,2}=-\infty}^{\infty}{}' \cos(2\pi\epsilon_1 q_1)\cos(2\pi\epsilon_2 q_2) E_1\left(\frac{\pi^2}{a}(q_1^2+q_2^2)\right) \end{aligned} \tag{29}$$

where

$$B(\epsilon_1,\epsilon_2) = \lim_{a\to 0} [T(\epsilon_1,\epsilon_2;a) - \pi \ln(1/a)] \tag{30}$$

Now, in the limit $\epsilon \to 0$, $T(\epsilon_1, \epsilon_2; a) = (1/\epsilon^2) - a + S(0, 0; a)$. Hence, in view of (25) and (26),

$$B(\epsilon \to 0) = (1/\epsilon^2) + C_2. \tag{31}$$

To obtain some other values of $B(\epsilon_1, \epsilon_2)$, we note that since

$$S(\tfrac{1}{2},\tfrac{1}{2};a) = \tfrac{1}{4}T'(0,0;4a) + \tfrac{1}{4}T(\tfrac{1}{2},\tfrac{1}{2};4a) - \tfrac{1}{2}T(0,\tfrac{1}{2};4a)$$

and

$$T'(0,0;a) = \tfrac{1}{4}T'(0,0;4a) + \tfrac{1}{4}T(\tfrac{1}{2},\tfrac{1}{2};4a) + \tfrac{1}{2}T(0,\tfrac{1}{2};4a)$$

we have, in the limit $a \to 0$,

$$4S(\tfrac{1}{2},\tfrac{1}{2};0) = C_2 + B(\tfrac{1}{2},\tfrac{1}{2}) - 2B(0,\tfrac{1}{2})$$

and

$$3C_2 = -8\pi \ln 2 + B(\tfrac{1}{2},\tfrac{1}{2}) + 2B(0,\tfrac{1}{2}).$$

Combining these results with (28), we obtain

$$B(0,\tfrac{1}{2}) = C_2 + 3\pi \ln 2; \qquad B(\tfrac{1}{2},\tfrac{1}{2}) = C_2 + 2\pi \ln 2. \tag{32}$$

Again, the asymptotic behaviour of the sum $T(\epsilon_1, \epsilon_2; a)$, as $a \to 0$, is readily obtained from (29)–(31).

We now multiply the two-dimensional version of (7) by $a^{-1/2}$ and integrate with respect to a, with the result

$$\sum_{l_{1,2}=-\infty}^{\infty}{}' \frac{\cos(2\pi\epsilon_1 l_1)\cos(2\pi\epsilon_2 l_2)}{(l_1^2+l_2^2)^{1/2}} \operatorname{erfc}[a(l_1^2+l_2^2)]^{1/2}$$

$$= 2(a/\pi)^{1/2} + P(\epsilon_1, \epsilon_2) - \sum_{q_{1,2}=-\infty}^{\infty} \frac{\operatorname{erfc}\{(\pi^2/a)[(q_1+\epsilon_1)^2+(q_2+\epsilon_2)^2]\}^{1/2}}{[(q_1+\epsilon_1)^2+(q_2+\epsilon_2)^2]^{1/2}} \quad (33)$$

where

$$P(\epsilon_1, \epsilon_2) = \sum_{l_{1,2}=-\infty}^{\infty}{}' \frac{\cos(2\pi\epsilon_1 l_1)\cos(2\pi\epsilon_2 l_2)}{(l_1^2+l_2^2)^{1/2}} \quad (34)$$

