On the double zeros of a partial theta function

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Abstract
The series \( \theta(q, x) := \sum_{j=0}^{\infty} q^{j(j+1)/2} x^j \) converges for \( q \in [0, 1) \), \( x \in \mathbb{R} \), and defines a partial theta function. For any fixed \( q \in (0, 1) \) it has infinitely many negative zeros. For \( q \) taking one of the spectral values \( \tilde{q}_1, \tilde{q}_2, \ldots \) (where \( 0.3092493386 \ldots = \tilde{q}_1 < \tilde{q}_2 < \cdots < 1 \), \( \lim_{j \to \infty} \tilde{q}_j = 1 \)) the function \( \theta(q, .) \) has a double zero \( y_j \) which is the rightmost of its real zeros (the rest of them being simple). For \( q \neq \tilde{q}_j \) the partial theta function has no multiple real zeros. We prove that \( \tilde{q}_j = 1 - \pi/2j + (\log j)/8j^2 + O(1/j^2) \) and \( y_j = -e^\pi e^{-(\log j)/4j} + O(1/j) \).

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1 Introduction
Consider the bivariate series \( \theta(q, x) := \sum_{j=0}^{\infty} q^{j(j+1)/2} x^j \). For each fixed \( q \) of the open unit disk it defines an entire function in \( x \) called a partial theta function. This terminology is explained by the fact that the Jacobi theta function is the sum of the series \( \sum_{j=-\infty}^{\infty} q^{j^2} x^j \) and one has \( \theta(q^2, x/q) = \sum_{j=0}^{\infty} q^{j^2} x^j \). There are different domains in which the function \( \theta \) finds applications: asymptotic analysis \([2]\), statistical physics and combinatorics \([16]\), Ramanujan type \( q \)-series \([17]\) and the theory of (mock) modular forms \([3]\). See also \([1]\) for more information about this function.

The function \( \theta \) satisfies the following functional equation:

\[ \theta(q, x) = 1 + qx \theta(q, qx) \] (1)

In what follows we consider \( q \) as a parameter and \( x \) as a variable. We treat only the case \( q \in (0, 1), \ x \in \mathbb{R} \). For each fixed \( q \) the function \( \theta(q, .) \) has infinitely many negative zeros. (It has no positive zeros because its Taylor coefficients are all positive.) There exists a sequence of values \( \tilde{q}_j \) of \( q \) (called spectral values) such that \( 0.3092493386 \ldots = \tilde{q}_1 < \tilde{q}_2 < \cdots < 1 \) (where \( \tilde{q}_j \to 1^- \) as \( j \to \infty \)) for which and only for which the function \( \theta(q, .) \) has a multiple real zero \( y_j \) (see \([12]\) and \([9]\)). This zero is negative, of multiplicity 2 and is the rightmost of its real zeros. The rest of them are simple. The function \( \theta(\tilde{q}_j, .) \) has a local minimum at \( y_j \). As \( q \) increases and passes from \( \tilde{q}_j \) to \( \tilde{q}_j^+ \), the rightmost two real zeros coalesce and give birth to a complex conjugate pair.

The double zero of \( \theta(\tilde{q}_1, .) \) equals \( -7.5032559833 \ldots \). The spectral value \( \tilde{q}_1 \) is of interest in the context of a problem due to Hardy, Petrovitch and Hutchinson, see \([4], [14], [5], [13], [6]\) and \([12]\). The following asymptotic formula and limit are proved in \([10]\):

\[ \tilde{q}_j = 1 - \pi/2j + o(1/j), \quad \lim_{j \to \infty} y_j = -e^{\pi} = -23.1407 \ldots \] (2)
In the present paper we make this result more precise:

**Theorem 1.** The following asymptotic estimates hold true:

\[
\tilde{q}_j = 1 - \frac{\pi}{2j} + \frac{\log j}{8j^2} + \frac{b}{j^2} + o\left(\frac{1}{j}\right),
\]

\[
y_j = -e^{\pi e^{-\frac{\log j}{4}} + \alpha/j + o\left(\frac{1}{j}\right)},
\]

where \( b \in [1.735469700\ldots, 3.327099360\ldots] \) and \( \alpha = -\frac{\pi}{4} - 2b + \frac{\pi^2}{4} \).

Hence \( \alpha \in [-4.972195782\ldots, -1.788936462\ldots] \).

The first several numbers \( y_j \) form a monotone decreasing sequence. We list the first five of them:

\(-7.5\ldots, -11.7\ldots, -14.0\ldots, -15.5\ldots, -16.6\ldots\).

The theorem implies that for \( j \) large enough the sequence must also be decreasing and gives an idea about the rate with which the sequences \( \{\tilde{q}_j\} \) and \( \{y_j\} \) tend to their limit values.

