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1974 J. Phys. A: Math. Nucl. Gen. 7 1568

(http://iopscience.iop.org/0301-0015/7/13/011)

J. Phys. A: Math., Nucl. Gen., Vol. 7, No. 13, 1974. Printed in Great Britain. © 1974

Exact results for some lattice sums in 2, 4, 6 and 8 dimensions

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Received 6 February 1974, in final form 29 April 1974

Abstract. A method developed by Glasser in 1973 is used to evaluate exactly lattice sums in 2, 4, 6 and 8 dimensions. Amongst the many results given are the Madelung sums. A certain three-dimensional sum first evaluated by Glasser but inaccurately presented, is given correctly.

1. Introduction

Glasser (1973a, b) has recently revived much interest in the exact evaluation of lattice sums. It should be explained here what is meant by the 'exact' value of a lattice sum. Here we say a multiple sum has been evaluated if it can be expressed as the product of simple sums such as Dirichlet series. For example it has been established that

$$\sum_{(l_1,l_2)\neq(0,0)} (l_1^2+l_2^2)^{-s} = 4\zeta(s)\beta(s) \tag{1.1}$$

where the sum on the left-hand side is over all integer values of l_1 and l_2 both positive and negative but excluding the case where both are zero. The right-hand side is the product of two well known Dirichlet series namely

$$\zeta(s) = \sum_{n=0}^{\infty} (n+1)^{-s}; \qquad \beta(s) = \sum_{n=0}^{\infty} (-1)^n(2n+1)^{-s}. \tag{1.2}$$

The right-hand side of (1) is thus regarded as the exact result.

Two methods were presented by Glasser (1973a, b) in his evaluation of lattice sums. One was an analytic approach, the other involved number-theoretic techniques. Both approaches were used by Glasser to obtain some two-dimensional sums. A three-dimensional sum was also determined partially by the analytic method leaving a certain two-dimensional sum, which was finally evaluated using the arithmetic method. Glasser also commented on how higher even dimensional sums could be evaluated using the analytic approach, and gave one four-dimensional example. Here we use and extend the analytic method only, to evaluate Glasser's three-dimensional sum, and to obtain exact results for many sums in 2, 4, 6 and 8 dimensions. One of the most fascinating facts about these results is that all but one of them are implicit in the monumental work of Jacobi—the *Fundamenta Nova Theoriae Ellipticarum Functionum* published in 1829. In this book Jacobi established some truly astonishing identities between products and powers of some infinite series. The basic series which are used here are defined following Whittaker and Watson (1958). These are:

$$\theta_2 = 2q^{1/4}(1+q^2+q^6+\ldots) = \sum_{-\infty}^{\infty} q^{(n-\frac{1}{2})^2} = 2\sum_{n=0}^{\infty} q^{(n+\frac{1}{2})^2} \tag{1.3}$$

$$\theta_3 = 1+2q+2q^4+2q^9+\ldots = \sum_{-\infty}^{\infty} q^{n^2} = 1+2\sum_{n=0}^{\infty} q^{n^2} \tag{1.4}$$

$$\theta_4 = 1-2q+2q^4-2q^9+\ldots = \sum_{-\infty}^{\infty} (-1)^n q^{n^2} = 1+2\sum_{n=0}^{\infty} (-1)^{n^2} q^{n^2} \tag{1.5}$$

$$\theta_1' = 2q^{1/4}(1-3q^2+5q^6-\ldots) = 2\sum_{n=0}^{\infty} (-1)^n(2n+1)q^{(n+\frac{1}{2})^2}. \tag{1.6}$$

We quote below a few of the important relations existing amongst these functions, thus

$$\theta_3(-q) = \theta_4(q) \tag{1.7}$$

$$\theta_3\theta_4 = \theta_4^2(q^2); \qquad \theta_2\theta_3 = \tfrac{1}{2}\theta_2^2(q^{1/2}) \tag{1.8}$$

$$\theta_1' = \theta_2\theta_3\theta_4 \tag{1.9}$$

(1.9) is one of Jacobi's identities.