In the limit $\epsilon \to 0$, we obtain the following result, which is symmetric with respect to the interchange $a \leftrightarrow (\pi^2/a)$,

$$\sum_{l_{1,2}=-\infty}^{\infty}{}' \frac{\operatorname{erfc}[a(l_1^2+l_2^2)]^{1/2}}{(l_1^2+l_2^2)^{1/2}}$$

$$= 2(\pi/a)^{1/2} + 2(a/\pi)^{1/2} + D - \sum_{q_{1,2}=-\infty}^{\infty}{}' \frac{\operatorname{erfc}[(\pi^2/a)(q_1^2+q_2^2)]^{1/2}}{(q_1^2+q_2^2)^{1/2}} \quad (35)$$

where

$$D = \lim_{\epsilon\to 0}[P(\epsilon_1, \epsilon_2) - (1/\epsilon)] = 4\zeta(\tfrac{1}{2})\beta(\tfrac{1}{2}) = -3{\cdot}900265. \quad (36)$$

For $a = \pi$, we get the following sum in a *closed* form:

$$\sum_{l_{1,2}=-\infty}^{\infty}{}' \frac{\operatorname{erfc}[\pi(l_1^2+l_2^2)]^{1/2}}{(l_1^2+l_2^2)^{1/2}} = 2 + 2\zeta(\tfrac{1}{2})\beta(\tfrac{1}{2}) = 0{\cdot}049868. \quad (37)$$

From (35) it follows that, in the limit $a \to 0$, the sum in question approaches the asymptotic value $2(\pi/a)^{1/2} + D$. Finally, we note the following special values of $P(\epsilon_1, \epsilon_2)$:

$$\begin{aligned} P(0, \tfrac{1}{2}) &= 2\sqrt{2}(\sqrt{2}-1)\zeta(\tfrac{1}{2})\beta(\tfrac{1}{2}) = -1{\cdot}142361 \\ P(\tfrac{1}{2}, \tfrac{1}{2}) &= 4(\sqrt{2}-1)\zeta(\tfrac{1}{2})\beta(\tfrac{1}{2}) = -1{\cdot}615543. \end{aligned} \quad (38)$$

From (33) it follows that

$$\sum_{q_{1,2}=-\infty}^{\infty} \frac{\operatorname{erfc}\{a[(q_1+\epsilon_1)^2+(q_2+\epsilon_2)^2]\}^{1/2}}{[(q_1+\epsilon_1)^2+(q_2+\epsilon_2)^2]^{1/2}}$$

$$= 2\left(\frac{\pi}{a}\right)^{1/2} + \sum_{l_{1,2}=-\infty}^{\infty}{}' \frac{\cos(2\pi\epsilon_1 l_1)\cos(2\pi\epsilon_2 l_2)}{(l_1^2+l_2^2)^{1/2}} \operatorname{erf}\left(\frac{\pi^2}{a}(l_1^2+l_2^2)\right)^{1/2} \quad (39)$$

In the limit $a \to 0$, we get for this sum the asymptotic value

$$2(\pi/a)^{1/2} + P(\epsilon_1, \epsilon_2). \quad (39a)$$

We shall now consider the sum

$$U(\epsilon_1, \epsilon_2; a) = \sum_{l_{1,2}=-\infty}^{\infty}{}' \frac{\cos(2\pi\epsilon_1 l_1)\cos(2\pi\epsilon_2 l_2)}{(l_1^2+l_2^2)^{1/2}} \exp[-a(l_1^2+l_2^2)^{1/2}]. \quad (40)$$

In order that Poisson's summation formula be applicable to this sum, we follow the technique of Fetter *et al* (1966) and write

$$U(\epsilon_1, \epsilon_2; a) = \lim_{\delta \to 0} U(\epsilon_1, \epsilon_2; a, \delta)$$

where

$$\begin{aligned} U(\epsilon_1, \epsilon_2; a, \delta) &= \frac{a}{2\pi^{1/2}} \sum_{l_{1,2}=-\infty}^{\infty}{}' \cos(2\pi\epsilon_1 l_1)\cos(2\pi\epsilon_2 l_2) \int_\delta^\infty p^{-3/2} \, \mathrm{e}^{-p-a^2(l_1^2+l_2^2)/4p} \, \mathrm{d}p \\ &= \frac{a}{2\pi^{1/2}} \int_\delta^\infty p^{-3/2} \, \mathrm{e}^{-p} \left(\sum_{l_{1,2}=-\infty}^{\infty} \cos(2\pi\epsilon_1 l_1)\cos(2\pi\epsilon_2 l_2) \, \mathrm{e}^{-a^2(l_1^2+l_2^2)/4p} - 1 \right) \mathrm{d}p. \end{aligned}$$

