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Evaluation of lattice sums using Poisson's summation formula III

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Abstract. Using Poisson's summation formula of dimensionality less than or equal to three, a number of slowly convergent three-dimensional lattice sums, which appear in the theory of ionic crystals, have been reduced to rapidly convergent two-dimensional sums. As a result we not only reproduce some of the formulae reported recently by Hautot and by Zucker but also obtain several new ones which exhibit a remarkably fast convergence.

1. Introduction

Recently we developed a method for the analytic evaluation of a class of lattice sums in arbitrary dimensions (Chaba and Pathria 1975, 1976; to be referred to as I and II, respectively). The central theme of this method was to convert a given slowly convergent sum into a rapidly convergent one by the application of Poisson's summation formula. Accordingly, the evaluation of a variety of sums appearing in the theoretical study of different physical systems was considerably facilitated; for reference to possible applications, see I and II.

In the present paper we report a further development of our method which leads to alternative forms for certain basic sums that appear in the theory of cubic lattices; some of these forms turn out to be reproductions of the ones reported recently by Hautot (1974, 1975) and by Zucker (1975, 1976) while others are new and, in general, exhibit a remarkably fast convergence. This is made possible by applying Poisson's summation formula, of dimensionality less than or equal to d, to a given d-dimensional sum in conjunction with the formulae

$$f(x;\alpha)=\sum_{m=-\infty}^{\infty}\frac{\cos(mx)}{m^2+\alpha^2}=\frac{\pi\cosh[(\pi-|x|)\alpha]}{\alpha\sinh(\pi\alpha)}\qquad(\alpha\neq 0)\tag{1}$$

and

$$\sum_{m=1}^{\infty}\frac{\cos(mx)}{m^2}=\frac{1}{2}\lim_{\alpha\to 0}\left(f(x;\alpha)-\frac{1}{\alpha^2}\right)=\frac{\pi^2}{6}-\frac{\pi|x|}{2}+\frac{x^2}{4}.\tag{2}$$

The notation employed in this paper is the same as in I and II, except that the summation variables are now designated as follows: m and n denote *all* integers, k and l denote *only odd* integers while p and q denote *only even* integers.

2. Evaluation of sums

We start with the two-dimensional sum

$$A(\epsilon_1, \epsilon_2) = \sum_{m_{1,2}=-\infty}^{\infty}{}' \frac{\cos(2\pi\epsilon_1 m_1)\cos(2\pi\epsilon_2 m_2)}{m_1^2 + m_2^2}, \tag{3}$$

where Σ' excludes the term with $m_1 = m_2 = 0$. For reasons of symmetry, it will be sufficient to consider $\epsilon_{1,2}$ in the range $(0, \frac{1}{2})$. Now, the summation over m_1 can be carried out using formula (1) for $m_2 \neq 0$ and formula (2) for $m_2 = 0$, with the result

$$A(\epsilon_1, \epsilon_2) = \pi^2(\tfrac{1}{3} - 2\epsilon_1 + 2\epsilon_1^2) + 2\pi \sum_{m=1}^{\infty} \frac{\cos(2\pi\epsilon_2 m)\cosh[(1-2\epsilon_1)\pi m]}{m \sinh(\pi m)}. \tag{4}$$

The original two-dimensional sum is thereby reduced to a one-dimensional sum. The following special cases may be noted (see equation (28) of II)

$$A(\tfrac{1}{2}, \tfrac{1}{2}) = -\pi \ln 2; \qquad \sum_{m=1}^{\infty} (-1)^m m^{-1} \operatorname{cosech}(\pi m) = -\tfrac{1}{2}\ln 2 + \tfrac{1}{12}\pi, \tag{5a}$$

$$A(0, \tfrac{1}{2}) = -\tfrac{1}{2}\pi \ln 2; \qquad \sum_{m=1}^{\infty} (-1)^m m^{-1} \coth(\pi m) = -\tfrac{1}{4}\ln 2 - \tfrac{1}{6}\pi, \tag{5b}$$

$$A(\tfrac{1}{2}, 0) = -\tfrac{1}{2}\pi \ln 2; \qquad \sum_{m=1}^{\infty} m^{-1} \operatorname{cosech}(\pi m) = -\tfrac{1}{4}\ln 2 + \tfrac{1}{12}\pi. \tag{5c}$$