These identities were not given in terms of the θ functions, but rather in terms of the complete elliptic integral of the first kind, $K(k)$, given by

$$K(k) = \int_0^1 \frac{\mathrm{d}x}{[(1-x^2)(1-k^2x^2)]^{1/2}}. \tag{1.10}$$

The relations between K and θ functions are:

$$\theta_3^2 = \frac{2K}{\pi}; \qquad \theta_4^2 = \frac{2k'K}{\pi}; \qquad \theta_2^2 = \frac{2kK}{\pi}, \tag{1.11}$$

where $k^2+k'^2 = 1$.

q is actually equal to $\exp(-\pi K'/K)$ where $K' = K(k')$, but here it is treated as a parameter.

2. Procedure for evaluating lattice sums

The method of evaluating lattice sums is first illustrated in obtaining the result of (1.1). The operation M is first defined as

$$M[f] = \frac{1}{\Gamma(s)}\int_0^{\infty} t^{s-1} f\,\mathrm{d}t. \tag{2.1}$$

Then

$$\begin{aligned}\sum_{(l_1,l_2)\neq(0,0)} (l_1^2+l_2^2)^{-s} &= M\left[\sum_{(l_1,l_2)\neq(0,0)} \exp[-(l_1^2+l_2^2)t]\right] \\ &= M[\theta_3^2(q)-1], \qquad q = \mathrm{e}^{-t}. \end{aligned} \tag{2.2}$$

Now Jacobi (1829, p 103, equation (4)) gives

$$\theta_3^2-1 = 4\sum_{n=0}^{\infty}\frac{q^{n+1}}{1+q^{2n+2}} = 4\sum_{n=0}^{\infty}\sum_{m=0}^{\infty}(-1)^m q^{(1+n)(1+2m)} \tag{2.3}$$

therefore

$$M[\theta_3^2-1] = \frac{4}{\Gamma(s)}\int_0^\infty t^{s-1}\sum_{n=0}^{\infty}\sum_{m=0}^{\infty}(-1)^m\exp[-(1+n)(1+2m)t]\,\mathrm{d}t$$

$$= 4\sum_{m=0}^{\infty}(-1)^m(2m+1)^{-s}\sum_{n=0}^{\infty}(n+1)^{-s} = 4\zeta(s)\beta(s). \tag{2.4}$$

We give one more example of what is essentially the Madelung sum for a four-dimensional cubic lattice. Thus

$$\sum_{(l_1,l_2,l_3,l_4)\neq(0,0,0,0)}(-1)^{l_1+l_2+l_3+l_4}(l_1^2+l_2^2+l_3^2+l_4^2)^{-s}$$

$$= M\left[\sum_{(l_1,l_2,l_3,l_4)\neq(0,0,0,0)}(-1)^{l_1+l_2+l_3+l_4}\exp[-(l_1^2+l_2^2+l_3^2+l_4^2)t]\right]$$

$$= M[\theta_4^4(q)-1] \qquad q = \mathrm{e}^{-t}. \tag{2.5}$$

Now Jacobi (p 104, equation (10)) gives,

$$\theta_4^4-1 = 8\sum_{n=0}^{\infty}(-1)^{n+1}\frac{(n+1)q^{n+1}}{1+q^{n+1}} = 8\sum_{n=0}^{\infty}\sum_{m=0}^{\infty}(-1)^{n+1}(n+1)q^{(n+1)(1+m)}(-1)^m$$

therefore

$$M[\theta_4^4-1] = 8\sum_{n=0}^{\infty}(-1)^{n+1}\frac{(n+1)}{(n+1)^s}\sum_{m=0}^{\infty}\frac{(-1)^m}{(1+m)^s} = -8\eta(s)\eta(s-1) \tag{2.6}$$

where

$$\eta(s) = \sum_{n=0}^{\infty}(-1)^n(n+1)^{-s} = (1-2^{1-s})\zeta(s). \tag{2.7}$$

Thus for $s = 2$ the sum given in (2.5) is equal to $-\frac{2}{3}\pi^2\ln 2$.