Poisson's formula may now be applied to the summation over $\boldsymbol{l}$ whereby this summation gets replaced by

$$\left(\frac{4\pi p}{a^2}\right) \sum_{q_{1,2}=-\infty}^{\infty} \exp\left(-\frac{4\pi^2 p}{a^2}[(q_1+\epsilon_1)^2 + (q_2+\epsilon_2)^2]\right).$$

Integration over p may now be carried out, with the result

$$\begin{aligned} U(\epsilon_1, \epsilon_2; a, \delta) &= \frac{2\pi}{a} \sum_{q_{1,2}=-\infty}^{\infty} \frac{\operatorname{erfc}[\![\delta^{1/2}\{1 + (4\pi^2/a^2)[(q_1+\epsilon_1)^2 + (q_2+\epsilon_2)^2]\}^{1/2}]\!]}{\{1 + (4\pi^2/a^2)[(q_1+\epsilon_1)^2 + (q_2+\epsilon_2)^2]\}^{1/2}} \\ &\quad - \frac{a}{2\pi^{1/2}} \Gamma(-\tfrac{1}{2}, \delta), \end{aligned}$$

where $\Gamma(n, \delta)$ is the incomplete gamma function. In the limit $\delta \to 0$, we have

$$\begin{aligned} U(\epsilon_1, \epsilon_2; a) = \lim_{\delta \to 0} \Bigg(&\sum_{q_{1,2}=-\infty}^{\infty} \frac{\operatorname{erfc}[\![\delta^{1/2}\{(4\pi^2/a^2)[(q_1+\epsilon_1)^2 + (q_2+\epsilon_2)^2]\}^{1/2}]\!]}{[(q_1+\epsilon_1)^2 + (q_2+\epsilon_2)^2]^{1/2}} \\ &- \frac{a}{\pi^{1/2}} \frac{\mathrm{e}^{-\delta}}{\delta^{1/2}} + a \operatorname{erfc}(\delta^{1/2}) \Bigg) - \sum_{q_{1,2}=-\infty}^{\infty} \Bigg(\frac{1}{[(q_1+\epsilon_1)^2 + (q_2+\epsilon_2)^2]^{1/2}} \\ &- \frac{1}{[(a^2/4\pi^2) + (q_1+\epsilon_1)^2 + (q_2+\epsilon_2)^2]^{1/2}} \Bigg). \end{aligned}$$

Using (39a), we finally obtain

$$\begin{aligned} U(\epsilon_1, \epsilon_2; a) = a + P(\epsilon_1, \epsilon_2) - \sum_{q_{1,2}=-\infty}^{\infty} \Bigg[&[(q_1+\epsilon_1)^2 + (q_2+\epsilon_2)^2]^{-1/2} \\ &- \left(\frac{a^2}{4\pi^2} + (q_1+\epsilon_1)^2 + (q_2+\epsilon_2)^2 \right)^{-1/2} \Bigg]; \end{aligned} \tag{41}$$

we note that $P(\epsilon_1, \epsilon_2) = U(\epsilon_1, \epsilon_2; 0)$. In retrospect we observe that equation (41) could also be obtained by taking a Laplace transform of (39) with respect to the variable $t = a$ and replacing the parameter s by $a^2/(4\pi^2)$.

