ON THE MATHEMATICS OF SALT

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Abstract. We describe the key analytic and computational properties of Madelung’s constants.

1. Introduction

Following Zucker [21] and others, we consider the three series

\[ J_3(2s) := \sum_{n=1}^{\infty} \frac{1}{(m^2 + n^2 + p^2)^s}, \quad M_3(2s) := \sum_{n=1}^{\infty} \frac{(-1)^{m+n+p}}{(m^2 + n^2 + p^2)^s}, \]

\[ N_3(2s) := \sum_{n=1}^{\infty} \frac{1}{((m + \frac{1}{2})^2 + (n + \frac{1}{2})^2 + (p + \frac{1}{2})^2)^s} \]

which for Re \( s > 3/2 \) are absolutely convergent.

2. Three Squares

Sums of an odd number of squares are notoriously less amenable to closed forms than those of an even number. In this section—which is largely a reworking of material in [3]—we primarily record some results for \( r_3(n) \), the number of representations of \( n \) as a sum of three squares. Following Hardy and Bateman, Hua in [14] gives the following formula for \( r_3(n) \). Let

\[ \chi_2(n) := \begin{cases} 
0 & \text{if } 4^{-a}n \equiv 7 \pmod{8}; \\
2^{-a} & \text{if } 4^{-a}n \equiv 3 \pmod{8}; \\
3 \cdot 2^{-1-a} & \text{if } 4^{-a}n \equiv 1, 2, 5, 6 \pmod{8} 
\end{cases} \]

where \( a \) is the highest power of 4 dividing \( n \).

Then

\[ r_3(n) = \frac{16\sqrt{n}}{\pi} L(-4n, 1) \chi_2(n) \]

\[ \times \prod_{p^2 | n} \left( \frac{p^{a^{-1}} - 1}{p^{-1} - 1} + p^{-a} \left( 1 - \frac{1}{p} \left( -\frac{p^{-2a}n}{p} \right) \right)^{-1} \right) \]

where \( \tau = \tau_p \) is the highest power of \( p^2 \) dividing \( n \).

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The Dirichlet series for \( r_4(n) \) deriving from for an even number of squares [2], but we are able to derive a nice expression in terms of Bessel functions. Let \( K_s \) be the modified Bessel function of the second kind. Then we have (see [20], p. 183)

\[
(2.2) \quad K_s(x) = \frac{1}{2} \left( \frac{x}{2} \right)^s \int_0^\infty e^{-t} \frac{e^{-x/2t}}{t^{s+1}} \, dt.
\]

By the substitution \( t = \frac{1}{u} \) in (2.2), we get

\[
(2.3) \quad K_s(x) = \frac{1}{2} \left( \frac{x}{2} \right)^s \int_0^\infty e^{-\frac{x^2}{4} - \frac{1}{4} u} u^{s-1} \, du.
\]

Let

\[
\theta_3(q) := \sum_{n=-\infty}^{\infty} q^{n^2}, \quad \theta_4(q) := \sum_{n=-\infty}^{\infty} (-1)^n q^{n^2}
\]

and

\[
\theta_2(q) := \sum_{n=-\infty}^{\infty} q^{(n+1/2)^2}
\]

be the classical Jacobean theta functions. In view of the Poisson summation formula [2], we have, for \( t > 0 \)

\[
\theta_3(e^{-\pi t}) = t^{-1/2} \theta_3(e^{-\pi t/2}) \quad \theta_2(e^{-\pi t}) = t^{-1/2} \theta_4(e^{-\pi t}).
\]

Since the Mellin transform of \( e^{-\alpha t} \) for \( \alpha \neq 0 \) is \( M_s(e^{-\alpha t}) = \Gamma(s) \alpha^{-s} \), so we have (letting \( q = e^{-\pi t} \))

\[
\mathcal{J}_3(2s) = 3 \sum_{n,m,p \in \mathbb{Z}} \frac{n^2}{(n^2 + m^2 + p^2)^{s+1}} = \frac{3\pi^{s+1}}{\Gamma(s+1)} \sum_{n,m,p \in \mathbb{Z}} n^2 M_{s+1}(q^{n^2+m^2+p^2})
\]

\[
= \frac{3\pi^{s+1}}{\Gamma(s+1)} M_{s+1} \left( \sum_{n \in \mathbb{Z}} n^2 q^{n^2} \theta_3^2(q) \right) = \frac{3\pi^{s+1}}{\Gamma(s+1)} \sum_{n \in \mathbb{Z}} n^2 \int_0^\infty e^{-n^2\pi t} \theta_3^2(q) t^{s-1} \, dt
\]

\[
+ \frac{3\pi^{s+1}}{\Gamma(s+1)} \sum_{n \in \mathbb{Z}} n^2 \int_0^\infty e^{-n^2\pi t} \, dt
\]