In a similar fashion many other lattice sums have been evaluated and presented in table 1. The d-dimensional sums have been defined as follows

$$S(m,n) = \sum_{(l_1,l_2,\ldots,l_d)\neq(0,0,\ldots,0)}(-1)^{l_1+l_2+\ldots+l_m}(l_1^2+l_2^2+\ldots+l_d^2)^{-s} \tag{2.8}$$

$$T(m,n) = \sum[l_1^2+l_2^2+\ldots+l_m^2+(l_{m+1}-\tfrac{1}{2})^2+\ldots+(l_d-\tfrac{1}{2})^2]^{-s} \tag{2.9}$$

$$U(m,n) = \sum(-1)^{l_1+l_2+\ldots+l_m}[l_1^2+\ldots+l_m^2+(l_{m+1}-\tfrac{1}{2})^2+\ldots+(l_d-\tfrac{1}{2})^2]^{-s} \tag{2.10}$$

where $m+n = d$ and the summations are over all integer values of $l_1\ldots l_d$ both positive, negative and zero excepting the case of $S(m,n)$ in which all the l_d equal to zero are excluded†. It then follows that

$$S(m,n) = M[\theta_4^m\theta_3^n-1] \tag{2.11}$$

$$T(m,n) = M[\theta_3^m\theta_2^n] \tag{2.12}$$

$$U(m,n) = M[\theta_4^m\theta_2^n]. \tag{2.13}$$

† Thus the four-dimensional Madelung sum given in (2.5) is $S(4, 0)$.

Table 1

Sum	q series†	Reference in Jacobi (1829)‡	Value in Dirichlet series
$S(0,1)$	$\theta_3 - 1 = 2\sum q^{(n+1)^2}$	p 184 (6)	$2\zeta(2s)$
$S(1,0)$	$\theta_4 - 1 = 2\sum(-1)^{n+1}q^{(n+1)^2}$	p 184 (8)	$-2\eta(2s)$
$T(0,1) = U(0,1)$	$\theta_2 = 2\sum q^{(n+\frac{1}{2})^2}$	p 184 (7)	$2^{2s+1}\lambda(2s)$
$S(0,2)$	$\theta_3^2 - 1 = 4\sum \dfrac{q^{n+1}}{1+q^{2n+2}}$	p 103 (4)	$4\zeta(s)\beta(s)$
$S(1,1)$	$\theta_4\theta_3 - 1 = 4\sum \dfrac{(-1)^{n+1}q^{2n+2}}{1+q^{4n+4}}$	p 103 (7)	$-4.2^{-s}\eta(s)\beta(s)$
$S(2,0)$	$\theta_4^2 - 1 = 4\sum \dfrac{(-1)^{n+1}q^{n+1}}{1+q^{2n+2}}$	p 103 (6)	$-4\eta(s)\beta(s)$
$T(1,1)$	$\theta_3\theta_2 = 2q^{1/4}\sum \dfrac{q^{n/2}}{1+q^{n+\frac{1}{2}}}$	Put $q^{1/2}$ for q in (5), p 103, -2	$2^{2s+1}\lambda(s)\beta(s)$
$T(0,2) = U(0,2)$	$\theta_2^2 = 4q^{1/2}\sum \dfrac{q^n}{1+q^{2n+1}}$	p 103 (5)	$4.2^s\lambda(s)\beta(s)$
$U(1,1)$	$\theta_4\theta_2 = 2q^{1/4}\sum(-1)^n\left(\dfrac{q^n}{1+q^{4n+1}} - \dfrac{q^{3n+2}}{1+q^{4n+3}}\right)$		$2^{2s+1}[A^2(s) - B^2(s)]$
$S(0,4)$	$\theta_3^4 - 1 = 8\sum \dfrac{(n+1)q^{n+1}}{1+(-q)^{n+1}}$	p 103 (8)	$8(1-2^{2-2s})\zeta(s-1)\zeta(s)$
$S(2,2)$	$\theta_4^2\theta_3^2 - 1 = 8\sum \dfrac{(-1)^{n+1}(n+1)q^{2n+2}}{1+q^{2n+2}}$	p 104 (12)	$-8.2^{-s}\eta(s-1)\eta(s)$
$S(4,0)$	$\theta_4^4 - 1 = 8\sum \dfrac{(-1)^{n+1}(n+1)q^{n+1}}{1+q^{n+1}}$	p 104 (10)	$-8\eta(s-1)\eta(s)$