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### 2 Plan of the proof of Theorem 1

For \( q \in (0, \tilde{q}_1) \) the function \( \theta(q,.) \) has only simple negative zeros which we denote by \( \xi_j \), where \( \cdots < \xi_2 < \xi_1 < 0 \) (see \[12\] and \[9\]). The following equality holds true for all values of \( q \in (0,1) \) (see \[11\]):

\[
\theta(q, x) = \prod_{j=1}^{\infty} \left(1 - \frac{x}{\xi_j}\right)
\]

For \( q \in [\tilde{q}_1, 1) \) the indexing of the zeros is such that zeros change continuously as \( q \) varies.

For \( q \in (0, \tilde{q}_1) \) all derivatives \( (\partial^k \theta/\partial x^k)(q,.) \) have only simple negative zeros. For \( k = 1 \) this means that the numbers \( t_s \) and \( w_s \), where the function \( \theta(q,.) \) has respectively local minima and maxima, satisfy the string of inequalities

\[
\cdots < t_{s+1} < \xi_{2s+1} < w_s < \xi_{2s} < t_s < \xi_{2s-1} < \cdots < 0.
\]

The above inequalities hold true for any \( q \in (0,1) \) whenever \( \xi_{2s-1} \) is real negative (which implies that this is also the case of \( \xi_j \) for \( j > 2s - 1 \)).

**Lemma 2.** Suppose that \( q \in (\tilde{q}_j, \tilde{q}_{j+1}) \) (we set \( \tilde{q}_0 = 0 \)). Then for \( s \geq j + 1 \) one has \( t_{s+1} \leq w_s/q \) and \( w_s \leq t_s/q \).

**Proof.** Equality (1) implies

\[
(\partial \theta/\partial x)(q, x) = xq^2(\partial \theta/\partial x)(q, qx) + \theta(q, qx).
\]

When \( qx = t_s \) and \( s \geq j + 1 \), then \( \theta(q, t_s) \leq 0 \), \( (\partial \theta/\partial x)(q, t_s) = 0 \) and \( (\partial \theta/\partial x)(q, t_s/q) \leq 0 \). Hence the local maximum is to the left of or exactly at \( t_s/q \), i.e. \( w_s \leq t_s/q \).
In the same way if one sets $qx = w_s$, one gets $\theta(q, w_s) \geq 0$, $(\partial \theta / \partial x)(q, w_s) = 0$ and $(\partial \theta / \partial x)(q, w_s/q) \geq 0$ and hence $t_{s+1} \leq w_s/q$.

**Notation 3.** (1) In what follows we are using the numbers $u_s := -q^{-2s+1/2}$ and $v_s := -q^{-2s-1/2}$.

(2) We denote by $\tilde{r}_s$ the solution to the equation $\theta(q, u_s) = 0$ and we set $z_s := -(\tilde{r}_s)^{-2s+1/2}$.

**Remark 4.** For $s$ sufficiently large the equation $\theta(q, u_s) = 0$ has a unique solution. This follows from part (2) of Lemma \[\text{L5}\].

It is shown in \[\text{L9}\] that

$$
\cdots < \xi_4 < w_2 < \xi_3 < -q^{-3} < \xi_2/q < v_1 < \xi_1/q < -q^{-2} < \xi_2 < u_1 < \xi_1 < -q^{-1} < 0 .
$$

These inequalities hold true for $q > 0$ sufficiently small and for any $q \in (0,1)$ if the index $j$ of $\xi_j$ is sufficiently large.

Comparing the inequalities \[\text{L5}\] and \[\text{L7}\] we see that $\xi_{2s+1} < w_s, v_s < \xi_{2s}$ and $\xi_{2s} < t_s, u_s < \xi_{2s-1}$. In this sense we say that a number $u_s$ (resp. $v_s$) corresponds to a local minimum (resp. maximum) of $\theta(q,.)$.

We prove the following theorems respectively in Sections \[\text{L5}\] and \[\text{L3}\].

**Theorem 5.** The following asymptotic estimates hold true:

$$
\tilde{r}_j = 1 - \pi/2j + (\log j)/8j^2 + b^*/j^2 + o(1/j^2) \quad \text{and} \quad z_j = -e^\pi e^{-(\log j)/4j + o^*/j + o(1/j)} ,
$$

where $b^* \in [1.735469700\ldots, 1.756303033\ldots]$ and $\alpha^* = -\pi/4 - 2b^* + \pi^2/4$.

hence $\alpha^* \in [-1.830603128\ldots, -1.788936462\ldots]$.

**Theorem 6.** For $j$ sufficiently large one has $0 < \tilde{r}_j \leq \tilde{q}_j \leq \tilde{r}_{j+1} < 1$.

Theorem \[\text{L1}\] follows from the above two theorems. Indeed, as

$$
1 - \pi/2j + (\log j)/8j^2 + O(1/j^2)) = \tilde{r}_j \leq \tilde{q}_j \quad \text{and} \quad 1 - \pi/2(j + 1) + (\log(j + 1))/8(j + 1)^2 + O(1/(j + 1)^2) = \tilde{r}_{j+1} \geq \tilde{q}_j
$$

one deduces immediately the equality $\tilde{q}_j = 1 - \pi/2j + o(1/j)$ (A). It is also clear that $\tilde{r}_{j+1} = 1 - \pi/2j + (\log j)/8j^2 + O(1/j^2)$.

