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New applications of Poisson's summation formula

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Abstract. Fourier expansions in modified Bessel functions are evaluated in terms of elementary functions. The results are obtained in the form of rapidly convergent series so that numerical computations are quite easy. This leads to the possibility of tabulating the modified Bessel functions in their critical domain. A physical application is also given: simple expansions giving the Madelung constant for cubic crystallographic structures are established; they involve only elementary functions and exhibit the greatest known accuracy.

1. Introduction

One of the most powerful methods for evaluating simple or multiple series is known as Poisson's summation rule. Having to sum the n-uple series:

$$S = \sum_{\text{all } k_i = -\infty}^{+\infty} \ldots \sum f(k_1, \ldots, k_n) \qquad (k_i \text{ integer}) \tag{1}$$

one has (Bochner 1932):

$$S = \sum_{\text{all } l_i = -\infty}^{+\infty} \ldots \sum g(l_1, \ldots, l_n) \qquad (l_i \text{ integer}) \tag{2}$$

where g is the Fourier transform of f:

$$g(y_1, \ldots, y_n) = \int_{-\infty}^{+\infty} \ldots \int \exp[2\mathrm{i}\pi(x_1y_1 + \ldots + x_ny_n)] f(x_1, \ldots, x_n)\, \mathrm{d}x_1 \ldots \mathrm{d}x_n. \tag{3}$$

Both series must converge uniformly. The Fourier integral of f must exist. Poisson's rule transforms the original series into another series whose convergence may be better. When the starting series is n-uple it is possible to modify it in many ways by using the m-dimensional Poisson formula (with $m \leqslant n$). One possibility may be much more interesting than the others since it leads to a better final expansion. In practice there is no general rule for deciding whether or not Poisson's rule will be useful. This is due to the fact that a 'good' expansion has to fulfil two distinct conditions:

(i) the general term of the expansion must decrease as rapidly as possible in order to ensure a rapid convergence;

(ii) the general term must be expressed in terms of elementary functions.

The first question to ask in examining a series (1) is: does f satisfy these two conditions? If not, then we must look for an m-dimensional Fourier transform of f which leads to a function g of the kind mentioned above. Tables of Fourier transforms exist which

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allow one to decide when to attempt this procedure. It is clear that the simplest function g obeying the two above conditions is the decreasing exponential. Now we know that if g is the Fourier transform of f, f is in turn the Fourier transform of g.

As an example let us examine the one-dimensional problem. We set:

$$g = \exp(-a|l|).$$

Its Fourier transform is $2a/(a^2+4\pi^2y^2)$. So we have:

$$\sum_{k=-\infty}^{+\infty} \frac{1}{a^2+4\pi^2k^2} = \frac{1}{2a}\sum_{l=-\infty}^{+\infty} \exp(-a|l|).$$

This relation is well known. Other g functions can be chosen such as: $g = \exp(-al^2)$ or $g = [1/(b^2+l^2)]\exp(-a|l|)$ and so forth, but the corresponding results are either well known or of very little interest in applied physics. In the two-dimensional problem, the function g can take the following forms:

$$g = \exp[-a(l_1^2+l_2^2)^{1/2}] \qquad \text{or} \qquad \exp[-a(l_1^2+l_2^2)] \text{ etc}\ldots.$$

Since the list is not limitative it is evident that each case promises to be interesting. Function f is easily derived from g by computing its two-dimensional Fourier transform. As shown in § 4 important new results can be obtained by considering

$$f(x, y) = [(2x-1)^2+(2y-1)^2]^{-1/2}K_\nu\{a[(2x-1)^2+(2y-1)^2]^{1/2}\}\cos bx \cos cy$$

where K is the modified Bessel function of the third kind (Abramowitz and Stegun 1965). Series of the type $\Sigma\Sigma_{x,y} f(x, y)$ are often encountered in applied physics.

We shall show that they can be evaluated with the aid of the two-dimensional Poisson formula. The final result will be written as an expansion in terms of elementary functions with remarkably rapid convergence.