From these results one readily obtains

$$\sum_{m=1}^{\infty} (-1)^m m^{-1} \tanh(\tfrac{1}{2}\pi m) = \tfrac{1}{4}\ln 2 - \tfrac{1}{4}\pi, \tag{6a}$$

$$\sum_{m=1}^{\infty} (-1)^m m^{-1} \coth(\tfrac{1}{2}\pi m) = -\tfrac{3}{4}\ln 2 - \tfrac{1}{12}\pi, \tag{6b}$$

$$\sum_{m=1}^{\infty} (-1)^m 2m^{-1}(e^{2\pi m} - 1)^{-1} = -\sum_{m=1}^{\infty} m^{-1} \operatorname{cosech}(2\pi m) = \tfrac{3}{4}\ln 2 - \tfrac{1}{6}\pi, \tag{6c}$$

$$\sum_{k=1}^{\infty} k^{-1} \operatorname{cosech}(\pi k) = \tfrac{1}{8}\ln 2, \qquad \sum_{p=2}^{\infty} p^{-1} \operatorname{cosech}(\pi p) = -\tfrac{3}{8}\ln 2 + \tfrac{1}{12}\pi; \tag{6d}$$

some of these results have already been reported by Hautot (1975) and by Zucker (1976). Finally, the asymptotic behaviour of $A(\epsilon_1, \epsilon_2)$, as $\epsilon = (\epsilon_1^2 + \epsilon_2^2)^{1/2} \to 0$, is given by

$$\lim_{\epsilon \to 0} A(\epsilon_1, \epsilon_2) = -2\pi \ln(\pi\epsilon) - \pi\eta, \tag{II(27)}$$

where

$$\eta = \ln\{[\Gamma(\tfrac{1}{4})]^4/(4\pi^3)\} = 0{\cdot}33160608. \tag{7}$$

It then follows from (4) that

$$\lim_{\epsilon \to 0} \sum_{m=1}^{\infty} m^{-1} \coth(\pi m)\cos(2\pi\epsilon m)$$

$$= \lim_{\epsilon \to 0} \sum_{m=1}^{\infty} m^{-1} \operatorname{cosech}(\pi m)\cosh[(1-2\epsilon)\pi m]$$

$$= -\ln(\pi\epsilon) - \tfrac{1}{6}\pi - \tfrac{1}{2}\eta. \tag{8}$$

We are now in a position to consider the three-dimensional sum

$$U(\vec{\epsilon}; a) = \sum_{m_{1,2,3}=-\infty}^{\infty}{}' \frac{\cos(2\pi\epsilon_1 m_1)\cos(2\pi\epsilon_2 m_2)\cos(2\pi\epsilon_3 m_3)\exp[-a(m_1^2+m_2^2+m_3^2)^{1/2}]}{(m_1^2+m_2^2+m_3^2)^{1/2}}. \tag{9}$$

For the part with $m_3 = 0$ we use equation (41) of II; for the remainder we apply the (two-dimensional) Poisson formula to summations over m_1 and m_2 and then carry out a straightforward summation over $m_3 \neq 0$. We get

$$\begin{aligned} U(\vec{\epsilon}; a) = a + &\sum_{m_{1,2}=-\infty}^{\infty}{}' \frac{\cos(2\pi\epsilon_1 m_1)\cos(2\pi\epsilon_2 m_2)}{(m_1^2+m_2^2)^{1/2}} \\ &- \sum_{m_{1,2}=-\infty}^{\infty} [\![[(m_1+\epsilon_1)^2+(m_2+\epsilon_2)^2]^{-1/2} \\ &- 2\pi\{a^2+4\pi^2[(m_1+\epsilon_1)^2+(m_2+\epsilon_2)^2]\}^{-1/2}]\!] \\ &+ 2\pi \sum_{m_{1,2}=-\infty}^{\infty} \frac{\cos(2\pi\epsilon_3)-\exp[-\gamma(m_1,m_2)]}{\gamma(m_1,m_2)[\cosh\gamma(m_1,m_2)-\cos(2\pi\epsilon_3)]}, \end{aligned} \tag{10}$$

where

$$\gamma(m_1, m_2) = \{a^2+4\pi^2[(m_1+\epsilon_1)^2+(m_2+\epsilon_2)^2]\}^{1/2}.$$

