J. Phys. A: Math. Gen., Vol. 9, No. 4, 1976. Printed in Great Britain. © 1976

Functional equations for poly-dimensional zeta functions and the evaluation of Madelung constants

I J Zucker
Department of Physics, University of Surrey, Guildford, Surrey, UK

Received 13 October 1975, in final form 15 December 1975

Abstract. The lattice sums required to evaluate Madelung constants of ionic crystals are very slowly convergent if summed directly. A method is given of transforming these sums to other series which not only are rapidly convergent but involve the use of elementary functions only.

1. Introduction

In a previous publication, henceforth referred to as I, Zucker (1975) showed how the Madelung constant, α, and other lattice sums for invariant cubic lattice complexes could be written as a linear combination of at most eight independent sums. For many common lattices only three of these sums sufficed. These were

$$b(2s)=\sum{}'(-1)^m(m^2+n^2+p^2)^{-s}, \tag{1.1}$$

$$c(2s)=\sum{}'(-1)^{m+n}(m^2+n^2+p^2)^{-s}, \tag{1.2}$$

$$d(2s)=\sum{}'(-1)^{m+n+p}(m^2+n^2+p^2)^{-s}. \tag{1.3}$$

A further useful sum, $a(2s)$, given by

$$a(2s)=\sum{}'(m^2+n^2+p^2)^{-s} \tag{1.4}$$

was also considered, but in I it was shown that

$$(2^{3-2s}-1)a(2s)=3b(2s)+3c(2s)+d(2s). \tag{1.5}$$

$\sum'$ implies the sums to be over all integer values of indices appearing, excluding only the case where they are simultaneously zero. To evaluate α the appropriate value of s is $\frac{1}{2}$ and typical results for some ionic crystals given in I were

$$\alpha(\mathrm{NaCl})=2d(1); \qquad \alpha(\mathrm{ZnS})=3[b(1)+d(1)]/2;$$
$$\alpha(\mathrm{CsCl})=[3b(1)+d(1)]/2=3[a(1)-c(1)]/2. \tag{1.6}$$

The values of α are all in terms of the basic cube side formed by one species of ion. The sums $b(1)-d(1)$ are very slowly convergent. Indeed $a(1)$ as defined by (1.4) diverges, but it has a value as determined by (1.5).

In a recent paper, Hautot (1974) developed a method used by van der Hoff and Benson (1953) which enabled such sums to be calculated very rapidly. The method used Hankel integral transforms and Schlömilch series. In a further paper Hautot (1975) developed his approach and transformed the sums into quickly convergent series involving elementary functions only. Here we shall re-derive Hautot's (1975) results without using Hankel transforms or Schlömilch series. The results will be derived from functional relations deduced for $a(2s)-d(2s)$, which incidentally enable us to evaluate these as functions of s for negative arguments. In addition to the functional equations the standard result

$$\sum_{-\infty}^{\infty}(-1)^m(m^2+b^2)^{-1}=(\pi \operatorname{cosech} \pi b)/b \tag{1.7}$$

will be used. This formula is found in many books on complex variable, e.g. Phillips (1951).

2. Functional equations for $a(2s)-d(2s)$

In I, $a(2s)-d(2s)$ were represented as Mellin transforms of Jacobian θ functions. Briefly recapitulating, let M_s be the Mellin operator defined by

$$\Gamma(s)\,M_s(f(t))=\int_0^{\infty} t^{s-1}f(t)\,dt \tag{2.1}$$

where $\Gamma(s)$ is the gamma function. Further let

$$\theta_2=\theta_2(q)=\sum_{-\infty}^{\infty} q^{(n-\frac{1}{2})^2}; \qquad \theta_3=\theta_3(q)=\sum_{-\infty}^{\infty} q^{n^2}; \qquad \theta_4=\theta_4(q)=\sum_{-\infty}^{\infty}(-1)^n q^{n^2}. \tag{2.2}$$

They yield the identities

$$\theta_3=\theta_3(q^4)+\theta_2(q^4); \qquad \theta_4=\theta_3(q^4)-\theta_2(q^4). \tag{2.3}$$