2. Evaluation of certain double Fourier series

We wish to evaluate the following sums (ν is an integer):

$$S_1(x, y, z; \nu) = \sum_{-\infty}^{+\infty}\sum{}' (m^2+n^2)^{-\nu/2}K_\nu[z(m^2+n^2)^{1/2}]\cos mx \cos ny \tag{4}$$

$$S_2(x, y, z; \nu) = \sum_{-\infty}^{+\infty}\sum [(2m-1)^2+(2n-1)^2]^{-\nu/2}K_\nu\{z[(2m-1)^2+(2n-1)^2]^{1/2}\} \times \cos(2m-1)x\cos(2n-1)y \tag{5}$$

$$S_3(x, y, z; \nu) = \sum_{-\infty}^{+\infty}\sum{}' (m^2+4n^2)^{-\nu/2}K_\nu[z(m^2+4n^2)^{1/2}]\cos mx \cos 2ny \tag{6}$$

$$S_4(x, y, z; \nu) = \sum_{-\infty}^{+\infty}\sum [4m^2+(2n-1)^2]^{-\nu/2}K_\nu\{z[4m^2+(2n-1)^2]^{1/2}\} \times \cos 2mx\cos(2n-1)y \tag{7}$$

$$S_5(x, y, z; \nu) = \sum_{-\infty}^{+\infty}\sum [m^2+(2n-1)^2]^{-\nu/2}K_\nu\{z[m^2+(2n-1)^2]^{1/2}\}\cos mx\cos(2n-1)y \tag{8}$$

$$S_6(x, y, z; \nu) = \sum_{-\infty}^{+\infty}\sum{}' (4m^2+4n^2)^{-\nu/2} K_\nu[z(4m^2+4n^2)^{1/2}] \cos 2mx \cos 2ny. \tag{9}$$

The symbol ν will be omitted when no confusion is possible. Simple arithmetical devices allow four relations to be found between these sums:

$$S_6(x, y, z) = 2^{-\nu} S_1(2x, 2y, 2z) \tag{10}$$

$$S_1(x, y, z) = 2^{-\nu} S_1(2x, 2y, 2z) + S_4(x, y, z) + S_4(y, x, z) + S_2(x, y, z) \tag{11}$$

$$S_1 = S_3 + S_5 \tag{12}$$

$$S_5 = S_2 + S_4. \tag{13}$$

We shall first evaluate S_2 and S_4. By adding them we shall find S_5 by (13). S_2 and S_4 being known, let us call $f(x, y, z) = S_4(x, y, z) + S_4(y, x, z) + S_2(x, y, z)$; then (11) allows us to write S_1 under the form:

$$S_1(x, y, z) = \sum_{l=0}^{\infty} 2^{-l\nu} f(2^l x, 2^l y, 2^l z). \tag{14}$$

When S_1 is known, S_6 can be deduced from (10) and S_3 follows from (12). So we need the values of S_2 and S_4.

2.1. Calculation of $S_2(x, y, z)$

S_2 is defined by equation (5). We use the one-dimensional Poisson formula. In view of this we need the Fourier transform $g(u)$ of the function of t:

$$f(t) = [(2t-1)^2 + (2n-1)^2]^{-\nu/2} K_\nu\{z[(2t-1)^2 + (2n-1)^2]^{1/2}\} \cos(2t-1)x \cos(2n-1)y$$

$$g(u) = \int_{-\infty}^{+\infty} f(t) \exp(2i\pi ut)\, \mathrm{d}t.$$

The value of this integral is given in the tables of Gradshteyn and Ryzhik (1965, 6.726-4, p 756). After performing all the calculations we find:

$$S_2(x, y, z; \nu) = \surd(2\pi) z^{-\nu} \sum_{\substack{-\infty \\ m}}^{+\infty} \sum_{\substack{1 \\ n}}^{\infty} (-1)^m [z^2 + (x+\pi m)^2]^{(2\nu-1)/4} (2n-1)^{(1-2\nu)/2} \cos(2n-1)y$$
$$\times K_{\nu-1/2}\{(2n-1)[z^2 + (x+\pi m)^2]^{1/2}\}. \tag{15}$$