Table 1 (*continued*)

Sum	q series†	Reference in Jacobi (1829)‡	Values in Dirichlet series
$T(0,4)=U(0,4)$	$\theta_2^4 = 16\sum\frac{(2n+1)q^{2n+1}}{1-q^{4n+2}}$	p 104 (9)	$16\lambda(s-1)\lambda(s)$
$T(2,2)$	$\theta_3^2\theta_2^2 = 4\sum\frac{(2n+1)q^{n+\frac12}}{1-q^{2n+1}}$	p 104 (13)	$4.2^s\lambda(s-1)\lambda(s)$
$U(2,2)$	$\theta_4^2\theta_2^2 = 4\sum\frac{(-1)^n(2n+1)q^{n+\frac12}}{1+q^{2n+1}}$	p 104 (11)	$4.2^s\beta(s-1)\beta(s)$
$S(0,6)$	$\theta_3^6-1 = 16\sum\frac{(n+1)^2q^{2n+1}}{1+q^{2n+2}}-4\sum\frac{(-1)^n(2n+1)^2q^{2n+1}}{1-q^{2n+1}}$	p 108 (42)+(44)	$16\zeta(s-2)\beta(s)-4\beta(s-2)\zeta(s)$
$S(2,4)$	$\theta_4^2\theta_3^4-1 = 4\sum\frac{(-1)^n(2n+1)^2q^{2n+1}}{1+q^{2n+1}}$	p 107 (41)	$4\beta(s-2)\eta(s)$
$S(3,3)$	$\theta_4^3\theta_3^3-1 = 16\sum\frac{(-1)^{n+1}(n+1)^2q^{(n+1)/2}}{1+q^{n+1}}+4\sum\frac{(-1)^n(2n+1)^2q^{n+\frac12}}{1+q^{n+\frac12}}$	put $q^{1/2}$ for q in (41)–(45), p 108	$-2^s[16\eta(s-2)\beta(s)-4\beta(s-2)\eta(s)]$
$S(4,2)$	$\theta_4^4\theta_3^2-1 = 4\sum\frac{(-1)^{n+1}(2n+1)^2q^{2n+1}}{1-q^{2n+1}}$	p 108 (44)	$-4\beta(s-2)\zeta(s)$
$S(6,0)$	$\theta_4^6-1 = 16\sum\frac{(-1)^{n+1}(n+1)^2q^{n+1}}{1+q^{2n+2}}+4\sum\frac{(-1)^n(2n+1)^2q^{2n+1}}{1+q^{2n+1}}$	p 108 (41)–(45)	$-16\eta(s-2)\beta(s)+4\beta(s-2)\eta(s)$
$T(0,6)=U(0,6)$	$\theta_2^6 = 4\sum\frac{(2n+1)^2q^{n+\frac12}}{1+q^{2n+1}}+4\sum\frac{(-1)^n(2n+1)^2q^{n+\frac12}}{1-q^{2n+2}}$	p 108 (40)–(43)	$4.2^s[\lambda(s-2)\beta(s)-\beta(s-2)\lambda(s)]$
$T(2,4)$	$\theta_3^2\theta_2^4 = 16\sum\frac{(n+1)^2q^{n+1}}{1+q^{2n+2}}$	p 108 (42)	$16\zeta(s-2)\beta(s)$
$T(3,3)$	$\theta_3^3\theta_2^3 = \frac12\sum\frac{(2n+1)^2q^{\frac12 n+\frac14}}{1+q^{n+\frac12}}-\frac12\sum\frac{(-1)^n(2n+1)q^{\frac12 n+\frac14}}{1-q^{n+\frac12}}$	Put $q^{1/2}$ for q in (40)–(43), 8	$2^{2s-1}[\lambda(s-2)\beta(s)-\beta(s-2)\lambda(s)]$