Letting $\epsilon_{1,2} \to 0$, we obtain with the help of (36)

$$U(0,0;a) = \sum_{l_{1,2}=-\infty}^{\infty}{}' \frac{\exp[-a(l_1^2+l_2^2)^{1/2}]}{(l_1^2+l_2^2)^{1/2}}$$

$$= \frac{2\pi}{a} + D + a - \sum_{q_{1,2}=-\infty}^{\infty}{}' \left[(q_1^2+q_2^2)^{-1/2} - \left(\frac{a^2}{4\pi^2}+q_1^2+q_2^2\right)^{-1/2}\right]. \tag{42}$$

For small a, one can obtain a complete asymptotic expansion of $U(0, 0; a)$ in powers of a^2 by using the Hardy sums

$$\sum_{q_{1,2}=-\infty}^{\infty}{}' (q_1^2+q_2^2)^{-s} = 4\zeta(s)\beta(s) \qquad (s>1), \tag{43}$$

which would appear among the coefficients of the expansion.

Similarly, by taking a Laplace transform of (33), we obtain

$$V(\epsilon_1, \epsilon_2; a) = \sum_{l_{1,2}=-\infty}^{\infty} \frac{\exp\{-a[(l_1+\epsilon_1)^2+(l_2+\epsilon_2)^2]^{1/2}\}}{[(l_1+\epsilon_1)^2+(l_2+\epsilon_2)^2]^{1/2}}$$

$$= \frac{2\pi}{a} + \sum_{q_{1,2}=-\infty}^{\infty}{}' \cos(2\pi\epsilon_1 q_1)\cos(2\pi\epsilon_2 q_2)\left(\frac{a^2}{4\pi^2}+q_1^2+q_2^2\right)^{-1/2} \tag{44}$$

In the limit $\epsilon_{1,2} \to 0$, $V(\epsilon_1, \epsilon_2; a) = (1/\epsilon) - a + U(0, 0; a)$; equations (42) and (44) then lead to a result identical with (36). For small a, (44) gives

$$V(\epsilon_1, \epsilon_2; a) = \frac{2\pi}{a} + P(\epsilon_1, \epsilon_2) - O(a^2). \tag{45}$$

We note that, since the right-hand side of (44) can be written as a complete sum over $\boldsymbol{q}$, this result can also be obtained by a direct application of the two-dimensional Poisson formula to the sum over $\boldsymbol{l}$.

Finally we obtain, by an appropriate manipulation of the identity

$$\sum_{l_{1,2}=-\infty}^{\infty} \exp[-a(l_1^2+l_2^2)] = \left(\frac{\pi}{a}\right) \sum_{q_{1,2}=-\infty}^{\infty} \exp\left(-\frac{\pi^2}{a}(q_1^2+q_2^2)\right),$$

the following formula (for $p \neq 0, 1$)

$$\sum_{l_{1,2}=-\infty}^{\infty}{}' \frac{\Gamma[p, a(l_1^2+l_2^2)]}{(l_1^2+l_2^2)^p}$$

$$= \frac{a^p}{p} + \frac{\pi}{(1-p)a^{1-p}} + D(p) - \pi^{2p-1} \sum_{q_{1,2}=-\infty}^{\infty}{}' \frac{\Gamma[1-p, (\pi^2/a)(q_1^2+q_2^2)]}{(q_1^2+q_2^2)^{1-p}}, \tag{46}$$

where $D(p)$ is given by

$$D(p) = 4\Gamma(p)\zeta(p)\beta(p). \tag{47}$$

For $p = \frac{1}{2}$, (46) reduces to (35), with $D(\frac{1}{2}) = \pi^{1/2}D$.

4. Lattice sums in three dimensions

Following the procedure of § 3, first of all we obtain

$$S(\boldsymbol{\epsilon}; a) = \sum_{\boldsymbol{R}}{}' \frac{\exp[2\pi i(\boldsymbol{\epsilon} \cdot \boldsymbol{R}) - aR^2]}{R^2} = a + S(\boldsymbol{\epsilon}; 0) - \pi \sum_{\boldsymbol{R}} \frac{\operatorname{erfc}(\pi a^{-1/2}|\boldsymbol{R}+\boldsymbol{\epsilon}|)}{|\boldsymbol{R}+\boldsymbol{\epsilon}|}. \tag{48}$$