For $a = 0$, we get (in the notation of II)

$$\begin{aligned} B(\vec{\epsilon}) &= \pi U(\vec{\epsilon}; 0) \\ &= \pi \sum_{m_{1,2}=-\infty}^{\infty}{}' \frac{\cos(2\pi\epsilon_1 m_1)\cos(2\pi\epsilon_2 m_2)}{(m_1^2+m_2^2)^{1/2}} \\ &+ \pi \sum_{m_{1,2}=-\infty}^{\infty} \frac{\cos(2\pi\epsilon_3)-\exp\{-2\pi[(m_1+\epsilon_1)^2+(m_2+\epsilon_2)^2]^{1/2}\}}{[(m_1+\epsilon_1)^2+(m_2+\epsilon_2)^2]^{1/2}[\![\cosh\{2\pi[(m_1+\epsilon_1)^2+(m_2+\epsilon_2)^2]^{1/2}\}-\cos(2\pi\epsilon_3)]\!]}. \end{aligned} \tag{11}$$

Now

$$\lim_{\epsilon\to 0} \sum_{m_{1,2}=-\infty}^{\infty}{}' \frac{\cos(2\pi\epsilon_1 m_1)\cos(2\pi\epsilon_2 m_2)}{(m_1^2+m_2^2)^{1/2}} = \frac{1}{\epsilon} + 4\zeta(\tfrac{1}{2})\beta(\tfrac{1}{2}) \qquad \text{II(36)}$$

and

$$\lim_{\epsilon\to 0} B(\vec{\epsilon}) = \frac{1}{\epsilon^2} + C_3, \qquad \text{II(56)}$$

where

$$\zeta(s) = \sum_{m=0}^{\infty} (m+1)^{-s}, \qquad \beta(s) = \sum_{m=0}^{\infty} (-1)^m (2m+1)^{-s}$$

and C_3 is a constant defined by

$$C_3 = \lim_{a\to 0}\left(\sum_{\boldsymbol{R}_3}{}' \frac{\exp(-aR^2)}{R^2} - 2\pi^{3/2}a^{-1/2}\right); \qquad \text{II(50)}$$

in Zucker's notation, $C_3 = a(2) = -8{\cdot}91363292$. Taking the limit $\epsilon \to 0$ in (11) and using the foregoing results, we obtain for C_3:

$$C_3 = \tfrac{1}{3}\pi^2 + 4\pi\zeta(\tfrac{1}{2})\beta(\tfrac{1}{2}) + 2\pi \sum_{m_{1,2}=-\infty}^{\infty}{}' (m_1^2+m_2^2)^{-1/2}\{\exp[2\pi(m_1^2+m_2^2)^{1/2}]-1\}^{-1}. \quad (12a)$$

Using equation (A.1) of the appendix, we obtain a very rapidly converging expression, namely:

$$C_3 = 4\pi \ln 2 - \tfrac{1}{3}\pi^2 + 4\pi\zeta(\tfrac{1}{2})\beta(\tfrac{1}{2}) - 2\pi\eta$$
$$+ 8\pi \sum_{m_{1,2}=1}^{\infty} (m_1^2+m_2^2)^{-1/2}\{\exp[2\pi(m_1^2+m_2^2)^{1/2}]-1\}^{-1}. \quad (12b)$$

For obtaining an accuracy of 1 in 10^9, it is sufficient to take only four terms of the final series in equation (12*b*).

We now consider other special values of $B(\epsilon_1, \epsilon_2, \epsilon_3)$. First of all, using equation (38) of II, we obtain

$$B(\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}) = 4(\sqrt{2}-1)\pi\zeta(\tfrac{1}{2})\beta(\tfrac{1}{2}) - 16\pi \sum_{k,l=1}^{\infty} (k^2+l^2)^{-1/2}\{\exp[\pi(k^2+l^2)^{1/2}]+1\}^{-1}. \quad (13)$$

Next, using equations (38) of II and (A.4), we get

$$B(0, \tfrac{1}{2}, \tfrac{1}{2}) = B(\tfrac{1}{2}, 0, \tfrac{1}{2})$$
$$= 2\sqrt{2}(\sqrt{2}-1)\pi\zeta(\tfrac{1}{2})\beta(\tfrac{1}{2}) - \pi\eta$$
$$- 16\pi \sum_{k=1}^{\infty}\sum_{p=2}^{\infty} (k^2+p^2)^{-1/2}\{\exp[\pi(k^2+p^2)^{1/2}]+1\}^{-1}. \quad (14a)$$