2.2. Calculation of $S_4(x, y, z)$

S_4 is defined by equation (7). The calculations are analogous; one finds:

$$S_4(x, y, z; \nu) = \surd(\pi)(2z)^{-\nu} \sum_{\substack{-\infty \\ m,n}}^{+\infty}\sum (-1)^n [z^2 + (y+\pi n)^2]^{(2\nu-1)/4} m^{(1-2\nu)/2} \cos 2mx$$
$$\times K_{\nu-1/2}\{2m[z^2 + (y+\pi n)^2]^{1/2}\}. \tag{16}$$

2.3. Discussion of equations (15) and (16): special cases $\nu = 0, 1$

Formulae (15) and (16) solve the problem of evaluating S_2 and S_4 in a satisfactory manner since the results are obtained in the form of two expansions in terms of elementary functions. The reader will recall that when ν is an integer $K_{\nu-1/2}$ is the product of a decreasing exponential and a polynomial. Moreover the asymptotic behaviour of K_ν ensures a rapid convergence. Two special cases are interesting: $\nu = 0$ and $\nu = 1$. In these cases equations (15) and (16) simplify in a neat way. We need the following classical formulae:

$$K_{1/2}(z) = K_{-1/2}(z) = \sqrt{(\pi/2z)}\exp(-z)$$

$$\sum_{n=1}^{\infty} (2n-1)^{-1}\cos(2n-1)y\exp[-(2n-1)a] = (1/4)\ln|(\cos y+\cosh a)(\cos y-\cosh a)^{-1}|$$

$$\sum_{n=1}^{\infty} (1/n)\cos ny\exp(-na) = -(1/2)\ln|1+\exp(-2a)-2\cos y\exp(-a)|.$$

After performing the calculations we find the following remarkable results:

$$S_2(x, y, z; 0) = (\pi/2)\sum_{m}{}_{-\infty}^{+\infty} (-1)^m[z^2+(x+\pi m)^2]^{-1/2}\frac{\sinh(z^2+(x+\pi m)^2]^{1/2}}{\sinh^2[z^2+(x+\pi m)^2]^{1/2}+\sin^2 y}\cos y \tag{17}$$

$$S_2(x, y, z; 1) = (\pi/4z)\sum_{m}{}_{-\infty}^{+\infty} (-1)^m \ln\left|\frac{\cos y+\cosh[z^2+(x+\pi m)^2]^{1/2}}{\cos y-\cosh[z^2+(x+\pi m)^2]^{1/2}}\right| \tag{18}$$

$$S_4(x, y, z; 0) = (\pi/2)\sum_{m}{}_{-\infty}^{+\infty} [z^2+(x+\pi m)^2]^{-1/2}\frac{\sinh[z^2+(x+\pi m)^2]^{1/2}}{\sinh^2[z^2+(x+\pi m)^2]^{1/2}+\sin^2 y}\cos y \tag{19}$$

$$S_4(x, y, z; 1) = (\pi/4z)\sum_{m}{}_{-\infty}^{+\infty} \ln\left|\frac{\cos y+\cosh[z^2+(x+\pi m)^2]^{1/2}}{\cos y-\cosh[z^2+(x+\pi m)^2]^{1/2}}\right|. \tag{20}$$

All these expansions are very well suited to the numerical computation of the Fourier series $S_1, \ldots, S_6$.

3. Evaluation of certain simple Fourier series

The preceding section dealt with double sums. In practice simple sums containing K_ν functions are often encountered. This will be apparent in § 4 which is devoted to applications. Supposing we wish to evaluate the Fourier series:

$$S = \sum_{m=0}^{\infty} K_0[(2m+1)z]\cos(2m+1)y = (1/2)\sum_{-\infty}^{+\infty} K_0[(2m+1)z]\cos(2m+1)y.$$