To obtain an estimate of the term $O(1/j^2)$ recall that

$$
\tilde{r}_j = 1 - \pi/2j + (\log j)/8j^2 + b^*/j^2 + o(1/j^2) \quad \text{and} \quad \tilde{r}_{j+1} = 1 - \pi/2j + (\log j)/8j^2 + (b^* + \pi/2)/j^2 + o(1/j^2)
$$

(we use the equality $1/(j+1) = 1/j - 1/(j+1)$). This implies $\tilde{q}_j = 1 - \pi/2j + (\log j)/8j^2 + b/j^2 + o(1/j^2)$, where $b \in [b^*, b^* + \pi/2]$ hence $b \in [1.735469700\ldots, 3.327099360\ldots]$. The quantities $\alpha$ and $\alpha^*$ are expressed by similar formulas via $b$ and $b^*$, see Theorems \[\text{L1}\] and \[\text{L5}\]. This gives the closed intervals to which $\alpha$ and $\alpha^*$ belong.

Section \[\text{L4}\] contains properties of the function $\psi$ used in the proofs. At first reading one can read only the statements of Theorem \[\text{L10}\] and Proposition \[\text{L11}\] from that section.
3 Proof of Theorem

We prove first the inequality \( \tilde{r}_j \leq \tilde{q}_j \). When \( q \) increases and becomes equal to a spectral value \( \tilde{q}_j \), then two negative zeros of \( \tilde{\theta} \) coalesce. The corresponding double zero of \( \tilde{\theta}(\tilde{q}_j,.) \) is a local minimum. It equals \( t_j \). Hence for some value of \( q \) not greater than \( \tilde{q}_j \) one has \( \tilde{\theta}(q,u_j) = 0 \). This value is \( \tilde{r}_j \), see Notation 8.

To prove the inequality \( \tilde{q}_j \leq \tilde{r}_{j+1} \) we use a result due to V. Katsnelson, see [7]:

The sum of the series \( \sum_{j=0}^{\infty} q^{(j+1)/2} x^j \) (considered for \( q \in (0,1) \) and \( x \) complex) tends to \( 1/(1-x) \) (for \( x \) fixed and as \( q \to 1^- \)) exactly when \( x \) belongs to the interior of the closed Jordan curve \( \{ e^{s+i\theta}, s \in [-\pi,\pi] \} \).

Hence in particular \( \tilde{\theta}(q,x) \) converges to \( 1/(1-x) \) as \( q \to 1^- \) for each fixed \( x \in (-e^\pi,0] \). This means that for \( j \) sufficiently large one has \( y_j < -23 \) (because the function \( 1/(1-x) \) has no zeros on \((-\infty,0]\) and \( 23 < e^\pi \)).

Proposition 7. For \( j \) sufficiently large one has \( \tilde{\theta}(\tilde{q}_j,v_j) > 1/3 \).

Before proving the proposition we deduce the inequality \((*)\) from it. Recall that \( \tilde{q}_j \geq \tilde{q}_1 > 0.3 \). Using equation (1) one gets

\[
\tilde{\theta}(\tilde{q}_j,v_{j+1}) = 1 + \tilde{q}_j u_{j+1} \tilde{\theta}(\tilde{q}_j,v_j) < 1 - 0.3 \times 23 \times (1/3) = -1.3 < 0 .
\]

Hence for \( q = \tilde{q}_j \) the value of \( \tilde{\theta}(q,u_{j+1}) \) is still negative, i.e. one has \( \tilde{\theta}(q,u_{j+1}) = 0 \) for some value \( q > \tilde{q}_j \).

Proof of Proposition 7. We deduce the proposition from the following two lemmas:

Lemma 8. Suppose that the quantity \( v_j \) is computed for \( q \) equal to the spectral value \( \tilde{q}_j \). Set \( \Xi_j := (-\tilde{q}_j^{-2j} - v_j(\tilde{q}_j))/(\tilde{q}_j^{-2j} + \tilde{q}_j^{-2j-1}) \). Then \( \lim_{j \to \infty} \Xi_j = 1/2 \).

The next lemma considers certain points of the graph of \( \tilde{\theta}(\tilde{q}_j,.) \). Recall that \( \tilde{\theta}(\tilde{q}_j,w_j) = 1 \) because for \( q = \tilde{q}_j \) one has \( \tilde{\theta}(\tilde{q}_j,t_j) = 0 \), \( w_j = t_j/\tilde{q}_j \) and by equation (1) \( \tilde{\theta}(\tilde{q}_j,w_j) = 1 + \tilde{q}_j w_j \cdot \tilde{\theta}(\tilde{q}_j,t_j) = 1 \).

Lemma 9. The point \( (v_j,\tilde{\theta}(\tilde{q}_j,v_j)) \) lies above or on the straight line passing through the two points \( (-\tilde{q}_j^{-2j},\tilde{\theta}(\tilde{q}_j,-\tilde{q}_j^{-2j})) \) and \( (w_j,\tilde{\theta}(\tilde{q}_j,w_j)) = (w_j,1) \).

