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Exact values for some two-dimensional lattice sums

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Abstract. Exact values are given for many two-dimensional lattice sums in terms of products of Dirichlet L-series. Madelung constants are included amongst the sums considered.

1. Introduction

In recent times interest in the exact evaluation of lattice sums has been revived, particularly by Glasser (1973a, b). The term 'exact' in this context means that a multiple sum has been expressed as a product of simple sums. For example, Hardy (1919) showed that

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

$(m, n \neq 0, 0)$ means summation over all positive and negative integer values of m and n but excluding the case $m = n = 0$. Thus in (1.1) the double sum on the left-hand side has been expressed as the product of two well known Dirichlet series on the right-hand side and we call this result exact. The Dirichlet series on the right-hand side of (1.1) are

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

We have investigated other two-dimensional lattice sums of which (1.1) is a special case. The sums considered were:

$$\begin{aligned}
Q &= Q(a, b, c) = Q(a, b, c : s) = \sum_{(m,n\neq 0,0)} (am^2+bmn+cn^2)^{-s} \\
Q^m &= Q^m(a, b, c) = Q^m(a, b, c : s) = \sum_{(m,n\neq 0,0)} (-1)^m(am^2+bmn+cn^2)^{-s} \\
Q^n &= Q^n(a, b, c) = Q^n(a, b, c : s) = \sum_{(m,n\neq 0,0)} (-1)^n(am^2+bmn+cn^2)^{-s} \\
Q^{mn} &= Q^{mn}(a, b, c) = Q^{mn}(a, b, c : s) = \sum_{(m,n\neq 0,0)} (-1)^{m+n}(am^2+bmn+cn^2)^{-s}.
\end{aligned} \tag{1.3}$$

Here a, b, c are relatively prime positive integers with $b \leqslant a \leqslant c$ and $b^2-4ac < 0$. Thus the lattice sum given in (1.1) is just $Q(1, 0, 1 : s)$. Figure 1 shows how two-dimensional space may be divided into parallelograms having sides of lengths $\sqrt{a}$ and $\sqrt{c}$ with angle θ between the sides, where $b = 2\sqrt{(ac)}\cos\theta$. Then $(am^2+bmn+cn^2)^{1/2}$ is the distance between any lattice point and an arbitrary origin on the lattice.

$Q(a, b, c)$ is also known as the Epstein zeta function and often denoted by $\zeta(s, Q)$. It has been investigated previously, but with regard as to where its zeros lie. Thus $Q(1, 0, 5)$

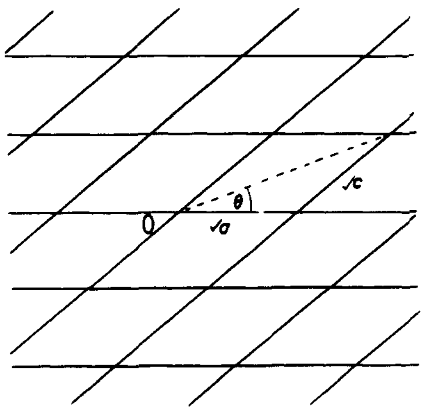

Figure 1.

was considered by Potter and Titchmarsh (1935) and Davenport and Heilbron (1936a, b) who obtained some general results concerning the location of zeros. Recently Smart (1973) attempted to evaluate Q. He was able to transform $Q(a, b, c)$ into other series but was only able to obtain $Q(1, 0, 1)$ and $Q(1, 1, 1)$ which were known previously. $Q(1, 0, 4)$ is also known and Glasser (1973b) obtained $Q(1, 0, 16)$, the latter being required to evaluate a certain three-dimensional sum. Apart from knowing $Q^m(1, 0, 1)$ and $Q^{mn}(1, 0, 1)$ little is known about Q^m, Q^n and Q^{mn}. Here we present many results for all the forms given by (1.3). The results have been expressed, not as products of simple Dirichlet series, but as sums of products of the less familiar Dirichlet L-series of which the simple Dirichlet series are special cases. The properties of L-functions represented by L-series are stated briefly in § 2.