If we evaluate this series through Poisson's one-dimensional rule, we should find without difficulty:

$$S = (\pi/4)\sum_{-\infty}^{+\infty} (-1)^n[z^2+(y+\pi n)^2]^{-1/2}.$$

The summand is now an elementary function but the convergence of the new series is very much worse than in the starting series. It is possible to re-arrange the terms in the summand in order to increase the rapidity of the convergence (Gradshteyn and Ryzhik 1965) but no remarkable result can be obtained in this way. The aim of this section is to show that S can be evaluated in an indirect way through Poisson's rule. The technique used is entirely analogous to that given in § 2. We start with the definition of S_4 and split it into two parts:

$$S_4(x, y, z; v) = 2 \sum_{n=1}^{\infty} (2n-1)^{-v} \cos(2n-1)y K_v[(2n-1)z]$$
$$+2 \sum_{m=1}^{\infty} \sum_{n=-\infty}^{+\infty} [4m^2+(2n-1)^2]^{-v/2} K_v\{z[4m^2+(2n-1)^2]^{1/2}\}$$
$$\times \cos 2mx \cos(2n-1)y.$$

The sum over n in the last term is evaluated with the aid of Poisson's formula. Finally one finds (for the sake of brevity only the special cases $v = 0$ and $v = 1$ are written):

$$\sum_0^{\infty} K_0[(2m+1)z] \cos(2m+1)y$$
$$= (\pi/4) \sum_{-\infty}^{+\infty} (-1)^m [z^2+(y+\pi m)^2]^{-1/2} \frac{\exp\{-[z^2+(y+\pi m)^2]^{1/2}\}+(-1)^m \cos y}{\cosh[z^2+(y+\pi m)^2]^{1/2}+(-1)^m \cos y} \tag{21}$$

$$\sum_0^{\infty} (2m+1)^{-1} K_1[(2m+1)z] \cos(2m+1)y$$
$$= (\pi/4z) \sum_{-\infty}^{+\infty} (-1)^m \ln|1+\exp\{-2[z^2+(y+\pi m)^2]^{1/2}\}$$
$$+2(-1)^m \cos y \exp\{-[z^2+(y+\pi m)^2]^{1/2}\}|. \tag{22}$$

Other sums of the same type can be deduced from (21) and (22) in the following way: let us calculate $H(y, z) = \Sigma_1^{\infty} K_0(mz) \cos my$. Equation (21) gives the value of

$$F(y, z) = \sum_0^{\infty} K_0[(2m+1)z] \cos(2m+1)y.$$

However,

$$F(y, z) = H(y, z) - H(2y, 2z),$$

thus

$$H(y, z) = \sum_{l=0}^{\infty} F(2^l y, 2^l z)$$

where F is given by (21).

4. Applications

4.1. The tabulation of $K_v(z)$ (v integer)

Equations (21) and (22) allow an accurate tabulation of K_0 and K_1 in their critical domain $3 < z < 10$. When $z < 3$ the power expansion in the neighbourhood of $z = 0$ is rapidly convergent. When $z > 10$ the asymptotic expansion is convenient (Watson

1966). Between these two limits one can use equations (21) and (22) as follows. Put $y = \pi/6$ in both equations. We obtain (*idem* for K_1)

$$K_0(z)\cos(\pi/6)+K_0(5z)\cos(5\pi/6)+K_0(7z)\cos(7\pi/6)+\ldots \sim (\sqrt{(3)}/2)K_0(z)$$

$$= (\pi/4)\sum_{-\infty}^{+\infty}(-1)^m[z^2+\pi^2(m+1/6)^2]^{-1/2} \times \frac{\exp\{-[z^2+\pi^2(m+1/6)^2]^{1/2}\}+(-1)^m(\sqrt{(3)}/2)}{\cosh[z^2+\pi^2(m+1/6)^2]^{1/2}+(-1)^m(\sqrt{(3)}/2)} \quad (23)$$

with a relative accuracy better than $K_0(15)/K_0(3) = 3\times10^{-6}$.

For greater accuracy, replace z by $5z$ in equation (23) and add the new equation to (23). The new expansion will give $K_0(z)$ with a relative accuracy better than $K_0(21)/K_0(3) = 6\times10^{-9}$ and so on for increasing accuracies. Once K_0 and K_1 are tabulated, the values of $K_2, K_3, \ldots$ can be deduced using the well known recurrence relations between the K_n.