However, if we take $\epsilon_1 = \epsilon_2 = \frac{1}{2}$ and $\epsilon_3 = 0$, we get instead

$$B(\tfrac{1}{2}, \tfrac{1}{2}, 0) = 4(\sqrt{2}-1)\pi\zeta(\tfrac{1}{2})\beta(\tfrac{1}{2}) + 16\pi \sum_{k,l=1}^{\infty} (k^2+l^2)^{-1/2}\{\exp[\pi(k^2+l^2)^{1/2}]-1\}^{-1}. \quad (14b)$$

Equating (14*a*) and (14*b*), we obtain the following sum in a *closed* form:

$$\sum_{k=1}^{\infty}\sum_{m=1}^{\infty} (k^2+m^2)^{-1/2}\{\exp[\pi(k^2+m^2)^{1/2}]+(-1)^m\}^{-1}$$
$$= \frac{4-3\sqrt{2}}{8}\zeta(\tfrac{1}{2})\beta(\tfrac{1}{2}) - \frac{1}{16}\eta = 0{\cdot}00884846. \quad (15)$$

Next, using equations (38) of II and (A.3), we get

$$B(0, \tfrac{1}{2}, 0) = B(\tfrac{1}{2}, 0, 0)$$
$$= \pi \ln 2 + 2\sqrt{2}(\sqrt{2}-1)\pi\zeta(\tfrac{1}{2})\beta(\tfrac{1}{2}) - \pi\eta$$
$$+ 16\pi \sum_{k=1}^{\infty}\sum_{p=2}^{\infty} (k^2+p^2)^{-1/2}\{\exp[\pi(k^2+p^2)^{1/2}]-1\}^{-1}. \quad (16a)$$

However, if we take $\epsilon_3 = \frac{1}{2}$ and let $\epsilon_1 = \epsilon_2 \to 0$, we get, using (36) of II and (A.2),

$$B(0, 0, \tfrac{1}{2}) = 10\pi \ln 2 - \pi^2 + 4\pi\zeta(\tfrac{1}{2})\beta(\tfrac{1}{2}) - 2\pi\eta$$
$$- 16\pi \sum_{p,q=2}^{\infty} (p^2+q^2)^{-1/2}\{\exp[\pi(p^2+q^2)^{1/2}]+1\}^{-1}. \quad (16b)$$

Equating (16*a*) and (16*b*), we obtain another sum in a *closed* form:

$$\sum_{p=2}^{\infty}\sum_{m=1}^{\infty}(p^2+m^2)^{-1/2}\{\exp[\pi(p^2+m^2)^{1/2}]+(-1)^m\}^{-1}$$
$$=\frac{9}{16}\ln 2-\frac{\pi}{16}+\frac{\sqrt{2}}{8}\zeta(\tfrac{1}{2})\beta(\tfrac{1}{2})-\frac{1}{16}\eta=0\cdot00045138. \tag{17}$$

Clearly, formulae (15) and (17) are more basic than the one reported by Hautot (1975), namely:

$$\sum_{m,n=1}^{\infty}(-1)^n(m^2+n^2)^{-1/2}\{\exp[\pi(m^2+n^2)^{1/2}]+(-1)^m\}^{-1}$$
$$=\frac{9}{16}\ln 2-\frac{\pi}{16}+\frac{\sqrt{2}-1}{2}\zeta(\tfrac{1}{2})\beta(\tfrac{1}{2}), \tag{18}$$

which follows quite simply by subtracting (15) from (17). On the other hand, adding (15) to (17), we obtain another result of this type:

$$\sum_{m,n=1}^{\infty}(m^2+n^2)^{-1/2}\{\exp[\pi(m^2+n^2)^{1/2}]+(-1)^m\}^{-1}$$
$$=\frac{9}{16}\ln 2-\frac{\pi}{16}-\frac{2-\sqrt{2}}{4}\zeta(\tfrac{1}{2})\beta(\tfrac{1}{2})-\frac{1}{8}\eta. \tag{19}$$

We now consider the sum

$$V(\vec{\epsilon};a)=\sum_{m_{1,2,3}=-\infty}^{\infty}\frac{\exp\{-a[(m_1+\epsilon_1)^2+(m_2+\epsilon_2)^2+(m_3+\epsilon_3)^2]^{1/2}\}}{[(m_1+\epsilon_1)^2+(m_2+\epsilon_2)^2+(m_3+\epsilon_3)^2]^{1/2}}. \tag{20}$$