The two lemmas imply that for \( j \) sufficiently large the following inequality holds true:

\[
\tilde{\theta}(\tilde{q}_j,v_j) - \tilde{\theta}(\tilde{q}_j,-\tilde{q}_j^{-2j}) \geq \Xi_j(\tilde{\theta}(\tilde{q}_j,w_j) - \tilde{\theta}(\tilde{q}_j,-\tilde{q}_j^{-2j})) > (1/3)(1 - \tilde{\theta}(\tilde{q}_j,-\tilde{q}_j^{-2j})) .
\]

Hence \( \tilde{\theta}(\tilde{q}_j,v_j) > 1/3 + (2/3) \tilde{\theta}(\tilde{q}_j,-\tilde{q}_j^{-2j}) \). It is shown in [9] (see Proposition 9 there) that for \( q \in (0,1) \) one has \( \tilde{\theta}(q,-q^{-s}) \in (0,q^s) \), \( s \in \mathbb{N} \). Hence \( \tilde{\theta}(\tilde{q}_j,v_j) > 1/3 \). ☐

Proof of Lemma 8. It is clear that \( (-\tilde{q}_j^{-2j} - v_j(\tilde{q}_j))/(\tilde{q}_j^{-2j} + \tilde{q}_j^{-2j-1}) = \sqrt{\tilde{q}_j}(1 - \sqrt{\tilde{q}_j})/(1 - \tilde{q}_j) = \sqrt{\tilde{q}_j}/(1 + \sqrt{\tilde{q}_j}) \). As \( j \to \infty \) one has \( \tilde{q}_j \to 1 \) and the above fraction tends to \( 1/2 \). ☐

Proof of Lemma 9. We are going to prove a more general statement from which the lemma follows. Suppose that \( w_s \leq x_2 < x_1 < x_0 \leq -q^{-2s} < -1 < 0 \) for some \( s \in \mathbb{N} \). Set \( \tilde{\theta}(q,x_0) = C \), \( \tilde{\theta}(q,x_1) = B \), \( \tilde{\theta}(q,x_2) = A \). Suppose that \( A > B > C > 0 \) and \( A \geq 1 \). We use the letters \( A \), \( B \) and \( C \) also to denote the points of the graph of \( \tilde{\theta}(q,.) \) with coordinates \( (x_0,C) \), \( (x_1,B) \) and \( (x_2,A) \).
We prove that the point $B$ is above or on the straight line $AC$.
Indeed, suppose that the point $B$ is below the straight line $AC$. Then

$$\frac{B - C}{|x_1 - x_0|} < \frac{A - B}{|x_2 - x_1|}$$

(9)

Consider the points $(x_0/q, C')$, $(x_1/q, B')$ and $(x_2/q, A')$ of the graph of $\theta(q,.)$. Equation (11) implies that

$$C' = 1 + x_0C, \quad B' = 1 + x_1B, \quad A' = 1 + x_2A.$$ 

In the same way for the points $(x_0/q^2, C'')$, $(x_1/q^2, B'')$ and $(x_2/q^2, A'')$ of the graph of $\theta(q,.)$ one gets

$$C'' = 1 + \frac{x_0}{q}C', \quad B'' = 1 + \frac{x_1}{q}B, \quad A'' = 1 + \frac{x_2}{q}A'$$

(10)

It is clear that $x_2/q^2 < x_1/q^2 < x_0/q^2 \leq -q^{-2s-2}$. By Lemma 2 one has

$$w_{s+1} \leq \frac{t_{s+1}}{q} \leq w_s/q^2 \leq x_2/q^2 \leq -q^{-2s-2}.$$ 

The inequalities $A > B > C > 0$ and $x_2 < x_1 < x_0 < -1$ imply $A' < B' < C'$, see (10). As $A \geq 1$ and $x_2 < -1$, one has $A' < 0$. Therefore $A'' = 1 + (x_2/q)A' > 1$.

It follows from $w_{s+1} \leq x_2/q^2 < x_1/q^2 < x_0/q^2 \leq -q^{-2s-2}$ that $B'' > 0$ and $C'' > 0$. (Indeed, $\theta(q,x) > 0$ for $x \in (-q^{-2s-1}, -q^{-2s})$, see [9].) If $B' < C' < 0$, then $x_2 < x_1 < x_0 < -1$ implies $A'' > B'' > C''$, see (10). If $B' < 0 \leq C'$, then again by (10) one gets $A'' > B'' > C''$.

If $0 \leq B' < C'$, then one obtains $A'' > B''$ and $A'' > C''$. If $B'' \leq C''$, then the point $B''$ lies below the straight line $A''C''$. In this case one can find a point $(x_1/q^2, B''_s)$ of the graph of $\theta(q,.)$ such that

$$w_{s+1} \leq x_2/q^2 < x_1/q^2 < x_0/q^2 \leq -q^{-2s-2} < -1 < 0, \quad A'' > B''_s > C'' > 0$$

and the point $B''_s$ lies below the straight line $A''B''$.