Two methods were used to obtain the results given here. One was the number theoretic method described by Glasser (1973b). This involved finding the number of representations of an integer by the binary quadratic form $am^2+bmn+cn^2$ and its associated reduced equivalent forms with discriminant b^2-4ac. This is a difficult approach, each form having to be considered individually and providing no information about Q^m, Q^n and Q^{mn}. Nevertheless, it produced some results which were not obtained by the second method. However, this second method using θ-functions—also described by Glasser (1973a) and elaborated by Zucker (1974a, b)—was more flexible, especially in producing new results from previously known ones. For example, if $Q(1, 0, c)$ was known then for odd c it was immediately possible to obtain $Q^{mn}(1, 0, c)$, or if c was even then $Q^m(1, 0, c)$ could be found. Again, knowing $Q(1, 0, c)$ it was possible to evaluate $Q(1, 0, 4c)$ by a set procedure provided that $c \equiv 2 \bmod (4)$, $3 \bmod (4)$ or $4 \bmod (8)$. By either method no completely general result was obtained. The details of the above calculations are somewhat complicated and will be given elsewhere.

2. The Dirichlet L-functions

The Dirichlet L-functions (Erdélyi 1955) may be defined for $\operatorname{Re} s > 1$ by the following series:

$$L_k = L_k(s) = \sum_{n=1}^{\infty} \frac{\chi(n)}{n^s} \tag{2.1}$$

where k is a fixed positive integer; $\chi(n)$ is a character (modulo k) and so satisfies the conditions

$$\begin{aligned} \chi(n+k) &= \chi(n) \\ \chi(m)\chi(n) &= \chi(mn) \\ \chi(n) &= 0 \qquad \text{if } k \text{ and } n \text{ have a common factor.} \end{aligned} \tag{2.2}$$

We are concerned only with L-functions having real characters when $\chi(n) = \pm 1$. The simplest series is for $k = 1$ when $\chi(n) = +1$ for all n. This gives the Riemann zeta function, the simplest L-function. We list below all the L-functions relevant to this communication together with alternative notation used by other authors (Fletcher *et al* 1962). Only the primitive L-series are given, ie those which cannot be expressed in terms of simpler L-series. We have also introduced the notation

$$(k, l) = \sum_{n=0}^{\infty} (kn+l)^{-s} \tag{2.3}$$

for the simple Dirichlet series, since with this notation the periodicity of a given L_k with k is exhibited.

$$\begin{aligned}
L_1 &= 1+2^{-s}+3^{-s}\ldots = (1,1) = \zeta(s) \\
L_3 &= 1-2^{-s}+4^{-s}-5^{-s}\ldots = (3,1)-(3,2) = g(s) \\
L_4 &= 1-3^{-s}+5^{-s}-7^{-s}\ldots = (4,1)-(4,3) = \beta(s) \\
L_5 &= 1-2^{-s}-3^{-s}+4^{-s}+6^{-s}\ldots = (5,1)-(5,2)-(5,3)+(5,4) \\
L_7 &= 1+2^{-s}-3^{-s}+4^{-s}-5^{-s}-6^{-s}\ldots = (7,1)+(7,2)-(7,3)+(7,4)-(7,5)-(7,6) \\
L_{8a} &= 1+3^{-s}-5^{-s}-7^{-s}\ldots = (8,1)+(8,3)-(8,5)-(8,7) = p(s) \\
L_{8b} &= 1-3^{-s}-5^{-s}+7^{-s}\ldots = (8,1)-(8,3)-(8,5)+(8,7) = q(s) \\
L_{12} &= 1-5^{-s}-7^{-s}+11^{-s}\ldots = (12,1)-(12,5)-(12,7)+(12,11) \\
L_{20} &= 1+3^{-s}+7^{-s}+9^{-s}-11^{-s}-13^{-s}-17^{-s}-19^{-s}\ldots \\
&= (20,1)+(20,3)+(20,7)+(20,9)-(20,11)-(20,13)-(20,17)-(20,19) \\
L_{24a} &= 1+5^{-s}+7^{-s}+11^{-s}-13^{-s}-17^{-s}-19^{-s}-23^{-s}\ldots \\
&= (24,1)+(24,5)+(24,7)+(24,11)-(24,13)-(24,17)-(24,19)-(24,23) \\
L_{24b} &= 1+5^{-s}-7^{-s}-11^{-s}-13^{-s}-17^{-s}+19^{-s}+23^{-s}\ldots \\
&= (24,1)+(24,5)-(24,7)-(24,11)-(24,13)-(24,17)+(24,19)+(24,23) \\
L_{40a} &= 1-3^{-s}+7^{-s}+9^{-s}+11^{-s}+13^{-s}-17^{-s}+19^{-s}-21^{-s}+23^{-s}-27^{-s}-29^{-s}-31^{-s} \\
&\quad -33^{-s}+37^{-s}-39^{-s}\ldots \\
&= (40,1)-(40,3)+(40,7)+(40,9)+(40,11)+(40,13)-(40,17)+(40,19) \\
&\quad -(40,21)+(40,23)-(40,27)-(40,29)-(40,31)-(40,33) \\
&\quad +(40,37)-(40,39).
\end{aligned} \tag{2.4}$$