Applying Poisson's summation formula in three dimensions, this sum takes the form

$$V(\vec{\epsilon};a)=4\pi\sum_{m_{1,2,3}=-\infty}^{\infty}\frac{\cos(2\pi\epsilon_1m_1)\cos(2\pi\epsilon_2m_2)\cos(2\pi\epsilon_3m_3)}{a^2+4\pi^2(m_1^2+m_2^2+m_3^2)}. \tag{21}$$

Summing over m_3, with the help of formula (1), we are left with a two-dimensional sum, namely:

$$V(\vec{\epsilon};a)=\pi\sum_{m_{1,2}=-\infty}^{\infty}\frac{\cos(2\pi\epsilon_1m_1)\cos(2\pi\epsilon_2m_2)\cosh[(1-2\epsilon_3)\xi(m_1,m_2)]}{\xi(m_1,m_2)\sinh\xi(m_1,m_2)}, \tag{22}$$

where

$$\xi(m_1,m_2)=[\tfrac{1}{4}a^2+\pi^2(m_1^2+m_2^2)]^{1/2}.$$

For $a\to 0$, we have (in the notation of II)

$$A(\vec{\epsilon})=\sum_{m_{1,2,3}=-\infty}^{\infty}{}'\frac{\cos(2\pi\epsilon_1m_1)\cos(2\pi\epsilon_2m_2)\cos(2\pi\epsilon_3m_3)}{m_1^2+m_2^2+m_3^2} \tag{23}$$

$$=\lim_{a\to 0}\pi\left(V(\vec{\epsilon};a)-\frac{4\pi}{a^2}\right) \tag{24}$$

$$= \pi^2(\tfrac{1}{3} - 2\epsilon_3 + 2\epsilon_3^2)$$
$$+ 2\pi \sum_{m=1}^{\infty} \frac{[\cos(2\pi\epsilon_1 m) + \cos(2\pi\epsilon_2 m)] \cosh[(1-2\epsilon_3)\pi m]}{m \sinh(\pi m)}$$
$$+ 4\pi \sum_{m_{1,2}=1}^{\infty} \frac{\cos(2\pi\epsilon_1 m_1)\cos(2\pi\epsilon_2 m_2)\cosh[(1-2\epsilon_3)\pi(m_1^2+m_2^2)^{1/2}]}{(m_1^2+m_2^2)^{1/2}\sinh[\pi(m_1^2+m_2^2)^{1/2}]}. \tag{25}$$

The following cases of $A(\epsilon_1, \epsilon_2, \epsilon_3)$ are of special interest.

First of all, using ($5a$), we obtain

$$A(\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}) = -2\pi \ln 2 + \tfrac{1}{6}\pi^2 + 4\pi \sum_{m_{1,2}=1}^{\infty} (-1)^{m_1+m_2}$$
$$\times (m_1^2+m_2^2)^{-1/2} \operatorname{cosech}[\pi(m_1^2+m_2^2)^{1/2}]. \tag{26}$$

Next, using ($5a$) and ($5c$), we get

$$A(0, \tfrac{1}{2}, \tfrac{1}{2}) = A(\tfrac{1}{2}, 0, \tfrac{1}{2})$$
$$= -\tfrac{3}{2}\pi \ln 2 + \tfrac{1}{6}\pi^2$$
$$+ 4\pi \sum_{m_{1,2}=1}^{\infty} (-1)^{m_1}(m_1^2+m_2^2)^{-1/2} \operatorname{cosech}[\pi(m_1^2+m_2^2)^{1/2}]. \tag{27}$$

However, if we take $\epsilon_1 = \epsilon_2 = \frac{1}{2}$ and $\epsilon_3 = 0$ and use ($5b$), we get instead

$$A(\tfrac{1}{2}, \tfrac{1}{2}, 0) = -\pi \ln 2 - \tfrac{1}{3}\pi^2 + 4\pi \sum_{m_{1,2}=1}^{\infty} (-1)^{m_1+m_2}$$
$$\times (m_1^2+m_2^2)^{-1/2} \coth[\pi(m_1^2+m_2^2)^{1/2}]. \tag{28}$$