Suppose that $A'' > B'' > C''$. We show that the point $B''$ is below the straight line $A''C''$. This is equivalent to proving that

$$\frac{(x_1/q) + (x_1^2/q)B - (x_0/q) - (x_0^2/q)C}{|x_1 - x_0|/q^2} < \frac{(x_2/q) + (x_2^2/q)A - (x_1/q) - (x_1^2/q)B}{|x_2 - x_1|/q^2}$$

or to proving the inequality

$$B(x_1^2/x_0^2)|x_2 - x_0| - C|x_2 - x_1| - A(x_2^2/x_0^2)|x_1 - x_0| < 0.$$ 

(11)

Inequality (11) can be given another presentation:

$$B|x_2 - x_0| - C|x_2 - x_1| - A|x_1 - x_0| < 0.$$ 

(12)

One can notice that inequality (11) (which we want to prove) is the sum of inequality (12) (which is true) and the inequality
\[ B \left( \frac{x^2}{x_0^2} - 1 \right) |x_2 - x_0| - A \left( \frac{x^2}{x_0^2} - 1 \right) |x_1 - x_0| < 0. \]  

(13)

So if we show that inequality (13) is true, then this will imply that inequality (11) is also true. Recall that \( x_2 < x_1 < x_0 < 0 \) and \( A > B > C > 0 \). Hence inequality (13) is equivalent to

\[ B(|x_1| + |x_0|) - A(|x_2| + |x_0|) < 0 \]

which is obviously true. We set \( B'' = B'' \) and \( x_1' = x_1 \).

For \( s \in \mathbb{N} \) we define in the same way the three points \( (x_0/q^{2s}, C^{(2s)}) \), \( (x_1^s/q^{2s}, B_s^{(2s)}) \) and \( (x_2/q^{2s}, A^{(2s)}) \) by the condition that they belong to the graph of \( \theta(q,.) \), \( w_s \leq x_2/q^{2s} < x_1^s/q^{2s} < x_0/q^{2s} < -q^{-2s} \), \( A^{(2s)} > B_s^{(2s)} > C^{(2s)} > 0 \) and the point \( B_s^{(2s)} \) lies below the straight line

![Graph of a partial theta function and the points A, B, C and C''](image)

Figure 1: Part of the graph of a partial theta function and the points A, B, C and C''.

This implies that the graph of \( \theta(q,.) \) has on each interval \( (-q^{-2s-2N}, -q^{-2s}), N \in \mathbb{N} \), at least \( O(4N) \) inflection points, twice as much as \( O(2N) \), the one that should be. (This contradiction proves the lemma.) Indeed, on Fig. 1 we show part of the graph of \( \theta(q,.) \) as it should look like (the sinusoidal curve) and the points C, B, A and C''. If the point B is below the straight line AC, then the change of convexity requires two more inflection points between a local minimum of \( \theta(q,.) \) and the local maximum to its left.
4 The function $\psi$

In the present section we consider the function $\psi(q) := 1 + 2\sum_{j=1}^{\infty}(-1)^jq^j$. It is real-analytic on $(-1,1)$. This function has been studied in [8] and the following theorem recalls the basic results about it. Part (1) is a well-known property while parts (2) – (7) are proved in [8].

**Theorem 10.** (1) By the Jacobi triple product identity the function $\psi$ can be expressed as follows (see [15], Chapter 1, Problem 56):

$$\psi(q) = \prod_{j=1}^{\infty} \frac{1-q^j}{1+q^j}$$

(2) The function $\psi$ is decreasing, i.e. $\psi' < 0$ for all $q \in (-1,1)$.

(3) For the endpoints of its interval of definition one has the limits $\lim_{q \to 1^+} \psi(q) = 0$, $\lim_{q \to 1^-} \psi(q) = +\infty$.

(4) The function $\psi$ is flat at 1, i.e. for any $l \in \mathbb{N}$, $\psi(q) = o((q-1)^l)$ as $q \to 1^-$.

(5) The function $\psi$ is convex, i.e. $\psi'' \geq 0$ for all $q \in (-1,1)$, with equality only for $q = 0$.

(6) Consider the function $\tau(q) := (q-1)\log \psi(q)$. It is increasing on $(0,1)$ and $\lim_{q \to 1^-} \tau(q) = \pi^2/4$. This implies that for any $\varepsilon > 0$ there exists $\delta > 0$ such that $e^{\pi^2(q-1)/\varepsilon} < \psi(q) \leq e^{\pi^2(q-1)/\varepsilon}$ for $q \in (1-\delta,1)$.

(7) As $q \to -1^+$, the growth rate of the function $\psi$ satisfies the conditions $\psi(q) = o((q+1)^{-1})$ and $(q+1)^\alpha / \psi(q) = o(1)$ for any $\alpha \in (-1,0)$.