4.2. The computation of the Madelung constant in crystal physics

Multiple sums frequently occur in crystal physics. One of the most famous is the Madelung sum. In the case of the NaCl structure this sum can be written as:

$$\alpha(\text{NaCl}) = \sum_{-\infty}^{+\infty}\sum\sum{}'(-1)^{m+n+p+1}(m^2+n^2+p^2)^{-1/2}$$

where the prime indicates that one excludes the case $m = n = p = 0$.

The three-dimensional Poisson formula cannot be used because of the omission of one term in the sum. After some calculations the one-dimensional Poisson formula leads to:

$$\alpha(\text{NaCl}) = 2\ln 2+4\sum_{\substack{-\infty\\ m,n}}^{+\infty}\sum{}'\sum_{k=0}^{\infty}(-1)^{m+n+1}K_0[\pi(2k+1)(m^2+n^2)^{1/2}]. \quad (24)$$

This formula is essentially analogous to the one discovered earlier by Madelung (1918). $K_n(z)$ is the modified Bessel function of the third kind (Abramowitz and Stegun 1965). The two-dimensional Poisson formula shows:

$$\sum_{\substack{-\infty\\ m,k}}\sum(-1)^{m+n}(m^2+n^2+p^2)^{-1/2}$$

$$= 2\sum_{\substack{-\infty\\ m,n}}^{+\infty}\sum[(2m+1)^2+(2n+1)^2]^{-1/2}\exp\{-p\pi[(2m+1)^2+(2n+1)^2]^{1/2}\}.$$

This formula was known to Shermann (1932). However, he was unable to go further in the computation of $\alpha(\text{NaCl})$ since this requires the evaluation of (Glasser 1973):

$$\sum_{-\infty}^{+\infty}\sum{}'(-1)^{m+n}(m^2+n^2)^{-1/2} = -4(1-\sqrt{2})\zeta(1/2)\beta(1/2), \quad (25)$$

ζ and β are Riemann's zeta and beta functions. Finally one has:

$$\alpha(\text{NaCl}) = 4(1-\sqrt{2})\zeta(1/2)\beta(1/2)+16\sum\sum_{0}^{\infty}[(2m+1)^2+(2n+1)^2]^{-1/2}$$
$$\times\{\exp\pi[(2m+1)^2+(2n+1)^2]^{1/2}+1\}^{-1}. \tag{26}$$

This formula was first established with the aid of Schlömilch series (Hautot 1974). We rediscover it here in a simpler way. It is interesting to compare equation (24) with equation (26). The expansion (24) converges rapidly on account of the asymptotic behaviour of $K_0(z) \sim (\pi/2z)^{1/2}\exp(-z)$. However, (24) needs the tabulation of K_0. This drawback does not exist with equation (26) since apart from the first term in the second member all the other terms only involve elementary functions.

It is possible to refine equation (26) in a beautiful way. In equation (24) we try to evaluate the double sum:

$$\sum\sum_{\substack{-\infty \\ m,n}}^{+\infty}{}'(-1)^{m+n+1}K_0[\pi(2k+1)(m^2+n^2)^{1/2}].$$

It is clear that this equals: $-S_1(\pi,\pi,z;0)$ with $z=(2k+1)\pi$. S_1 is computed with the aid of (14), (17) and (19). We find

$$S_1(\pi,\pi,z;0) = (\pi/2)\sum_{l=0}^{\infty}\sum_{\substack{-\infty \\ m}}^{+\infty}[2+(-1)^m]\cos(2^l\pi)[2^{2l}z^2+(2^l+m)^2\pi^2]^{-1/2}$$
$$\times\operatorname{cosech}[2^{2l}z^2+(2^l+m)^2\pi^2]^{1/2}.$$