The limiting case $\epsilon \to 0$ has already appeared in I:

$$S(0; a) = \frac{2\pi^{3/2}}{a^{1/2}} + C_3 + a - \pi \sum_{\boldsymbol{R}}{}' \frac{\operatorname{erfc}(\pi a^{-1/2} R)}{R}, \tag{49}$$

where

$$C_3 = \lim_{a\to 0} (S(0; a) - 2\pi^{3/2} a^{-1/2}) = -8{\cdot}913633. \tag{50}$$

Comparing (48) and (49), one obtains the asymptotic behaviour of the sum $S(\boldsymbol{\epsilon}; 0)$:

$$\lim_{\epsilon\to 0} S(\boldsymbol{\epsilon}; 0) = \frac{\pi}{\epsilon} + C_3. \tag{51}$$

The following special values of $S(\boldsymbol{\epsilon}; 0)$ may also be noted (Zucker 1975, Zasada and Pathria 1976):

$$S(0, 0, \tfrac{1}{2}; 0) = -0{\cdot}301380, \qquad S(0, \tfrac{1}{2}, \tfrac{1}{2}; 0) = -1{\cdot}830045,$$
$$S(\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}; 0) = -2{\cdot}519356. \tag{52}$$

The asymptotic behaviour of $S(\boldsymbol{\epsilon}; a)$, as $a \to 0$, is readily obtained from (48). We also obtain the following asymptotic result:

$$\lim_{a\to 0}\left(\sum_{\boldsymbol{R}} \frac{\operatorname{erfc}(a^{1/2}|\boldsymbol{R}+\boldsymbol{\epsilon}|)}{|\boldsymbol{R}+\boldsymbol{\epsilon}|}\right) = \frac{\pi}{a} + \frac{S(\boldsymbol{\epsilon}; 0)}{\pi}. \tag{53}$$

Next we obtain

$$T(\boldsymbol{\epsilon}; a) = \sum_{\boldsymbol{R}} \frac{\exp[-a(\boldsymbol{R}+\boldsymbol{\epsilon})^2]}{(\boldsymbol{R}+\boldsymbol{\epsilon})^2}$$
$$= \frac{2\pi^{3/2}}{a^{1/2}} + B(\boldsymbol{\epsilon}) - \pi \sum_{\boldsymbol{R}}{}' \frac{\exp[2\pi i(\boldsymbol{\epsilon} \cdot \boldsymbol{R})] \operatorname{erfc}(\pi a^{-1/2} R)}{R} \tag{54}$$

where

$$B(\boldsymbol{\epsilon}) = \lim_{a\to 0} (T(\boldsymbol{\epsilon}; a) - 2\pi^{3/2} a^{-1/2}) = \pi \sum_{\boldsymbol{R}}{}' \frac{\exp[2\pi i(\boldsymbol{\epsilon} \cdot \boldsymbol{R})]}{R}. \tag{55}$$

Now, in the limit $\epsilon \to 0$, $T(\boldsymbol{\epsilon}; a) = (1/\epsilon^2) - a + S(0; a)$. Hence, in view of (49) and (50),

$$B(\epsilon \to 0) = \frac{1}{\epsilon^2} + C_3. \tag{56}$$

The following special values of $B(\boldsymbol{\epsilon})$ may also be noted (Zucker 1975):

$$B(0, 0, \tfrac{1}{2}) = -2{\cdot}432806, \qquad B(0, \tfrac{1}{2}, \tfrac{1}{2}) = -4{\cdot}650782, \qquad B(\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}) = -5{\cdot}490136. \tag{57}$$

The asymptotic behaviour of $T(\boldsymbol{\epsilon}; a)$, as $a \to 0$, is readily obtained from (54) and (55)