Set $D := 1/2 + \log 2 + \pi^2/8 = 2.426847731 \ldots$. Property (6) can be further detailed:

**Proposition 11.** For $q$ close to 1 the function $\tau$ is of the form

$$\tau = \pi^2/4 + (1/2)(1-q)\log(1-q) - K(1-q) + o(1) - q$$

with

$$K \in [D, D + 1/12] = [2.426847731 \ldots, 2.510181064 \ldots].$$

Hence $\psi = e^{\pi^2\tau} = e^{K(1 + o(1))} (1-q)^{-\frac{1}{2}} e^{\frac{\pi^2}{\sqrt{D}}}.$

**Proof.** The logarithm of the $j$th factor of the right-hand side of formula (14) equals

$$\log \left( \frac{1-q^j}{1+q^j} \right) = (-2) \left( q^j + \frac{q^{3j}}{3} + \frac{q^{5j}}{5} + \cdots \right).$$

This means that

$$\log \psi(q) = \sum_{j=1}^{\infty} \left( q^j + \frac{q^{3j}}{3} + \frac{q^{5j}}{5} + \cdots \right)$$

$$= \sum_{j=1}^{\infty} \frac{q^{2k+1}}{2k+1}.$$ 

Hence $\tau(q) := (q-1)\log \psi(q) = 2\sum_{k=0}^{\infty} \zeta_k(q)$, where

$$\zeta_k(q) := \frac{q^{2k+1}}{(2k+1)(1+q+q^2+\cdots+q^{2k})} = \frac{q^{2k+1}(1-q)}{(2k+1)(1-q^{2k+1})}.$$
Lemma 12. For $q \in (0, 1]$ the following inequalities hold true:

$$q^{2k+1}/(2k + 1)^2 \leq \zeta_k(q) \leq q^{k+1}/(2k + 1)^2$$

with equalities only for $q = 1$.

Proof of Lemma 12. The inequalities result from $1 + q + \cdots + q^{2k} \leq 2k + 1$ and $q^{k+j} + q^{k-j} \geq 2q^k$ hence $1 + q + \cdots + q^{2k} \geq (2k + 1)q^k$ (with equalities only for $q = 1$).

The above lemma gives the idea to compare the function $\tau$ (for $q$ close to 1) with the function $h(q) := 2 \sum_{k=0}^{\infty} q^{k+1}/(2k + 1)^2$. The lemma implies the following result:

$$h(q^2)/q \leq \tau(q) \leq h(q) \quad (\tau(q) = h(q)) \iff (q = 1) \quad (17)$$

Our next step is to compare the asymptotic expansions of the functions $\tau$ and $h$ close to 1:

Lemma 13. For $q$ close to 1 the following equality holds:

$$h(q) = \pi^2/4 + (1/2)(1-q) \log(1-q) - D(1-q) + O((1-q)^2 \log(1-q)) \quad (18)$$

Proof of Lemma 13. Notice first that $\lim_{q \to 1^-} \tau(q) = h(1) = \pi^2/4$ and that $h = h_1 + h_2$, where

$$h_1 := 2 \sum_{k=0}^{\infty} q^{k+1}/(2k + 1)(2k + 2) \quad \text{and} \quad h_2 := 2 \sum_{k=0}^{\infty} q^{k+1}/(2k + 1)^2(2k + 2).$$

Equation (15) implies $\log((1+q)/(1-q)) = 2 \sum_{k=0}^{\infty} q^{2k+1}/(2k + 1)$. Integrating both sides of this equality yields

$$(1+q)\log(1+q) + (1-q)\log(1-q) = 2 \sum_{k=0}^{\infty} q^{2k+2}/(2k + 1)(2k + 2).$$

Thus $h_1 = (1+q^{1/2})\log(1+q^{1/2}) + (1-q^{1/2})\log(1-q^{1/2})$. The first summand is real analytic in a neighbourhood of 1 and equals $2\log 2 - (1/2)(1 + \log 2)(1-q) + O((1-q)^2)$. The second one is equal to

$$[(1-q)/(1+q^{1/2})](\log(1-q) - \log(1+q^{1/2}))$$

$$= (1-q)[(1/2 + O(1-q))\log(1-q) - (\log(1+q^{1/2}))/((1+q^{1/2}))]$$

$$= (1/2)(1-q)\log(1-q) + (1/2)(\log 2)(1-q) + O((1-q)^2 \log(1-q)).$$

About the function $h_2$ one can notice that there exist the limits $\lim_{q \to 1^-} h_2$ and $\lim_{q \to 1^-} h_2'$ (the latter equals $\pi^2/8$). This implies formula (18).