The first term of (2.4) is

\[
= \frac{6\pi^{s+1}}{\Gamma(s+1)} \sum_{m=1}^\infty r_2(m)(\pi m)^s \sum_{n=1}^\infty n^2 \int_0^\infty e^{-n^2\pi t - \pi m} t^{s-1} \, dt
\]

\[
= \frac{6\pi^{s+1}}{\Gamma(s+1)} \sum_{m=1}^\infty r_2(m)(\pi m)^s \sum_{n=1}^\infty n^2 \int_0^\infty e^{-n^2\pi t - \pi m} t^{s-1} \, dt, \quad (x = \frac{t}{\pi m})
\]

\[
= \frac{12\pi^{s+1}}{\Gamma(s+1)} \sum_{m=1}^\infty r_2(m)m^{s/2} \sum_{n=1}^\infty \frac{1}{n^{s-2}} K_s(2\pi n \sqrt{m})
\]

by (2.3) and the second term is

\[
\frac{6\pi^{s+1}}{\Gamma(s+1)} \sum_{n=1}^\infty \frac{1}{n^{2s-2} \pi^s} \int_0^\infty e^{-x^2} x^{s-1} \, dx = \frac{6\pi}{s} \zeta(2s-2).
\]
This proves the following result in which \( o_2(n) \) counts the number of representations of a number as the sum of two odd squares, while \( \zeta_{1/2}(s) := \sum_{n=1}^{\infty} (n - 1/2)^{-s} = (2s - 1)\zeta(s) \), of representations of a number as the sum of two odd squares.

**Theorem 2.1.** For all \( s \)

\[
J_3(2s) = \frac{6\pi}{s} \zeta(2s - 2) + \frac{12\pi^{s+1}}{\Gamma(s + 1)} \sum_{k > 0} k^{s} K_s(2\pi \sqrt{k}) \sum_{n^2 | k} \frac{r_2(k/n^2)}{n^{2s-2}}.
\]

Equivalently

\[
J_3(2s) = \frac{6\pi}{s} \zeta(2s - 2) + \frac{3 (2\pi)^{s+1}}{2 \Gamma(s + 1)} \sum_{m=1}^{\infty} (-1)^m r_2(m) m^{s/2} \sum_{\substack{e \in \text{even} \atop c > 0 \text{ odd}}} \frac{1}{e^{s-2} K_s(e \pi \sqrt{m})} - \left(\frac{4}{3}\right)^s.
\]

Correspondingly,

\[
N_3(2s) = \frac{6\pi}{s} \zeta_{1/2}(2s - 2) + \frac{3 (2\pi)^{s+1}}{2 \Gamma(s + 1)} \sum_{m=1}^{\infty} (-1)^m r_2(m) m^{s/2} \sum_{o > 0 \text{ odd}} \frac{1}{o^{s-2} K_s(o \pi \sqrt{m})} - \left(\frac{4}{3}\right)^s.
\]

and

\[
M_3(2s) = -\frac{3\pi^{s+1}}{\Gamma(s + 1)} \sum_{m=1}^{\infty} o_2(m) m^{s/2} \sum_{\substack{e \in \text{even} \atop c > 0 \text{ odd}}} \frac{(-1)^{e/2}}{e^{s-2} K_s\left(c \frac{\pi}{2} \sqrt{m}\right)}.
\]

Equivalently

\[
M_3(2s) = -\frac{24 (\frac{\pi}{2})^{s+1}}{\Gamma(s + 1)} \sum_{k > 0} k^{s} K_s(\pi \sqrt{k}) \sum_{n^2 | k} (-1)^n o_2(k/n^2) \frac{n^{2s-2}}{n^{2s-2}}.
\]

**Proof.** The final two sets of formulas follow as those for \( J_3 \) on replacing \( \theta_3 \) by \( \theta_2 \) or \( \theta_4 \) in appropriate places. For example,

\[
M_3(2s) = \sum_{(n,m,p) \in \mathbb{Z}^3 - \{(0,0,0)\}} (-1)^{n+m+p} (n^2 + m^2 + p^2)^s = 3 \sum_{(n^2 + m^2 + p^2)^{s+1}} (-1)^{n+m+p} n^2 m^2 p^2.
\]