Hence we obtain:

$$\alpha(\text{NaCl}) = 2\ln 2-2\sum\sum_{\substack{0 \\ k,l}}^{\infty}\sum_{\substack{-\infty \\ m}}^{+\infty}[2+(-1)^m]\cos(2^l\pi)[(2k+1)^2 2^{2l}+(2^l+m)^2]^{-1/2}$$
$$\times\operatorname{cosech}\pi[(2k+1)^2 2^{2l}+(2^l+m)^2]^{1/2}.$$

We split the l-sum into two parts:

$$\sum_{l=0}^{\infty} = (l=0)+\sum_{l=1}^{\infty}.$$

Taking into account the identity:

$$\sum_{k=1}^{\infty}f(4k^2) = \sum_{l=1}^{\infty}\sum_{k=0}^{\infty}f[2^{2l}(2k+1)^2]$$

we find after some manipulations:

$$\alpha(\text{NaCl}) = 2\ln 2+2\sum_{k=0}^{\infty}(2k+1)^{-1}\operatorname{cosech}(2k+1)\pi-6\sum_{k=1}^{\infty}(2k)^{-1}\operatorname{cosech}2k\pi$$
$$+12\sum\sum_{1}^{\infty}\{[(2k-1)^2+(2m-1)^2]^{-1/2}\operatorname{cosech}\pi[(2k-1)^2+(2m-1)^2]^{1/2}$$
$$-(4k^2+4m^2)^{-1/2}\operatorname{cosech}\pi(4k^2+4m^2)^{1/2}\}.$$

The simple series can be evaluated exactly (see appendix). Finally the following useful expansion is obtained:

$$\alpha(\mathrm{NaCl}) = (9/2)\ln 2-(\pi/2)+12\sum_{1}^{\infty}\sum\{[(2k-1)^2+(2m-1)^2]^{-1/2}$$

$$\times \operatorname{cosech} \pi[(2k-1)^2+(2m-1)^2]^{1/2}-(4k^2+4m^2)^{-1/2}\operatorname{cosech}\pi(4k^2+4m^2)^{1/2}\} \tag{27}$$

which appears to be the best known expansion for $\alpha(\mathrm{NaCl})$. Consider a numerical example: three terms in the double series give:

$$\alpha(\mathrm{NaCl}) \simeq (9/2)\ln 2-(\pi/2)$$

$$+12[(\operatorname{cosech}\pi\sqrt{2})/\sqrt{2}+2(\operatorname{cosech}\pi\sqrt{10})/\sqrt{10}-(\operatorname{cosech}\pi\sqrt{8})/\sqrt{8}]$$

$$= 1{\cdot}74756(28) \qquad \text{accurate to } 10^{-6}.$$

Nine terms in the series give α with ten figures.

The Madelung constant for the other fundamental cubic structures (caesium chloride and zinc blende) can be evaluated in a similar way. We know that (Hautot 1974):

$$\alpha(\mathrm{CsCl}) = 2\alpha(\mathrm{NaCl})-12\sum_{1}^{\infty}(2k-1)^{-1}\operatorname{cosech}\pi(2k-1)-24\sum_{1}^{\infty}\sum[(2k-1)^2+m^2]^{-1/2}$$

$$\times\operatorname{cosech}\pi[(2k-1)^2+m^2]^{1/2}$$

$$\alpha(\mathrm{ZnS}) = \alpha(\mathrm{CsCl})+3\ln 2-6\sum_{1}^{\infty}k^{-1}\operatorname{cosech}k\pi\ +12\sum_{1}^{\infty}\sum(-1)^{k+1}$$

$$\times(k^2+m^2)^{-1/2}\operatorname{cosech}\pi(k^2+m^2)^{1/2}.$$

Evaluating the simple series (see appendix) and combining with (27) we find:

$$\alpha(\mathrm{CsCl}) = (15/2)\ln 2-\pi-24\sum_{1}^{\infty}\sum(k^2+4m^2)^{-1/2}\operatorname{cosech}\pi(k^2+4m^2)^{1/2} \tag{28}$$

$$\alpha(\mathrm{ZnS}) = 12\ln 2-(3\pi/2)-36\sum_{1}^{\infty}\sum(k^2+4m^2)^{-1/2}\operatorname{cosech}\pi(k^2+4m^2)^{1/2}$$

$$+12\sum_{1}^{\infty}\sum[k^2+(2m-1)^2]^{-1/2}\operatorname{cosech}\pi[k^2+(2m-1)^2]^{1/2}. \tag{29}$$