Lemma 14. For $q \in (0, 1)$ it is true that

$$h(q) - \tau(q) \leq (1-q)/12. \quad (19)$$

Proposition 11 results from the last two lemmas.
Proof of Lemma 14. To prove formula (19) set $R := 1/(2k + 1)^2(1 + q + \cdots + q^{2k})$ and $S_l := 1 + q + \cdots + q^l$. Hence
\[
\frac{1}{2k + 1} \left( \frac{q^{k+1}}{2k + 1} - \frac{q^{2k+1}}{1 + q + \cdots + q^{2k}} \right) = (q^{k+1}(1 + q + \cdots + q^{2k}) - (2k + 1)q^{2k+1})R
= \left( \sum_{j=0}^{k-1} (q^{k+1+j} + q^{3k+1-j} - 2q^{2k+1}) \right) R
= \left( \sum_{j=0}^{k-1} q^{k+1+j}(1 - q^{k-j})^2 \right) R
= q^{k+1}(1 - q)^2 \left( \sum_{j=0}^{k-1} q^j (1 + q + \cdots + q^{k-j-1})^2 \right) R
= q^{k+1}(1 - q)^2 \left( \sum_{j=0}^{k-1} q^j \left( \sum_{\nu=0}^{k-j-1} q^\nu S_{2k-2j-2-2\nu} \right) \right) R.
\]
(20)
The sums $S_l$ enjoy the following property:
\[
(l - 1)S_l \geq (l + 1)qS_{l-2}.
\]
Indeed, this is equivalent to $(l - 1)(1 + q^l) \geq 2qS_{l-2}$. The last inequality follows from $1 + q^r \geq q + q^{-1}$ (i.e. $(1 - q)(1 - q^{-1}) \geq 0$) applied for suitable choices of the exponent $r$. Equation (21) implies the next property (whenever the indices are meaningful):
\[
(l - 2\nu + 1)S_l \geq (l + 1)q^{\nu}S_{l-2\nu}.
\]
Using equation (22) one can notice that the right-hand side of (21) is not larger than
\[
q^{k+1}(1 - q)^2 \left( \sum_{j=0}^{k-1} q^j \left( \sum_{\nu=0}^{k-j-1} \frac{2k - 2j - 1 - 2\nu}{2k - 2j - 1} S_{2k-2j-2} \right) \right) R
\leq q^{k+1}(1 - q)^2 \left( \sum_{j=0}^{k-1} \left( \sum_{\nu=0}^{k-j-1} \frac{2k - 2j - 1 - 2\nu}{2k - 2j - 1} \left( \frac{2k - 2j - 1}{2k - 1} S_{2k-2} \right) \right) \right) R
= q^{k+1}(1 - q)^2 \left( \sum_{j=0}^{k-j-1} \frac{2k - 2j - 1 - 2\nu}{2k - 1} S_{2k-2} \right) R
= q^{k+1}(1 - q)^2 \left( \sum_{j=0}^{k-j-1} \frac{(k - j)^2}{2k - 1} S_{2k-2} \right) R
= q^{k+1}(1 - q)^2 \frac{k(k+1)(2k+1)}{6(2k-1)(2k+1)^2} S_{2k-2}
\leq q^{k}(1 - q)^2 \frac{k(k+1)}{6(2k+1)^2}.
\]
At the last line we used property (21) with $l = 2k$. The last fraction is less than 1/24. Hence $h(q) - \tau(q) \leq (1 - q)^2 \sum_{k=0}^{\infty} q^k/12 = (1 - q)/12.$
5 Proof of Theorem \[5\]

We follow the same path of reasoning as the one used in \[10\]. In this section we use the results of \[10\] and \[8\]. Set

$$\lambda_s(q) := \sum_{j=2s}^{\infty} (-1)^j q^{j^2/2}, \quad \chi_s(q) := \lambda_s(q)/q^{2s^2} = \sum_{j=2s}^{\infty} (-1)^j q^{j^2/2-2s^2} = \sum_{j=0}^{\infty} (-1)^j q^{(j^2+4js)/2}. $$

The equation \( \theta(q, -q^{-2s+1}/2) = 0 \) is equivalent to (see \[10\])

$$\psi(q^{1/2}) = \lambda_s(q) = q^{2s^2} \chi_s(q). \quad (23)$$

The following lemma is also proved in \[10\]:

**Lemma 15.** (1) One has \( \lim_{q \to 1^-} \lambda_s(q) = \lim_{q \to 1^-} \chi_s(q) = 1/2. \)

(2) For \( s \in \mathbb{N} \) sufficiently large the graphs of the functions \( \psi(q^{1/2}) \) and \( \lambda_s(q) \) (considered for \( q \in (0, 1) \)) intersect at exactly one point belonging to \( (0, 1) \) and at 1.

(3) For \( q \in \mathbb{N} \) the inequality \( \lambda_s(q) \geq \lambda_{s+1}(q) \) holds true with equality for \( q = 0 \) and \( q = 1. \)

(4) For \( q \in (0, 1) \) one has \( 1/2 \leq \chi_s(q) \leq 1. \)

Part (2) of the lemma implies that for each \( s \) sufficiently large the number \( \tilde{r}_s \) is correctly defined. Part (3) implies that the numbers \( \tilde{r}_s \) form an increasing sequence. Indeed, this follows from \( \psi(q^{1/2}) \) being a decreasing function, see part (2) of Theorem \[10\].