Since \( M_s(e^{-\alpha t}) = \Gamma(s) \alpha^{-s} \), we have (letting \( q = e^{-\pi t} \))

\[
M_3(2s) = \frac{3\pi^{s+1}}{\Gamma(s + 1)} \sum_{(n,m,p) \in \mathbb{Z}^3 - \{(0,0,0)\}} (-1)^{n+m+p} n^2 M_{s+1}(q^{n^2 + m^2 + p^2})
\]

\[
= \frac{3\pi^{s+1}}{\Gamma(s + 1)} M_{s+1} \left( \sum_{n \in \mathbb{Z} - \{0\}} (-1)^n n^2 q^2 \theta_2^2(q) \right)
\]
as \( \theta_4(q) = \sum_{n \in \mathbb{Z}} (-1)^n q^{n^2} \). Since \( \theta_2(e^{-\pi t}) = t^{-1/2} \theta_4(e^{-\alpha/t}) \), so it is

\[
\mathcal{M}_3(2s) = \frac{3\pi^{s+1}}{\Gamma(s+1)} \sum_{n \in \mathbb{Z} \setminus \{0\}} (-1)^n n^2 q^{n^2} t^{-1} \theta_2^2(e^{-\pi t/s})
\]

\[
= \frac{3\pi^{s+1}}{\Gamma(s+1)} \sum_{n \in \mathbb{Z} \setminus \{0\}} (-1)^n n^2 \int_0^\infty e^{-n^2 \pi t \theta_2^2(e^{-\pi t/s})} s-1 dt
\]

\[
= \frac{3\pi^{s+1}}{\Gamma(s+1)} \sum_{n \in \mathbb{Z} \setminus \{0\}} (-1)^n n^2 \sum_{m,p \in \mathbb{Z}} \int_0^\infty e^{-\frac{\pi}{4}((m+\frac{1}{2})^2+(p+\frac{1}{2})^2)-n^2 \pi t s^{-1}} dt
\]

\[
= \frac{3\pi^{s+1}}{\Gamma(s+1)} \sum_{n \in \mathbb{Z} \setminus \{0\}} (-1)^n n^2 \sum_{m,p \in \mathbb{Z}} \int_0^\infty e^{-\frac{\pi}{4}((2m+1)^2+(2p+1)^2)-n^2 \pi t s^{-1}} dt
\]

as \( o_2(m) \) counts representations of \( m \) as a sum of two odd squares. Hence we have

\[
\mathcal{M}_3(2s) = \frac{6\pi^{s+1}}{\Gamma(s+1)} \sum_{n=1}^\infty (-1)^n n^2 \sum_{m=1}^\infty o_2(m) \int_0^\infty e^{-n^2 \pi t - \frac{\pi}{4} t s^{-1}} dt \]

\[
= \frac{6\pi^{s+1}}{\Gamma(s+1)} \sum_{m=1}^\infty o_2(m) \left( \frac{\pi m}{4} \right)^s \sum_{n=1}^\infty (-1)^n n^2 \int_0^\infty e^{-n^2 \pi t \sqrt{n}} -1/x s^{-1} dx, \quad (x = 4t/m)
\]

\[
= \frac{6\pi^{s+1}}{\Gamma(s+1)} \sum_{m=1}^\infty o_2(m) \left( \frac{\pi m}{4} \right)^s \sum_{n=1}^\infty (-1)^n n^2 \cdot 2 \left( \frac{2}{n \pi \sqrt{m}} \right)^s K_s(\pi n \sqrt{m})
\]

\[
= \frac{3\pi^{s+1}}{\Gamma(s+1)} \sum_{m=1}^\infty o_2(m) m^{s/2} \sum_{n=1}^\infty \left( \frac{-1}{(2n)^{s-2}} \right) K_s(\pi n \sqrt{m})
\]

as

\[
K_s(x) = \frac{1}{2} (\frac{x}{2})^s \int_0^\infty e^{-\frac{x^2}{4u} - \frac{1}{2} u} s^{-1} du.
\]

There are corresponding formulae for Zucker’s \( c_3 \) and \( b_3 \) in which one or both of \( o, u \) are required to be even. Moreover, the Bessel functions are elementary when \( s \) is a half-integer. Most nicely, for ‘jellium’, which is the Wigner sum analogue of Madelung’s constant, we have

\[
\mathcal{J}_3(1) = 3\pi \sum_{m>0} r_2(m) \text{cosech}^2(\pi \sqrt{m}) - \pi,
\]

along with

\[
\mathcal{M}_3(1) = -12\pi \sum_{m>0} o_2(m) \text{cosech}^2 \left( \frac{\pi}{2} \sqrt{m} \right),
\]

and

\[
\mathcal{N}_3(1) = 3\pi \sum_{m>0} (-1)^m r_2(m) \text{cosech}^2 (\pi \sqrt{m}) - 3\pi \log 2 - \frac{2}{\sqrt{3}},
\]

in each of which the exponential convergence is entirely apparent. There is a corresponding formula for \( \sum(-1)^n r_3(n)/n^s \) which corresponds to Madelung’s constant
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(see p. 301 in [2]). For a survey of other rapidly convergent lattice sums of this type see [2] and [5].