Then

$$a(2s)=M_s(\theta_3^3-1) \tag{2.4}$$

$$b(2s)=M_s(\theta_3^2\theta_4-1) \tag{2.5}$$

$$c(2s)=M_s(\theta_3\theta_4^2-1) \tag{2.6}$$

$$d(2s)=M_s(\theta_4^3-1) \qquad \text{with } q=e^{-t}. \tag{2.7}$$

An important property of M_s is that

$$M_s(f(q^k))=k^{-s}M_s(f(q)), \qquad q=e^{-t}. \tag{2.8}$$

These formulae were all discussed in I. Here some further well known results are required, namely the relations

$$t^{1/2}\theta_3(e^{-\pi t})=\theta_3(e^{-\pi/t}); \qquad t^{1/2}\theta_2(e^{-\pi t})=\theta_4(e^{-\pi/t}), \tag{2.9}$$

which are forms of the Poisson summation formula. The application of (2.8) and (2.9) to (2.4)–(2.7) together with the use of (2.3) when necessary will yield relations between

$a(2s)-d(2s)$ and $a(3-2s)-d(3-2s)$. The method is illustrated by applying it to the simpler 1- and 2-dimensional sums first.

Consider the 1-dimensional sum

$$A(1{:}2s)=\sum{}'(m^2)^{-s}=\mathrm{M}_s(\theta_3-1). \tag{2.10}$$

From (2.8) one has

$$\begin{aligned}\mathrm{M}_s(\theta_3-1)&=\pi^s\mathrm{M}_s[\theta_3(\mathrm{e}^{-\pi t}-1)]=\pi^s\mathrm{M}_s[t^{-1/2}\theta_3(\mathrm{e}^{-\pi/t})-1]\\&=K(\tfrac{1}{2},s)M_{\frac{1}{2}-s}(\theta_3-1)\end{aligned} \tag{2.11}$$

where

$$K(D/2,s)=\frac{\pi^{2s-D/2}\Gamma(D/2-s)}{\Gamma(s)}$$

and D is the dimensionality of the sum. Thus (2.11) gives

$$A(1{:}2s)=K(\tfrac{1}{2},s)A(1{:}1-2s). \tag{2.12}$$

But $A(1{:}2s)$ is just the Riemann zeta function, $\zeta(2s)$, and (2.12) is nothing but the well-known functional relation for $\zeta(2s)$. Indeed the above derivation is one of the standard methods of obtaining the relation and is demonstrated, for example, in Titchmarsh (1951). $\zeta(2s)$ has a simple pole at $2s=1$. (2.12) allows us to analytically continue $\zeta(2s)$ to values of $2s<1$.

Consider now the 2-dimensional sum

$$A(2{:}2s)=\sum\sum{}'(m^2+n^2)^{-s}=\mathrm{M}_s(\theta_3^2-1) \tag{2.13}$$

which could be considered as a 2-dimensional zeta function. Using the same method as before we have

$$A(2{:}2s)=K(1{:}s)A(2{:}2-2s). \tag{2.14}$$

It so happens that $A(2{:}2s)$ can be decomposed into a product of simple sums (Hardy 1919) thus

$$A(2{:}2s)=4\zeta(s)\beta(s),\qquad \text{where } \beta(s)=\sum_0^\infty(-1)^n(2n+1)^{-s}. \tag{2.15}$$

(2.14) after some rearrangement then yields the elegant relation

$$\frac{\Gamma(s)\zeta(s)\beta(s)}{\pi^s}=\frac{\Gamma(1-s)\zeta(1-s)\beta(1-s)}{\pi^{1-s}}. \tag{2.16}$$

$A(2{:}2s)$ has a simple pole at $s=1$ and again the functional equation enables us to continue the function for $s<1$.

Now $a(2s)=A(3{:}2s)$ is the 3-dimensional analogue of the zeta function. As far as is known it cannot be decomposed into a product of simple sums as can $A(2{:}2s)$. Nevertheless its functional relation is easily derived giving

$$a(2s)=K(3/2,s)a(3-2s). \tag{2.17}$$

$a(2s)$ has a simple pole at $s=3/2$ and (2.17) allows us to analytically continue $a(2s)$ into the region $s<3/2$. Functional relations for $b(2s)-d(2s)$ may be derived similarly but using somewhat more algebra. They are