Table 1 (*continued*)

Sum	q series†	Reference in Jacobi (1829)‡	Values in Dirichlet series
$T(4,2)$	$\theta_3^4\theta_2^2 = 4\sum \frac{(2n+1)^2 q^{n+\frac{1}{2}}}{1+q^{2n+1}}$	p 107 (40)	$4.2^s\lambda(s-2)\beta(s)$
$U(2,4)$	$\theta_4^2\theta_2^4 = 16\sum \frac{(-1)^{n+1}(n+1)^2 q^{n+1}}{1+q^{2n+2}}$	p 108 (45)	$16\eta(s-2)\beta(s)$
$U(3,3)$	$\theta_4^3\theta_2^3 = q^{3/4}\sum(-1)^n\left(\frac{(4n+3)^2 q^n}{1+q^{4n+3}} - \frac{(4n+1)^2 q^{3n}}{1+q^{4n+1}}\right)$		$2^{2s}[A(s)B(s-2) - A(s-2)B(s)]$
$U(4,2)$	$\theta_4^4\theta_2^2 = 4\sum \frac{(-1)^n(2n+1)^2 q^{n+\frac{1}{2}}}{1-q^{2m+1}}$	p 108 (42)	$4.2^s\beta(s-2)\lambda(s)$
$S(0,8)$	$\theta_3^8 - 1 = 16\sum \frac{(n+1)^3 q^{n+1}}{1-(-q)^{n+1}}$	p 115 (8)	$16(1-2^{1-s}+2^{4-2s})\zeta(s-3)\zeta(s)$
$S(4,4)$	$\theta_4^4\theta_3^4 - 1 = 16\sum \frac{(-1)^{n+1}(n+1)^3 q^{2n+2}}{1-q^{2n+2}}$	Put q^2 for q in (7), p 115	$-16.2^{-s}\eta(s-3)\zeta(s)$
$S(8,0)$	$\theta_4^8 - 1 = 16\sum \frac{(-1)^{n+1}(n+1)^3 q^{n+1}}{1-q^{n+1}}$	p 115 (7)	$-16\eta(s-3)\zeta(s)$
$T(0,8) = U(0,8)$	$\theta_2^8 = 256\sum \frac{(n+1)^3 q^{2n+2}}{1-q^{4n+4}}$	p 111 (5)	$256.2^{-s}\zeta(s-3)\lambda(s)$
$T(4,4)$	$\theta_3^4\theta_2^4 = 16\sum \frac{(n+1)^3 q^{n+1}}{1-q^{2n+2}}$	p 111 (3)	$16\zeta(s-3)\lambda(s)$
$U(4,4)$	$\theta_4^4\theta_2^4 = 16\sum \frac{(-1)^{n+1}(n+1)^3 q^{n+1}}{1-q^{2n+2}}$	p 111 (4)	$-16\eta(s-3)\lambda(s)$

† All the sums are from $n = 0$ to ∞.

‡ References in Jacobi (1829) are given by page number (p) and relevant equation ( ).

In table 1 we list all the sums that have been evaluated, together with their associated q series, reference to the *Fundamenta Nova* and the result in terms of Dirichlet series. The following Dirichlet series defined below have also been used in the table. These are

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

$$A(s) = \sum_{n=0}^{\infty} (-1)^n(4n+1)^{-s} \qquad B(s) = \sum_{n=0}^{\infty} (-1)^n(4n+3)^{-s}. \tag{2.14}$$

All the Dirichlet series used here are convergent for $s > 0$ except for $\zeta(s)$ and $\lambda(s)$ which converge for $s > 1$.