Examining equations (27), (28) and (29) we see that they are connected by the curious relation:

$$\alpha(\mathrm{ZnS}) = \alpha(\mathrm{NaCl})+\alpha(\mathrm{CsCl}).$$

It seems that this simple formula has never been mentioned in the literature. The numerical values of α are calculated from (27), (28) and (29):

$$\alpha(\mathrm{NaCl}) = 1{\cdot}74756459463$$

$$\alpha(\mathrm{CsCl}) = 2{\cdot}03536150945$$

$$\alpha(\mathrm{ZnS}) = 3{\cdot}78292610408.$$

5. The Madelung constant in finite form?

Is it possible to go further than equations (27), (28) and (29)? The problem has been suggested by Glasser (1973) in the following terms: is it possible to express α exactly in finite form? Up to now the answer has been negative because this would require the exact evaluation of double series such as:

$$\sum_{1}^{\infty}\sum (k^2+m^2)^{-1/2}\operatorname{cosech}\pi(k^2+l^2)^{1/2} = ?$$

This has never been performed successfully. The sole series of this kind that we have succeeded in summing is the following:

$$\sum_{1}^{\infty}\sum (-1)^k(k^2+m^2)^{-1/2}[\exp\pi(k^2+m^2)^{1/2}+(-1)^m]^{-1}$$
$$= (9/16)\ln 2-(\pi/16)-(1/2)(1-\sqrt{2})\zeta(1/2)\beta(1/2) = -0{\cdot}0083970802.$$

The proof is left to the reader: starting with equation (25) and using successive applications of the one-dimensional Poisson formula and of equation (21) one obtains the above result.

6. Conclusion

Poisson's summation formula has been used to sum certain Fourier series. In definite cases one obtains better expansions than those previously established. Many sums occurring in crystal physics can be evaluated with improved accuracy through this procedure.

Appendix

In § 4 we had to sum exactly some unusual series. Here we prove the following curious relations:

$$\sum_{1}^{\infty} k^{-1}\operatorname{cosech} k\pi = (\pi/12)-(1/4)\ln 2 \qquad (30)$$

$$\sum_{1}^{\infty} (2k)^{-1}\operatorname{cosech} 2k\pi = (\pi/12)-(3/8)\ln 2. \qquad (31)$$

More generally let us calculate:

$$f(z) = \sum_{1}^{\infty} k^{-1}\operatorname{cosech} kz$$
$$= 2\sum_{n=0}^{\infty}\sum_{k=1}^{\infty} k^{-1}\exp[-(2n+1)kz]$$
$$= -\ln\prod_{n=0}^{\infty}\{1-\exp[-(2n+1)z]\}^2.$$

Infinite products of this kind are encountered in the theory of elliptic functions (Whittaker and Watson 1963). Using traditional notations for the complete elliptic integral of the first kind $K(k)$ of modulus $k(k'^2 = 1-k^2;\ K' = K(k'))$ one finds:

$$f(z) = -(1/3)\ln 2+(z/12)-(1/6)\ln[k^{-1}(1-k^2)] \tag{32}$$

with $z = \pi(K'/K)$. A theorem of Abel allows us to calculate k exactly in finite form provided K'/K is of the form $(a+b\sqrt{m})/(a'+b'\sqrt{n})$ where all six numbers are integers (Whittaker and Watson 1963). To calculate (30) we note that $z = \pi$ so that $K' = K$. Then knowing that $k = 1/\sqrt{2}$, by (32) we get:

$$f(\pi) = (\pi/12)-(1/4)\ln 2.$$

To calculate (31) we note that $z = 2\pi$ so that $K' = 2K$. Then $k = 3-2\sqrt{2}$ and by (32) we get:

$$f(2\pi) = (\pi/6)-(3/4)\ln 2.$$

Numerous series of this type can be evaluated exactly in a similar way.

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