$$b(2s)=2^{-2s}K(3/2,s)[a(3-2s)+b(3-2s)-c(3-2s)-d(3-2s)] \tag{2.18}$$

$$c(2s)=2^{-2s}K(3/2,s)[a(3-2s)-b(3-2s)-c(3-2s)+d(3-2s)] \tag{2.19}$$

$$d(2s)=2^{-2s}K(3/2,s)[a(3-2s)-3b(3-2s)+3c(3-2s)-d(3-2s)]. \tag{2.20}$$

If s is put equal to $\frac{1}{2}$ then $K(\frac{3}{2},\frac{1}{2})=\pi^{-1}$. With the aid of (1.5) the following relations are found

$$3a(1)=3b(1)+3c(1)+d(1); \qquad a(2)=3b(2)+3c(2)+d(2);$$
$$\pi a(1)=a(2); \qquad \pi b(1)=2b(2)+c(2); \qquad \pi c(1)=b(2)+c(2)+d(2);$$
$$\pi d(1)=3c(2). \tag{2.21}$$

Of all eight unknowns $a(1)-d(1)$ and $a(2)-d(2)$, only three are independent. Hence all may be found knowing say $b(2)-d(2)$. In their form (1.1)–(1.3) they are hardly more rapidly convergent than $b(1)-d(1)$, but using (1.7) they can be converted into speedily convergent sums of elementary functions. This is now illustrated with $c(2)$. This may be decomposed using the result $\Sigma_{-\infty}^{\infty} f(n^2)=f(0)+2\Sigma_1^{\infty} f(n^2)$ thus

$$c(2)=\sum{}'(-1)^{m+n}(m^2+n^2+p^2)^{-1}=S_1+S_2+S_3+S_4. \tag{2.22}$$

$$S_1=-\sum{}'(-1)^m m^{-2}; \qquad S_2=\sum{}'(-1)^m(m^2+p^2)^{-1};$$

$$S_3=\sum{}'(-1)^{m+n}(m^2+n^2)^{-1};$$

$$S_4=4\sum_{-\infty}^{\infty}\sum_{1}^{\infty}\sum_{1}^{\infty}(-1)^{m+n}(m^2+n^2+p^2)^{-1}.$$

S_1 is just $\pi^2/6$. S_2 and S_3 can be derived from the results of Glasser (1973) and Zucker (1974) yielding $S_2=-\frac{1}{2}\pi\ln 2$ and $S_3=-\pi\ln 2$. Using (1.7), S_4 becomes

$$S_4=4\pi\sum_1^{\infty}\sum_1^{\infty}\frac{(-1)^n\operatorname{cosech}(n^2+p^2)^{1/2}\pi}{(n^2+p^2)^{1/2}}. \tag{2.23}$$

Hence $d(1)$ becomes

$$d(1)=\frac{3c(2)}{\pi}=\frac{\pi}{2}-\frac{9}{2}\ln 2+12\sum_1^{\infty}\sum_1^{\infty}\frac{(-1)^n\operatorname{cosech}(n^2+p^2)^{1/2}\pi}{(n^2+p^2)^{1/2}}. \tag{2.24}$$

This is precisely the result given by Hautot (1975). (Hautot (1975) has α(NaCl)$=-d(1)$. The reason for this is that he defines α(NaCl) in terms of the *nearest neighbour* distance rather than in terms of the side of the basic cube formed by one particular ion. The negative sign is simply due to his definition of α as a positive quantity.) In a similar way it may be shown that

$$c(1)=\frac{\pi}{2}-\frac{9}{2}\ln 2+4\sum_1^{\infty}\sum_1^{\infty}[1+(-1)^n+(-1)^{n+p}]\frac{\operatorname{cosech}(n^2+p^2)^{1/2}\pi}{(n^2+p^2)^{1/2}}, \tag{2.25}$$

$$b(1)=\frac{\pi}{2}-\frac{7}{2}\ln 2+4\sum_1^{\infty}\sum_1^{\infty}[2+(-1)^n]\frac{\operatorname{cosech}(n^2+p^2)^{1/2}\pi}{(n^2+p^2)^{1/2}}. \tag{2.26}$$