We also obtain the following asymptotic result:

$$\lim_{a\to 0}\left(\sum_{\boldsymbol{R}}{}' \frac{\exp[2\pi \mathrm{i}(\boldsymbol{\epsilon}\cdot\boldsymbol{R})]\,\mathrm{erfc}(a^{1/2}R)}{R}\right)=\frac{B(\boldsymbol{\epsilon})}{\pi}+2\left(\frac{a}{\pi}\right)^{1/2} \tag{58}$$

Before proceeding further we wish to point out that some interesting relationships can be established by breaking the given sums $S(\boldsymbol{\epsilon}; a)$ and $T(\boldsymbol{\epsilon}; a)$ into sub-sums; for instance, one obtains

$$A(0,0,\tfrac{1}{2})=\tfrac{1}{3}[C_3-A(\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2})-B(\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2})] \tag{59a}$$

$$A(0,\tfrac{1}{2},\tfrac{1}{2})=\tfrac{1}{3}B(\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2}) \tag{59b}$$

$$B(0,0,\tfrac{1}{2})=\tfrac{1}{3}[2C_3-2A(\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2})-B(\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2})] \tag{59c}$$

and

$$B(0,\tfrac{1}{2},\tfrac{1}{2})=\tfrac{1}{3}[C_3+2A(\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2})]; \tag{59d}$$

here, $A(\boldsymbol{\epsilon})$ stands for $S(\boldsymbol{\epsilon}; 0)$. Thus, for $\epsilon_{1,2,3}=0$ or $\frac{1}{2}$, a knowledge of only three numbers, such as C_3, $A(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ and $B(\frac{1}{2},\frac{1}{2},\frac{1}{2})$, suffices. In passing, we note that equations (59) lead to the following derived relationships, which have also been noted by Zucker (1975):

$$3A(0,0,\tfrac{1}{2})+3A(0,\tfrac{1}{2},\tfrac{1}{2})+A(\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2})=C_3 \tag{60a}$$

and

$$3B(0,0,\tfrac{1}{2})+3B(0,\tfrac{1}{2},\tfrac{1}{2})+B(\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2})=3C_3. \tag{60b}$$

Next, taking Laplace transforms of identities (54) and (48), respectively, we obtain

$$\begin{aligned}U(\boldsymbol{\epsilon}; a)&=\sum_{\boldsymbol{R}}{}' \frac{\exp[2\pi\mathrm{i}(\boldsymbol{\epsilon}\,.\,\boldsymbol{R})-aR]}{R}\\ &=\frac{B(\boldsymbol{\epsilon})}{\pi}+a-\frac{a^2}{4\pi^3}\sum_{\boldsymbol{R}}\left[(\boldsymbol{R}+\boldsymbol{\epsilon})^2\left(\frac{a^2}{4\pi^2}+(\boldsymbol{R}+\boldsymbol{\epsilon})^2\right)\right]^{-1}\end{aligned} \tag{61}$$

and

$$\begin{aligned}V(\boldsymbol{\epsilon}; a)&=\sum_{\boldsymbol{R}} \frac{\exp(-a|\boldsymbol{R}+\boldsymbol{\epsilon}|)}{|\boldsymbol{R}+\boldsymbol{\epsilon}|}\\ &=\frac{4\pi}{a^2}+\frac{A(\boldsymbol{\epsilon})}{\pi}-\frac{a^2}{4\pi^3}\sum_{\boldsymbol{R}}{}'\exp[2\pi\mathrm{i}(\boldsymbol{\epsilon}\,.\,\boldsymbol{R})]\left[R^2\left(\frac{a^2}{4\pi^2}+R^2\right)\right]^{-1};\end{aligned} \tag{62}$$

we note that $B(\boldsymbol{\epsilon})=\pi U(\boldsymbol{\epsilon}; 0)$.