It might be thought that other combinations of simple Dirichlet series would produce L-functions. For example,

$$L_6 = 1-5^{-s}+7^{-s}-11^{-s}\ldots = (6,1)-(6,5) = h(s)$$

has characters, but it may be shown that this series is just $(1+2^{-s})L_3$ and hence is not primitive. The list of primitive L-functions of real character given above is complete up to L_{8b}. As illustrated for some k there is no primitive function whilst for other values there may be more than one. If k is prime there is just one primitive L-function. There are of course many non-primitive functions and one occurs so often in our results that we will give it below. This is

$$L_2 = 1-2^{-s}+3^{-s}\ldots = (1-2^{1-s})L_1 = (2,1)-(2,2) = \eta(s). \tag{2.5}$$

All the above L-series except L_1 consist of equal numbers of positive and negative terms. It may be shown that apart from L_1 they all converge for $\operatorname{Re} s > 0$. Further all the functions obey a reflection formula, namely

$$L_k(s) = 2^s\pi^{s-1}k^{-s+\frac{1}{2}}\Gamma(1-s)\cos(s\pi/2)L_k(1-s) \qquad \text{if } \chi(k-1) = -1 \tag{2.6a}$$

$$L_k(s) = 2^s\pi^{s-1}k^{-s+\frac{1}{2}}\Gamma(1-s)\sin(s\pi/2)L_k(1-s) \qquad \text{if } \chi(k-1) = +1. \tag{2.6b}$$

This enables us to evaluate the L-functions for all real s. Indeed it may be shown that the L-functions are all entire single-valued functions of real s, except for $L_1(s)$ which has a simple pole at $s = 1$.

Each L-function takes on values given in terms of powers of π for positive integral values of s. The values are known for either even s, $\chi(k-1) = +1$ or odd s, $\chi(k-1) = -1$, but never both. For example,

$$L_1(2s) = \frac{1}{2}\frac{(2\pi)^{2s}}{2s!}|B_{2s}(0)|, \qquad L_4(2s+1) = \frac{1}{2}\left(\frac{\pi}{2}\right)^{2s+1}\frac{1}{2s!}|E_{2s}(0)| \tag{2.7}$$

where $B_{2s}(x)$ and $E_{2s}(x)$ are the Bernoulli and Euler polynomials as defined by Abramowitz and Stegun (1965). It is always possible to evaluate $L_k(1)$ in known transcendentals. For k as a prime p, a theorem of Dirichlet states that if

$$p \equiv 3 \bmod(4), \qquad L_p(1) = \frac{\pi}{\sqrt{p}} \times h(-p)$$

and if

$$p \equiv 1 \bmod(4), \qquad L_p(1) = \frac{2}{\sqrt{p}} \ln \epsilon_0 \times h(p)$$

where $h(p)$ is the number of classes of the quadratic forms with discriminant p and ϵ_0 is the fundamental unit in the algebraic number field $Q(\sqrt{p})$.

Known values of the L-functions are given in table 1 for various values of s. The values of $L_k(\frac{1}{2})$ have been evaluated by direct summation of the series using either the Euler or Euler–Mclaurin summation formulae. $L_1(\frac{1}{2}) = \zeta(\frac{1}{2})$ was found by evaluating $\eta(\frac{1}{2})$. Titchmarsh (1951) has shown that the series for $\eta(s)$ sums to $(1-2^{1-s})\zeta(s)$ for *all s*, hence $\zeta(\frac{1}{2}) = -(\sqrt{2}+1)\eta(\frac{1}{2})$. We note that $\eta(1) = \ln 2$, although $\zeta(1)$ diverges.

Results for various $Q(a, b, c : s)$ in terms of L_k are presented in table 2.

3. Discussion

The results in table 2 are not meant to be complete in any way. Even where we have left gaps in the table, this does not imply that the exact result cannot be found. Again the omission altogether of a form such as $Q(1, 0, 13)$ does not imply that an exact result

Table 1.