As Hautot (1975) points out, the cosech sums are rapidly convergent. For example $d(1)$ is given to ten decimal places with just nine terms. $b(1)-d(1)$ may thus be rapidly calculated and hence Madelung constants for simple crystals may be found. In I five other sums were also considered and found necessary to evaluate α for more complex cubic lattices. These sums were

$$e(2s)=\sum(-1)^m[m^2+(n-\tfrac{1}{2})^2+(p-\tfrac{1}{2})^2]^{-s}$$
$$f(2s)=\sum(-1)^{m+n}[m^2+n^2+(p-\tfrac{1}{2})^2]^{-s}$$
$$g(2s)=8\sum(-1)^{m+n+p}[(2m-\tfrac{1}{2})^2+(2n-\tfrac{1}{2})^2+(2p-\tfrac{1}{2})^2]^{-s}$$
$$h(2s)=4\sum(-1)^{n+p}[m^2+(2n-\tfrac{1}{2})^2+(2p-\tfrac{1}{2})^2]^{-s}$$
$$j(2s)=4\sum(-1)^{m+n+p}[m^2+(2n-\tfrac{1}{2})^2+(2p-\tfrac{1}{2})^2]^{-s}.$$

It may be shown for these sums that

$$e(1)=\pi^{-1}f(2);\qquad f(1)=\pi^{-1}e(2);\qquad g(1)=\sqrt{2}\pi^{-1}g(2);$$
$$h(1)=\pi^{-1}(h(2)+j(2));\qquad j(1)=\pi^{-1}(h(2)-j(2)).$$

$e(2)-j(2)$ may all be re-expressed in terms of quickly convergent cosech sums using (1.7) and one obtains

$$e(1)=2\ln(1+\sqrt{2})+4\sum_{1}^{\infty}\sum_{1}^{\infty}\frac{(-1)^n\operatorname{cosech}[n^2+(p-\frac{1}{2})^2]^{1/2}\pi}{[n^2+(p-\frac{1}{2})^2]^{1/2}}$$

$$f(1)=4\sum_{1}^{\infty}\sum_{1}^{\infty}\frac{\operatorname{cosech}[(n-\frac{1}{2})^2+(p-\frac{1}{2})^2]^{1/2}\pi}{[(n-\frac{1}{2})^2+(p-\frac{1}{2})^2]^{1/2}}$$

$$g(1)=4\sqrt{2}\sum_{-\infty}^{\infty}\sum_{-\infty}^{\infty}\frac{(-1)^n\operatorname{cosech}[\frac{1}{2}(2n-\frac{1}{2})^2+(p-\frac{1}{2})^2]^{1/2}\pi}{[\frac{1}{2}(2n-\frac{1}{2})^2+(p-\frac{1}{2})^2]^{1/2}}$$

$$h(1)=4\ln(1+\sqrt{2})+8\sum_{1}^{\infty}\sum_{1}^{\infty}\frac{\operatorname{cosech}[2n^2+(p-\frac{1}{2})^2]^{1/2}\pi}{[2n^2+(p-\frac{1}{2})^2]^{1/2}}$$

$$j(1)=8\sum_{1}^{\infty}\sum_{1}^{\infty}\frac{\operatorname{cosech}[(n-\frac{1}{2})^2+2(p-\frac{1}{2})^2]^{1/2}\pi}{[(n-\frac{1}{2})^2+2(p-\frac{1}{2})^2]^{1/2}}$$

all of which may be rapidly calculated.

3. Discussion

Hautot (1975) deduced a relation between α(NaCl), α(CsCl) and α(ZnS). This relation is implicit in (1.6) and has been stated or implied before e.g. Naor (1958 and unpublished date), Bertaut (1954), Fumi and Tosi (1957) and Sakamoto (1958). Relations between Madelung constants of many simple crystals exist, since they are merely linear combinations of $b(1)$, $c(1)$ and $d(1)$.

The method of obtaining functional equations can be applied to higher dimensional sums without difficulty. For example the simplest D dimensional analogue to the zeta function is

$$A(D{:}2s)=\sum{}'(m_1^2\ldots+m_D^2)^{-s}=\mathrm{M}_s[\theta_3^D-1] \tag{3.1}$$

and this obeys the relation

$$A(D{:}2s)=K(D/2,\,s)A(D-2s{:}2s). \tag{3.2}$$

$A(D{:}2s)$ has a simple pole at $2s=D$ and the above result allows us to analytically continue $A(D{:}2s)$ into the region $2s<D$. There are, of course, more complicated sums analogous to $b(2s)-d(2s)$, the number increasing as D becomes larger. Analogous results to (1.5) and (2.18)–(2.20) may be obtained.