Combining (28) with the formula

$$\sum_{m_{1,2}=1}^{\infty} (-1)^{m_1+m_2}(m_1^2+m_2^2)^{-1/2} = \ln 2 + (\sqrt{2}-1)\zeta(\tfrac{1}{2})\beta(\tfrac{1}{2}), \tag{29}$$

we obtain a very rapidly converging form:

$$A(\tfrac{1}{2}, \tfrac{1}{2}, 0) = 3\pi \ln 2 - \tfrac{1}{3}\pi^2 + 4(\sqrt{2}-1)\pi\zeta(\tfrac{1}{2})\beta(\tfrac{1}{2})$$
$$+ 8\pi \sum_{m_{1,2}=1}^{\infty} (-1)^{m_1+m_2}(m_1^2+m_2^2)^{-1/2}\{\exp[2\pi(m_1^2+m_2^2)^{1/2}]-1\}^{-1}. \tag{30}$$

Next, we obtain

$$A(0, 0, \tfrac{1}{2}) = -\pi \ln 2 + \tfrac{1}{6}\pi^2 + 4\pi \sum_{m_{1,2}=1}^{\infty} (m_1^2+m_2^2)^{-1/2} \operatorname{cosech}[\pi(m_1^2+m_2^2)^{1/2}]. \tag{31}$$

However, if we take $\epsilon_3 = 0$ and $\epsilon_1 = 0$, $\epsilon_2 = \frac{1}{2}$ (or $\epsilon_3 = 0$ and $\epsilon_1 = \frac{1}{2}$, $\epsilon_2 = 0$), we encounter divergencies which, in the end, get cancelled. This requires a cautious use of the formulae ($5b$), (8) and II(38), along with the standard result,

$$\sum_{m=1}^{\infty} m^{-1}\cos(2\pi\epsilon m) = -\ln[2\sin(\pi\epsilon)]. \tag{32}$$

We finally obtain

$$A(0,\tfrac{1}{2},0)=A(\tfrac{1}{2},0,0)$$
$$=\tfrac{7}{2}\pi\ln 2-\tfrac{1}{3}\pi^2+2\sqrt{2}(\sqrt{2}-1)\pi\zeta(\tfrac{1}{2})\beta(\tfrac{1}{2})-\pi\eta$$
$$+8\pi\sum_{m_{1,2}=1}^{\infty}(-1)^{m_1}(m_1^2+m_2^2)^{-1/2}\{\exp[2\pi(m_1^2+m_2^2)^{1/2}]-1\}^{-1}, \qquad (33)$$

which again is very rapidly convergent. In a private communication, Zucker has informed us of another form for $A(0,0,\tfrac{1}{2})$ (equal to $b(2)$ in his notation) which converges even faster than (33).

3. Applications and conclusions

The results reported here find immediate application in the evaluation of Madelung constants and other related sums for different lattice structures. For instance, the Madelung constant for NaCl is given by

$$\alpha(\mathrm{NaCl})=-\pi^{-1}B(\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2}). \qquad (34)$$

Substituting (13) into (34), we recover the result first established by Hautot (1974) with the aid of the Schlömlich series. However, $\alpha(\mathrm{NaCl})$ is also given by, see II(59*b*),

$$\alpha(\mathrm{NaCl})=-3\pi^{-1}A(0,\tfrac{1}{2},\tfrac{1}{2}). \qquad (35)$$

Substituting (27) into (35), we recover instead the more recent formula derived by Hautot (1975) and by Zucker (1976). If, on the other hand, we substitute (30) into (35), we obtain a new expression for $\alpha(\mathrm{NaCl})$ which, to our knowledge, is the most rapidly converging expression reported to date:

$$\alpha(\mathrm{NaCl})=-9\ln 2+\pi-12(\sqrt{2}-1)\zeta(\tfrac{1}{2})\beta(\tfrac{1}{2})$$
$$-24\sum_{m_{1,2}=1}^{\infty}(-1)^{m_1+m_2}(m_1^2+m_2^2)^{-1/2}\{\exp[2\pi(m_1^2+m_2^2)^{1/2}]-1\}^{-1}. \qquad (36)$$

As in the case of equation (12*b*) for C_3, only four terms of the final series (instead of Hautot's nine) suffice for obtaining an accuracy of 1 in 10^9. It may be mentioned here that equation (36) has also been derived independently by Zucker (private communication).