	0	$\frac{1}{2}$	1	2	3	4	2^s+1	$2s$
L_1	$-\frac{1}{2}$	$-1{\cdot}4603545$	∞	$\pi^2/6$		$\pi^4/90$		$\frac{1}{2}\frac{(2\pi)^{2s}}{2s!}\lvert B_{2s}(0)\rvert$
L_2	$\frac{1}{2}$	$0{\cdot}6048986$	$\ln 2$	$\pi^2/12$		$7\pi^4/720$		$L_2=(1-2^{1-s})L_1$
L_3	$\frac{1}{3}$	$0{\cdot}4808676$	$\pi/3\surd 3$		$4\pi^3/81\surd 3$		$\frac{1}{\surd 3}\frac{(2\pi)^{2s+1}}{(2s+1)!}\lvert B_{2s+1}(1/3)\rvert$	
L_4	$\frac{1}{2}$	$0{\cdot}6676946$	$\pi/4$		$\pi^3/32$		$\frac{1}{2}\left(\frac{\pi}{2}\right)^{2s+1}\frac{1}{(2s+1)!}\lvert E_{2s}(0)\rvert$	
L_5	0	$0{\cdot}2317509$	$(2/\surd 5)\ln[(1+\surd 5)/2]$	$4\pi^2/25\surd 5$		$8\pi^4/375\surd 5$		$\frac{2}{\surd 5}\frac{(2\pi)^{2s}\lvert B_{2s}(1/5)\rvert}{2s!}$ $+\frac{1}{\surd 5}(1-5^{1-2s})L_1(2s)$
L_7	1	$1{\cdot}1465857$	$\pi/\surd 7$		$32\pi^3/343\surd 7$			
L_{8a}	1	$1{\cdot}1004214$	$\pi/2\surd 2$		$3\pi^3/64\surd 2$		$\frac{1}{2\surd 2}\frac{\pi^{2s+1}}{2s!}\lvert E_{2s}(1/4)\rvert$	

Table 1. (Continued.)

L_{8b}	0	0·3736917	$\sqrt{\tfrac{1}{2}}\ln(1+\sqrt{2})$	$\pi^2/8\sqrt{2}$		$11\pi^4/768\sqrt{2}$		$\frac{1}{2\sqrt{2}}\frac{\pi^{2s}}{(2s-1)!}\lvert E_{2s-1}(1/4)\rvert$
L_{12}	0	0·4985570	$\sqrt{\tfrac{1}{3}}\ln(2+\sqrt{3})$	$\pi^2/6\sqrt{3}$		$23\pi^4/1296\sqrt{3}$		$\frac{1}{2\sqrt{3}}\frac{\pi^{2s}}{(2s-1)!}\lvert E_{2s-1}(1/6)\rvert$
L_{20}	2	1·679671	$\pi/\sqrt{5}$		$3\pi^3/40\sqrt{5}$		$\frac{1}{\sqrt{5}}\frac{\pi^{2s+1}}{2s!}\lvert E_{2s}(1/10)\rvert + \frac{1}{\sqrt{5}}(1-5^{-2s})L_4(2s+1)$	
L_{24a}	2	1·5719151	$\pi/\sqrt{6}$		$23\pi^3/288\sqrt{6}$		$\frac{1}{\sqrt{6}}\frac{\pi^{2s+1}}{2s!}\lvert E_{2s}(1/12)\rvert + \frac{1}{\sqrt{3}}(1-3^{-2s})L_{8a}(2s+1)$	
L_{24b}	0	0·7094581	$\sqrt{\tfrac{2}{3}}\ln(\sqrt{2}+\sqrt{3})$	$\pi^2/4\sqrt{6}$		$29\pi^4/1152\sqrt{6}$		$\frac{1}{\sqrt{6}}\frac{\pi^{2s}}{(2s-1)!}\lvert E_{2s-1}(1/12)\rvert - \frac{1}{\sqrt{3}}(1+3^{1-2s})L_{8b}(2s)$
L_{40a}	2	1·2737015	$\pi/\sqrt{10}$		$79\pi^3/800\sqrt{10}$			

Table 2.