Acknowledgments

Thanks are due to Polly Frankfort for suggesting this approach.

Appendix

Hautot (1975) gives the values of some series of the form

$$\sum_{n=1}^{\infty}\frac{\operatorname{cosech}\pi n\lambda}{n}=-\tfrac{1}{3}\ln 2+\frac{\lambda\pi}{12}-\tfrac{1}{6}\ln[k^{-1}(1-k^2)], \tag{A.1}$$

where $\lambda=K'/K$ and $K(k)$ is the complete elliptic integral of the first kind with modulus k. $K'=K(k')$ where $(k')^2=1-k^2$. He states a theorem of Abel's saying that k may be found in finite form if K'/K is of the form $(a+b\surd m)/(c+d\surd n)$ where a, b, c, d, m and n are all integers. The word 'finite' needs amplification. Abel's theorem states that under the above conditions k is the root of an algebraic equation with integral coefficients. Thus k cannot be necessarily expressed in radicals.

Another way of expressing the series in (A.1) is by using (1.7), whence it may be shown that

$$\sum_{n=1}^{\infty}\frac{\operatorname{cosech}\lambda\pi n}{n}=\frac{\lambda\pi}{12}+\frac{\lambda}{2\pi}\sum_{(m,n\neq 0,0)}\sum(-1)^m(m^2+\lambda^2n^2)^{-1} \tag{A.2}$$

and

$$\sum_{n=1}^{\infty}(-1)^n\frac{\operatorname{cosech}\lambda\pi n}{n}=\frac{\lambda\pi}{12}+\frac{\lambda}{2\pi}\sum_{(m,n\neq 0,0)}\sum(-1)^{m+n}(m^2+\lambda^2n^2)^{-1}. \tag{A.3}$$

The double series on the right-hand sides of (A.2) and (A.3) have been evaluated in a number of cases by Zucker and Robertson (1975) and yield Hautot's results for $\lambda=1$ and 2. Other examples are

$$\sum_{n=1}^{\infty}(-1)^n\frac{\operatorname{cosech}3\pi n}{n}=\frac{\pi}{4}-\frac{\ln 2}{2}-\tfrac{1}{3}\ln(2+\surd 3) \tag{A.4}$$

$$\sum_{n=1}^{\infty}\frac{\operatorname{cosech}4\pi n}{n}=\frac{\pi}{3}-\tfrac{7}{8}\ln 2-\tfrac{1}{2}\ln(1+\surd 2) \tag{A.5}$$

$$\sum_{n=1}^{\infty}(-1)^n\frac{\operatorname{cosech}5\pi n}{n}=\frac{5\pi}{12}-\frac{\ln 2}{2}-2\ln\left(\frac{1+\surd 5}{2}\right). \tag{A.6}$$

Other results such as

$$\sum_{-\infty}^{\infty} \frac{(-1)^n \operatorname{cosech}(3n-1)\pi}{3n-1} = \tfrac{1}{9} \ln 8(2-\sqrt{3}) \tag{A.7}$$

may also be obtained.

References

Bertaut F 1954 *C. R. Acad. Sci., Paris* **239** 234–5
Fumi F G and Tosi M P 1957 *Phil. Mag.* **2** 284
Glasser M L 1973 *J. Math. Phys.* **14** 409–13
Hardy G H 1919 *Mess. Math.* **49** 85–91
Hautot A 1974 *J. Math. Phys.* **15** 1722–7
—— 1975 *J. Phys. A: Math. Gen.* **8** 853–62
van der Hoff B M E and Benson G C 1953 *Can. J. Phys.* **31** 1087–94
Naor P 1958 *Z. Krist.* **110** 112–26
Phillips E G 1951 *Functions of a Complex Variable* (Edinburgh: Oliver and Boyd) p 135
Sakamoto Y 1958 *J. Chem. Phys.* **28** 164–5
Titchmarsh E C 1951 *The Theory of the Riemann Zeta Function* (Oxford: Oxford University Press) chap 2
Zucker I J 1974 *J. Phys. A: Math., Nucl. Gen.* **7** 1568–75
—— 1975 *J. Phys. A: Math. Gen.* **8** 1734–45
Zucker I J and Robertson M M 1975 *J. Phys. A: Math. Gen.* **8** 874–81