In the limiting case $\epsilon\to 0$, we get, using (56) and (51) respectively,

$$U(0; a)=V'(0; a)=\sum_{\boldsymbol{R}}{}'\frac{\exp(-aR)}{R}=\frac{4\pi}{a^2}+\frac{C_3}{\pi}+a-\frac{a^2}{4\pi^3}\sum_{\boldsymbol{R}}{}'\left[R^2\left(\frac{a^2}{4\pi^2}+R^2\right)\right]^{-1}, \tag{63}$$

which leads to the following asymptotic formulae:

$$\lim_{a\to 0}\left(\sum_{\boldsymbol{R}}{}'\frac{\exp(-aR)}{R}\right)=\frac{4\pi}{a^2}+\frac{C_3}{\pi}+a-\mathrm{O}(a^2) \tag{63a}$$

and

$$\lim_{a\to\infty}\left\{\sum_{\boldsymbol{R}}{}'\left[R^2\left(\frac{a^2}{4\pi^2}+R^2\right)\right]^{-1}\right\}=\frac{4\pi^3}{a}+\frac{4\pi^2C_3}{a^2}+\frac{16\pi^4}{a^4}-\mathrm{O}(\mathrm{e}^{-a}). \tag{63b}$$

Corresponding results for $\epsilon\neq 0$ can be obtained from (61) and (62).

Finally we have (for $p\neq 0, \frac{3}{2}$)

$$\sum_{\boldsymbol{R}}{}'\frac{\Gamma(p, aR^2)}{R^{2p}}=\frac{a^p}{p}+\frac{\pi^{3/2}}{(\frac{3}{2}-p)a^{\frac{3}{2}-p}}+E(p)-\pi^{2p-\frac{3}{2}}\sum_{\boldsymbol{R}}{}'\frac{\Gamma(\frac{3}{2}-p, \pi^2R^2/a)}{R^{3-2p}} \tag{64}$$

where $E(p)$ is related to the sum $\Sigma_{\boldsymbol{R}}' R^{-2p}$ and may be evaluated by substituting suitable values of a in (64); see also Zucker (1975). The special case $a=\pi, p=\frac{3}{4}$ is worth noting:

$$\sum_{\boldsymbol{R}}{}'\frac{\Gamma(\frac{3}{4}, \pi R^2)}{R^{3/2}}=\frac{4}{3}\pi^{3/4}+\frac{1}{2}E(\tfrac{3}{4}). \tag{65}$$

5. Applications and concluding remarks

The sums evaluated in the preceding sections appear in several physical problems, some of which have been mentioned in the introduction. They have been of particular relevance in our recent work on Bose–Einstein condensation in finite systems. For instance, Chaba and Pathria (1975a) have employed (25) for evaluating the sum $\Sigma_{l_{1,2}}' K_0[\mu(l_1^2+l_2^2)^{1/2}]$ which appeared in their analysis of the two-dimensional problem (see equations (11) and (14) of I). More recently, Chaba and Pathria (1976) and Zasada and Pathria (1976) have employed (49) and (63) in a similar analysis of the three-dimensional problem. In each case the use of these formulae has enabled us to discuss successfully the growth of a condensate component in the given system and to view the phenomenon of Bose–Einstein condensation in terms of a 'collapse of the lattice points of the thermogeometric space of the given system towards its origin (Greenspoon and Pathria 1974)'.

It will be noticed that the sum in (63) is equivalent to the screened Coulomb potential, at the origin, owing to an infinitely extended lattice distribution of point charges. In the limit $a\to 0$, this sum assumes the asymptotic value $(4\pi/a^2)+C_3/\pi$. Noting that

$$\int_{\boldsymbol{R}}\frac{\mathrm{e}^{-aR}}{R}\,\mathrm{d}^3R=\frac{4\pi}{a^2},$$

we find that C_3 is a measure of the electric potential at a given lattice point when a unit positive charge is placed at each of the other lattice points while a balancing negative charge is distributed uniformly throughout the space (Harris and Monkhorst 1970). Such an interpretation comes naturally from the expression (63); it remains obscure in evaluations such as of Hautot (1974). Generalizations (61) and (62) also admit of similar interpretations.