The only q series not given by Jacobi is that for $\theta_2\theta_4$. The series for $\theta_2^3\theta_4^3$ also requires some care to formulate. The series for $\theta_2\theta_4$ was obtained by Zucker (to be published) via a long argument using Glasser's (1973b) result for the lattice sum

$$\sum_{(l_1,l_2)\neq(0,0)} (l_1^2+16l_2^2)^{-s} \tag{2.15}$$

which was obtained employing number theoretic techniques. Subsequently the q series for $\theta_2\theta_4$ was derived directly without recourse to number theory. With this series the result of Glasser (1973b) for a certain three-dimensional result namely

$$T = 4\sum_{n=1}^{\infty}\sum_{m=1}^{\infty}\sum_{l=1}^{\infty} (-1)^m[n^2+m^2+(l-\tfrac{1}{2})^2]^{-s} \tag{2.16}$$

was re-evaluated. It is easily shown that

$$2T = M[(\theta_3-1)(\theta_4-1)\theta_2] = M[\theta_2\theta_3\theta_4-\theta_2\theta_3-\theta_2\theta_4+\theta_2]. \tag{2.17}$$

Using identity (9) we find $M[\theta_2\theta_3\theta_4] = 2^{2s+1}\beta(2s-1)$ thus

$$2T = 2^{2s+1}\beta(2s-1)-T(1,1)-U(1,1)+T(0,1)$$

therefore

$$T = 2^{2s}[\beta(2s-1)-A^2(s)+B^2(s)-\lambda(s)\beta(s)+\lambda(2s)]. \tag{2.18}$$

This differs from Glasser's (1973b) result in some details. Both the left-hand side and the right-hand side of (2.18) have been independently evaluated numerically for several values of s, and the result given above found to be correct.

3. Discussion

Glasser (1973b) has pointed out that (2.18) appears to be the first exact result for a three-dimensional lattice sum so far obtained. However, I am less optimistic than he over the possibility of obtaining other exact three-dimensional results. The problem of finding $S(0, 3)$ or $S(0, d)$ can be put in another way. Let $\tau_d(n)$ be the number of ways of representing any positive integer as a sum of d squares. Then it is easily shown that $\tau_d(n)$ is the coefficient of q^n in θ_3^d. Thus Jacobi (1829) solved the problem for $d = 2, 4, 6$ and 8 when $\tau_d(n)$ can be expressed in terms of divisors of n. For example,

$$\begin{aligned} \tau_8(n) &= \sum \delta^3 && \text{for odd } n, \\ \tau_8(n) &= 8\sum \delta_e^3 - 8\sum \delta_o^3 && \text{for even } n \end{aligned} \tag{3.1}$$

where δ denotes a divisor of n, δ_e an even divisor and δ_o an odd divisor of n. Hardy (1918) states that $\tau_d(n)$ may be evaluated 'within the limits of human capacity for calculation for *any* even value of d'. Glaisher (1907) has worked out systematically all cases up to $d = 18$, though for $d > 8$ more recondite arithmetic functions than simple divisor sums have to be used to express $\tau_d(n)$. But for odd d the problem is much more difficult belonging 'to one of the most unfamiliar and difficult chapter in theory of numbers'. Hardy (1918) does actually give 'exact' results for θ_3^3, θ_3^5 and θ_3^7, but they involve multiple sums. The M operation on these will not produce simplifications as illustrated in § 2.

There are some suggestions, however, that can be made concerning three-dimensional sums. For instance the Madelung sums for $d = 1, 2$ and 4 are

$$S(1,0) = -2\eta(2s), \qquad S(2,0) = -4\eta(s)\beta(s), \qquad S(4,0) = -8\eta(s-1)\eta(s) \tag{3.2}$$

and similarly the Lennard-Jones and Ingham (1925) sums are

$$S(0,1) = 2\zeta(2s), \qquad S(0,2) = 4\zeta(s)\beta(s), \qquad S(0,4) = 8(1-2^{2-2s})\zeta(s-1)\zeta(s). \tag{3.3}$$

It might thus be conjectured that $S(3,0) = -6\eta(s-\frac{1}{2})J(s)$ and $S(0,3) = 6\zeta(s-\frac{1}{2})K(s)$ where $J(s)$ and $K(s)$ are as yet unknown Dirichlet series. A numerical investigation of this conjecture is now being carried out.

Acknowledgments

The author expresses his thanks to Dr M L Glasser for stimulating and continuing correspondence, to Dr G S Joyce (King's College) for help and suggestions and to Mrs B Zucker and Mrs K Saloman for initial impetus.

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