There is a corresponding formula for \( J_N(2s) \), for all \( N \geq 2 \), in which we obtain a Bessel-series in \( r_{N-1}(m) \):

\[
J_N(2s) = \sum_{n>0} \frac{r_N(n)}{n^s} = \frac{2N \Gamma(s - \frac{N+3}{2})}{\Gamma(s+1)} \pi^{\frac{N+1}{2}} \zeta(2s - N + 1)
\]

\[
+ \frac{4N \pi^{s+1}}{\Gamma(s+1)} \sum_{m>0} \frac{m\pi^s r_{N-1}(m)}{m^s} \sum_{n>0} \frac{n^{\frac{N+1}{2}}}{n^s} K_{s - \frac{N-3}{2}} (2n\pi\sqrt{m}).
\]

(2.10)

There is an equally attractive integral representation (see [20] p. 172) for:

\[
K_s(x) = \left( \frac{2}{x} \right)^s \frac{\Gamma(s + 1/2)}{\Gamma(1/2)} \int_0^\infty \frac{\cos(xt)}{(1 + t^2)^{s+1/2}} dt
\]

at least when \( x > 1/2 \). This leads to

\[
\sum_{n>0} \frac{r_s(n)}{n^s} = 2\beta \left( s + \frac{1}{2}, \frac{1}{2} \right) \sum_{m>0} r_2(m) \int_0^\infty \frac{C_{s-2}(\sqrt{mt})}{(1 + t^2)^{s+1/2}} dt
\]

where

\[
C_s(x) = \sum_{n>0} \frac{\cos(2\pi nx)}{n^s}
\]

is a Clausen-type function. For \( s = 2k \), even integer, this evaluates to

\[
C_{2k}(x) = \frac{(-1)^{k-1} (2\pi)^{2k}}{2 (2k)!} B_{2k}(x)
\]

where \( B_k \) is a Bernoulli polynomial.

Obviously this also extends to reworkings of (2.10). For example, the \( N = 2 \) case yields

\[
4\beta \left( s + \frac{1}{2}, \frac{1}{2} \right) \zeta(2s - 1) + \frac{16 \pi^{1+s}}{\Gamma(s+1)} \sum_{n=1}^\infty \frac{\sigma_{2s-1}(n)}{n^{s-\frac{1}{2}}} K_{s+\frac{1}{2}} (2n\pi) = 4 \zeta(s) \beta(s).
\]

This in turn, with \( s = 2 \), becomes

\[
4\pi^3 \sum_{n=1}^\infty \sigma_3(n) e^{-2n\pi} \left( 1 + \frac{3}{2} \frac{1}{n\pi} + \frac{3}{4} \frac{1}{n^2\pi^2} \right) \frac{1}{n} = \frac{2}{3} n^2 G - \frac{3}{2} \zeta(3),
\]

where \( G := \sum_{n>0} (-1)^n (2n + 1)^{-2} \) is Catalan’s constant.

There is a puissant formula for \( \theta_3^2 \) due to Andrews [1] (given with a typographical error in [2] p. 286). It is

\[
(2.11) \quad \theta_3^2(q) = 8 \sum_{n=0}^\infty \sum_{j=0}^{2n} \left( \frac{1 + q^{4n+2}}{1 - q^{4n+2}} \right) q^{(2n+1)^2 - (j+1/2)^2}.
\]

Lamentably we have not been able to use it to study \( J_3 \) or \( M_3 \) any further than was achieved in [5].
3. More to Come

The functional equations for $J, M, N$ are

$$\pi^{-3/2-s} \Gamma \left( \frac{3}{2} - s \right) J_3(3 - 2s) = \pi^{-s} \Gamma(s) J_3(2s),$$

$$\pi^{-3/2-s} \Gamma \left( \frac{3}{2} - s \right) M_3(3 - 2s) = \pi^{-s} \Gamma(s) N_3(2s),$$

and dually

$$\pi^{-3/2-s} \Gamma \left( \frac{3}{2} - s \right) N_3(3 - 2s) = \pi^{-s} \Gamma(s) M_3(2s).$$

These may be proved by exactly the method used in [2, (3.6.6)] to show that

$$\pi^{-s-1/2} \Gamma \left( \frac{1-s}{2} \right) \zeta(1-s) = \pi^{-s/2} \Gamma \left( \frac{s}{2} \right) \zeta(s).$$

This involves writing the righthand side, call it $I_{3+k}(s)$, for $k = 0, \pm 1$, as an integral

$$I_{3+k}(s) = \frac{1}{2s} + \frac{1}{3 - 2s} + \int_1^\infty \frac{t^{2s} g_{3+k}(t) + t^{3-2s} g_{3-k}(t)}{t} dt$$

where the function $g_k$ is given by $g_k = \frac{\theta_{2k-1}}{k}$. The invariance is now apparent and the integral is analytic for Re $s > 3/2$. The other cases are similar, but Poisson summation now involves a switch from $\theta_2$ to $\theta_4$ in one of the.

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