As mentioned in the introduction, our work has a direct bearing on the determination of Madelung constants and other related sums that appear in the theory of cubic lattices. For instance,

(i)

$$\alpha(\mathrm{NaCl})=\sum{}'\frac{(-1)^{l_1+l_2+l_3+1}}{(l_1^2+l_2^2+l_3^2)^{1/2}}=-U(\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2};0)=-\pi^{-1}B(\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2}). \tag{66}$$

(ii)

$$\alpha(\mathrm{CsCl}) = \sum{}^{*}\left(\frac{1}{[(l_1+\frac{1}{2})^2+(l_2+\frac{1}{2})^2+(l_3+\frac{1}{2})^2]^{1/2}} - \frac{1}{(l_1^2+l_2^2+l_3^2)^{1/2}}\right),$$

where the summation Σ^* implies that the term with $l_1 = l_2 = l_3 = 0$ is excluded from the latter part of the sum. We find that

$$\alpha(\mathrm{CsCl}) = \lim_{a\to 0}\,[V(\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2};a) - V'(0,0,0;a)] = \pi^{-1}[A(\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2}) - C_3]. \quad (67)$$

(iii)

$$\alpha(\mathrm{ZnS}) = \sum{}^{*}\left(\frac{3}{[(l_1+\frac{1}{4})^2+(l_2+\frac{3}{4})^2+(l_3+\frac{3}{4})^2]^{1/2}} + \frac{1}{[(l_1+\frac{1}{4})^2+(l_2+\frac{1}{4})^2+(l_3+\frac{1}{4})^2]^{1/2}}\right.$$
$$\left. - \frac{3}{[l_1^2+(l_2+\frac{1}{2})^2+(l_3+\frac{1}{2})^2]^{1/2}} - \frac{1}{(l_1^2+l_2^2+l_3^2)^{1/2}}\right)$$
$$= \lim_{a\to 0}\,[3V(\tfrac{1}{4},\tfrac{3}{4},\tfrac{3}{4};a) + V(\tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{4};a) - 3V(0,\tfrac{1}{2},\tfrac{1}{2};a) - V'(0,0,0;a)]$$
$$= \pi^{-1}[3A(\tfrac{1}{4},\tfrac{3}{4},\tfrac{3}{4}) + A(\tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{4}) - 3A(0,\tfrac{1}{2},\tfrac{1}{2}) - C_3]. \quad (68)$$

Now, it is straightforward to show that

$$A(\tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{4}) = A(\tfrac{1}{4},\tfrac{3}{4},\tfrac{3}{4}) = \tfrac{1}{4}A(\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2}). \quad (69)$$

In view of the relations (59*b*) and (69), equation (68) takes the form

$$\alpha(\mathrm{ZnS}) = \pi^{-1}[A(\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2}) - B(\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2}) - C_3]. \quad (70)$$

It follows that

$$\alpha(\mathrm{ZnS}) = \alpha(\mathrm{NaCl}) + \alpha(\mathrm{CsCl}), \quad (71)$$

as has been reported by several authors; see Zucker (1976).

In conclusion we wish to remark that most of the results reported in this paper are in the form of identities, valid for all $a > 0$, and relate a given sum to another one in the same dimensionality. The usefulness of these results lies in the fact that, for small values of a, the given sum, in general, is slowly convergent whereas the sum to which it is related converges rapidly. The formula in question then provides a useful asymptotic expansion of the given sum for small values of a. On the other hand, the same identity, for large values of a, provides an asymptotic expansion of the sum appearing on the right-hand side, for now it is the sum on the left-hand side of the identity that converges rapidly. This dual aspect of the Poisson summation formula makes it invaluable for handling a variety of summations that appear in the theoretical study of different physical problems.

Acknowledgments

One of us (ANC) thanks the Universidade Federal da Paraíba for granting him the leave of absence during which this work was carried out. Financial assistance provided by the National Research Council of Canada and by the University of Waterloo is also gratefully acknowledged.

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