Next, the Madelung constant for CsCl is given by, see II(59), II(60) and II(67),

$$\alpha(\mathrm{CsCl})=\pi^{-1}[A(\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2})-C_3] \qquad (37)$$
$$=-3\pi^{-1}[A(0,0,\tfrac{1}{2})+A(0,\tfrac{1}{2},\tfrac{1}{2})] \qquad (38)$$
$$=-\tfrac{3}{2}\pi^{-1}[B(0,0,\tfrac{1}{2})+A(0,\tfrac{1}{2},\tfrac{1}{2})]. \qquad (39)$$

Substituting (27) and (31) into (38), we recover the recent formula of Hautot (1975). If, on the other hand, we substitute (16*b*) and (30) into (39), we obtain

$$\alpha(\mathrm{CsCl})=-\tfrac{39}{2}\ln 2+2\pi-6\sqrt{2}\zeta(\tfrac{1}{2})\beta(\tfrac{1}{2})+3\eta$$
$$+24\sum_{k=1}^{\infty}\sum_{p=2}^{\infty}(k^2+p^2)^{-1/2}\operatorname{cosech}[2\pi(k^2+p^2)^{1/2}]$$
$$-12\sum_{m,n=1}^{\infty}[1+(-1)^{m+n}](m^2+n^2)^{-1/2}\{\exp[4\pi(m^2+n^2)^{1/2}]-1\}^{-1}. \qquad (40)$$

The remarkable feature of this result is that the closed part alone provides an accuracy of 1 in 10^5. The inclusion of only one term of the first series on the right-hand side improves the accuracy to 1 in 10^7; further inclusion of one term of the second series makes it 1 in 10^9.

At this stage we wish to remark that the considerable improvement in the convergence of the series expansions reported here implies the following useful reductions:

$$\sum_{k,l=1}^{\infty} (k^2+l^2)^{-1/2}\{\exp[\pi(k^2+l^2)^{1/2}]+1\}^{-1}$$
$$= -\frac{9}{16}\ln 2+\frac{\pi}{16}-\frac{\sqrt{2}-1}{2}\zeta(\tfrac{1}{2})\beta(\tfrac{1}{2})-\frac{3}{2}(S_1-2S_2+S_3), \tag{41}$$

$$\sum_{k,l=1}^{\infty} (k^2+l^2)^{-1/2}\operatorname{cosech}[\pi(k^2+l^2)^{1/2}]$$
$$= -\tfrac{9}{8}\ln 2+\tfrac{1}{8}\pi-(\sqrt{2}-1)\zeta(\tfrac{1}{2})\beta(\tfrac{1}{2})-(S_1-6S_2+3S_3), \tag{42}$$

$$\sum_{k=1}^{\infty}\sum_{p=2}^{\infty} (k^2+p^2)^{-1/2}\operatorname{cosech}[\pi(k^2+p^2)^{1/2}]$$
$$=\frac{9}{8}\ln 2-\frac{\pi}{8}+\frac{\sqrt{2}}{4}\zeta(\tfrac{1}{2})\beta(\tfrac{1}{2})-\frac{1}{8}\eta-(S_1+4S_2-3S_3), \tag{43}$$

and

$$\sum_{p,q=2}^{\infty} (p^2+q^2)^{-1/2}\operatorname{cosech}[\pi(p^2+q^2)^{1/2}]=S_1+2S_2-S_3, \tag{44}$$

where

$$S_1=\sum_{k,l=1}^{\infty} (k^2+l^2)^{-1/2}\{\exp[2\pi(k^2+l^2)^{1/2}]-1\}^{-1}, \tag{45}$$

$$S_2=\sum_{k=1}^{\infty}\sum_{p=2}^{\infty} (k^2+p^2)^{-1/2}\{\exp[2\pi(k^2+p^2)^{1/2}]-1\}^{-1}, \tag{46}$$

and

$$S_3=\sum_{p,q=2}^{\infty} (p^2+q^2)^{-1/2}\{\exp[2\pi(p^2+q^2)^{1/2}]-1\}^{-1}. \tag{47}$$

Clearly, the series (45)–(47) converge much more rapidly than the ones appearing on the left-hand sides of (41)–(43).

In the end we observe that the formulae reported here enable us to render the important lattice sum

$$U(0;a)=\sum_{\boldsymbol{R}_3}{}' R^{-1}\exp(-aR) \tag{48}$$

into a very useful form which contains only two-dimensional sums that are far more tractable than the original sum itself. For this we employ equation (10) for $U(\vec{\epsilon};a)$ and let $\epsilon \to 0$. Using II(36), we obtain