a, b, c	$Q(a,b,c)$	$Q^m(a,b,c)$	$Q^n(a,b,c)$	$Q^{mn}(a,b,c)$
1, 0, 1	$4L_1L_4$	$-4\times 2^{-s}L_2L_4$	$-4\times 2^{-s}L_2L_4$	$-4L_2L_4$
1, 1, 1	$6L_1L_3$	$-2(1+2^{1-s})L_2L_3$	$-2(1+2^{1-s})L_2L_3$	$-2(1+2^{1-s})L_2L_3$
1, 0, 2	$2L_1L_{8a}$	$-2L_2L_{8a}$	$2L_4L_{8b}-2^{1-s}L_2L_{8a}$	$-2L_4L_{8b}-2^{1-s}L_2L_{8a}$
1, 0, 3	$2(1+2^{1-2s})L_1L_3$	$-2L_4L_{12}-2^{1-2s}(1+2^{1-s})L_2L_3$	$2L_4L_{12}-2^{1-2s}(1+2^{1-s})L_2L_3$	$-2(1+2^{1-s})L_2L_3$
1, 0, 4	$2(1-2^{-s}+2^{1-2s})L_1L_4$	$-2(1+2^{-s})L_2L_4$	$-2^{2-3s}L_2L_4+2L_{8a}L_{8b}$	$-2^{2-3s}L_2L_4-2L_{8a}L_{8b}$
1, 0, 5	$L_1L_{20}+L_4L_5$			$-L_2L_{20}-(1+2^{1-s})L_4L_5$
1, 0, 6	$L_1L_{24a}+L_3L_{8b}$	$-L_2L_{24a}-(1+2^{1-s})L_3L_{8b}$		
2, 0, 3	$L_1L_{24a}-L_3L_{8b}$		$-L_2L_{24a}+(1+2^{1-s})L_3L_{8b}$	
1, 0, 7	$2(1-2^{1-s}+2^{1-2s})\,L_1L_7$			$-2L_2L_7$
1, 0, 8	$(1-2^{-s}+2^{1-2s})L_1L_{8a}+L_4L_{8b}$	$-(1+2^{-s})L_2L_{8a}-L_4L_{8b}$		

a, b, c	$Q(a,b,c)$
1, 1, 2	$2L_1L_7$
3, 2, 3	$(1-2^{-s}+2^{1-2s})L_1L_{8a}-L_4L_{8b}$
2, 2, 3	$L_1L_{20}-L_4L_5$
1, 0, 9	$(1+3^{1-2s})L_1L_4+L_3L_{12}$
1, 0, 10	$L_1L_{40a}+L_5L_{8a}$
1, 0, 12	$L_4L_{12}+(1+2^{-2s}+2^{2-4s})L_1L_3$
1, 0, 16	$(1-2^{-s}+2^{1-2s}+2^{1-3s}+2^{2-4s})L_1L_4-L_{8a}L_{8b}$
1,0, 24	$2^{-1}[(1-2^{-s}+2^{1-2s})L_1L_{24a}+L_4L_{24b}+L_{8a}L_{12}+(1+2^{-s}+2^{1-2s})L_3L_{8b}]$
1, 0, 25	$(1-2\times 5^{-s}+5^{1-2s})L_1L_4+L_5L_{20}$
1, 0, 48	$2^{-1}[(1+2^{-2s}+2^{1-4s}+2^{3-6s})L_1L_3+L_{8a}L_{24b}+L_{8b}L_{24a}+(1+2^{1-2s})L_4L_{12}]$

cannot be found. Unfortunately we have no criterion at all to tell us whether any given $Q(a, b, c)$ can be written down exactly in the sense meant here. Further we cannot pretend that the results obtained are of any physical significance, since $Q(a, b, c)$ may be directly summed very easily on any computer. There is, however, some aesthetic value in expressing multiple sums in known transcendental numbers, eg

$$\sum_{(m,n\neq 0,0)} (-1)^m(m^2+mn+n^2)^{-1} = -\frac{4\pi \ln 2}{3\sqrt{3}}$$

$$\sum_{(m,n\neq 0,0)} (-1)^{m+n}(m^2+5n^2)^{-1} = -\frac{\pi}{\sqrt{5}}\ln(1+\sqrt{5})$$

and they also provide checks for computer programs.

The results of most probable interest are those for the triangular lattice $Q(1, 1, 1)$ and for the rectangular lattices $Q(1, 0, c)$, in particular when c is a perfect square. Further the sums $Q^{mn}(a, b, c:\frac{1}{2})$ are the Madelung constants for the particular lattice, ie the sum obtained for the Coulomb interaction of a unit charge at the origin with alternative positive and negative charges placed at the other lattice points.

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