Recall that the constant \( K \) was introduced by Proposition \[11\] Set \( q := \tilde{r}_s = 1 - h_s/s. \) Consider the equalities \[23\]. The left-hand side is representable in the form

$$e^K (1 + o(1)) \left[ (1 - q)^{-1/2}/(1 + \sqrt{q})^{-1/2} \right] e^{\pi^2/(4q+o(q))},$$

see Proposition \[11\]. Hence \( \log \psi(q^{1/2}) \) is of the form

$$\left( \pi^2/4 \right) (-s/h_s)(2 - (1/2)(h_s/s) + o(h_s/s)) - (1/2) \log(h_s/s) + (1/2) \log 2 + K + o(1)$$

$$= -(\pi^2/2)(s/h_s) + (1/2) \log s - (1/2) \log h_s + L + o(1),$$

where \( L := K + (1/2) \log 2 + \pi^2/8. \) The right-hand side of \[23\] equals \( (1 - h_s/s)^{2s^2} \chi_s(1 - h_s/s). \)

Hence its logarithm is of the form

\[
(2s^2) \log(1 - h_s/s) + \log(\chi_s(1 - h_s/s)) = -(2s^2)(h_s/s + h_s^2/2s^2 + O(1/s^3)) - \log 2 + o(1)
\]

$$= -2sh_s - (h_s)^2 - \log 2 + o(1).$$

(we use \( \chi_s = 1/2 + o(1) \), see part (1) of Lemma \[15\] hence \( \log h_s = \log(\pi/2 + o(1)) \)). Set \( h_s := \pi/2 + d_s. \) Hence \( d_s = o(1), \) see equality (A) after Theorem \[6\] and

$$-(\pi^2/2)(s/(\pi/2 + d_s)) + (1/2) \log s - (1/2) \log(\pi/2) + L + o(1)$$

$$= -2s(\pi/2 + d_s) - (\pi/2 + d_s)^2 - \log 2 + o(1)$$

10
or equivalently

\[ -(\pi^2/2)s + (\pi/2 + d_s)((\log s)/2 - (\log(\pi/2))/2 + L) + o(1) \]

Hence

\[ ((\pi/2 + d_s)/2)\log s = -2s\pi d_s - 2s(d_s)^2 + O(1) \]
i.e. \( d_s = -((\log s)/8s)(1 + o(1)) \). Set \( d_s := -((\log s)/8s + g_s) \). Using equation (24) one gets

\[ -(\pi^2/2)s + (\pi/2 - (\log s)/8s + g_s)((\log s)/2 - (\log(\pi/2))/2 + L) + o(1) \]

\[ = -2s(\pi/2 - (\log s)/8s + g_s)^2 - (\pi/2 - (\log s)/8s + g_s)^3 - (\pi/2 - (\log s)/8s + g_s)\log 2 \] (25)

To find the main asymptotic term in the expansion of \( g_s \) we have to leave only the linear terms in \( g_s \) and the terms independent of \( g_s \) (because \( g_s^2 = o(g_s) \)). The left-hand side of equation (25) takes the form:

\[ -(\pi^2/2)s + (\pi/4)(\log s) - (\pi/4)\log(\pi/2) + (\pi/2)L + g_s((\log s)/2)(1 + o(1)) + o(1) \].

The right-hand side equals

\[ -2s(\pi/2)^2 + \pi(\log s)/4 - 2s\pi g_s - \pi^3/8 - (3\pi^2/4)g_s - (\pi/2)\log 2 - g_s\log 2 + o(1) \].

The terms \( s \) and \( \log s \) cancel. The remaining terms give the equality

\[ ((\log s)/2)(1 + o(1)) + 2s\pi + O(1)g_s \]

\[ = (\pi/4)\log(\pi/2) - (\pi/2)L - \pi^3/8 - (\pi/2)\log 2 + o(1) \].

Hence \( g_s = (1/s)(M + o(1)) \), where

\[ M := (\log(\pi/2))/8 - L/4 - \pi^2/16 - (\log 2)/4 = (\log(\pi/8))/8 - L/4 - \pi^2/16 \].

Now recall that

\[ L = K + (1/2)\log 2 + \pi^2/8 \quad \text{and} \quad K \in [2.426847731 \ldots, 2.510181064 \ldots] \].

Hence \( M = -b^* = (\log(\pi/16))/8 - 3\pi^2/32 - K/4 \), so \( b^* \in [1.735469700 \ldots, 1.756303033 \ldots] \).

Thus we have proved the first of formulas (8). To prove the second one it suffices to notice that

\[ z_s = -(\bar{r}_s)^{-2s+1/2} = -(1 - \pi/2s + (\log s)/8s^2 + b^*/s^2 + \cdots)^{-2s+1/2} \].

Set \( \Phi := \pi/2s - (\log s)/8s^2 - b^*/s^2 + \cdots \). Hence

\[ z_s = -e^{(-2s+1/2)\log(1-\Phi)} = e^{(-2s+1/2)(-\Phi-\Phi^2/2-\cdots)} = e^{\pi}e^{-(\log s)/4s+\alpha^*/s+\cdots} \]

with \( \alpha^* = -\pi/4 - 2b^* + \pi^2/4 \in [-1.830603128 \ldots, -1.788936462 \ldots] \).
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