$$U(0;a) = (2\pi/a)\coth(\tfrac{1}{2}a) + 4\zeta(\tfrac{1}{2})\beta(\tfrac{1}{2}) + a - \sum_{m_{1,2}=-\infty}^{\infty}{}' \{(m_1^2+m_2^2)^{-1/2}$$
$$-2\pi[a^2+4\pi^2(m_1^2+m_2^2)]^{-1/2}\} + 4\pi \sum_{m_{1,2}=-\infty}^{\infty}{}' [a^2+4\pi^2(m_1^2+m_2^2)]^{-1/2}$$
$$\times\{\exp[a^2+4\pi^2(m_1^2+m_2^2)]^{1/2}-1\}^{-1}, \tag{49}$$

valid for all $a > 0$. While the second sum on the right-hand side converges very rapidly, the first sum can be expressed as a power series in a^2 by using the Hardy sums,

$$\sum_{m_{1,2}=-\infty}^{\infty}{}' (m_1^2+m_2^2)^{-s} = 4\zeta(s)\beta(s) \qquad (s>1), \tag{50}$$

which would appear among the coefficients of the expansion. For $a \ll 1$, we obtain, using (12*a*),

$$U(0;a) = \frac{4\pi}{a^2} + \frac{C_3}{\pi} + a - O(a^2), \tag{51}$$

in agreement with II(63*a*).

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Appendix

We consider the sum

$$S_- = \sum_{m=1}^{\infty} m^{-1}(e^{2\pi m}-1)^{-1},$$

which may be written as

$$S_- = \sum_{m=1}^{\infty}\sum_{n=1}^{\infty} m^{-1} e^{-2\pi mn} = -\sum_{n=1}^{\infty} \ln(1-e^{-2\pi n}) = -\tfrac{1}{6}\ln\prod_{n=1}^{\infty}(1-e^{-2\pi n})^6.$$

Using Jacobi's formula in traditional notation (see Whittaker and Watson 1927), namely:

$$\prod_{n=1}^{\infty}(1-q^{2n})^6 = 2\pi^{-3}q^{-1/2}\kappa\kappa' K^3,$$

with $q = e^{-\pi}$, we obtain

$$\kappa = \kappa' = 1/\sqrt{2} \qquad \text{and} \qquad K = [\Gamma(\tfrac{1}{4})]^2/(4\sqrt{\pi}),$$

whence

$$S_- = \tfrac{1}{2}\ln 2 - \tfrac{1}{12}\pi - \tfrac{1}{4}\eta \qquad \left(\eta = \ln\frac{[\Gamma(\frac{1}{4})]^4}{4\pi^3} = 0{\cdot}33160608\right). \tag{A.1}$$

Similarly

$$S_+ = \sum_{m=1}^{\infty} m^{-1}(e^{2\pi m}+1)^{-1} = -\tfrac{5}{4}\ln 2 + \tfrac{1}{4}\pi + \tfrac{1}{4}\eta. \tag{A.2}$$

We note that $S_+ + S_- = -\frac{3}{4}\ln 2 + \frac{1}{6}\pi$, in agreement with (6*c*).

Using the same method, we obtain other results such as

$$\sum_{k=1}^{\infty} k^{-1}(e^{\pi k}-1)^{-1} = \tfrac{1}{8}\ln 2 - \tfrac{1}{8}\eta \tag{A.3}$$

$$\sum_{k=1}^{\infty} k^{-1}(e^{\pi k}+1)^{-1} = \tfrac{1}{8}\eta. \tag{A.4}$$

Adding (A.3) and (A.4), we get

$$\sum_{k=1}^{\infty} k^{-1}\operatorname{cosech}(\pi k) = \tfrac{1}{8}\ln 2, \tag{A.5}$$

in agreement with (6*d*). Other combinations yield the following results:

$$\sum_{m=1}^{\infty} m(e^{\pi m}-1)^{-1} = \tfrac{3}{8}\ln 2 - \tfrac{1}{24}\pi - \tfrac{1}{4}\eta \tag{A.6}$$

$$\sum_{m=1}^{\infty} m(e^{\pi m}+1)^{-1} = -\tfrac{5}{8}\ln 2 + \tfrac{1}{8}\pi + \tfrac{1}{4}\eta. \tag{A.7}$$

Clearly, several other sums can be evaluated, or constructed, with the help of the foregoing results.

In passing we quote the remarkable sum (Whittaker and Watson 1927)

$$\sum_{k=1}^{\infty} e^{-\pi k^2} = \frac{(2^{1/4}-1)\Gamma(1/4)}{2^{11/4}\pi^{3/4}}, \tag{A.8}$$

which does not really fall into the class of sums studied in this paper; it is quoted just for the readers' delight.

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