# Log-concavity of the derivatives of the Jacobi theta kernel: small orders, exceptional orders and infinitely many failures

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Luminary Oddities

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**Abstract**

Coffey and Csordas (Mathematics of Computation, 2013, Conjecture 2.5; restated by Csordas as Open Problem 4.13) conjectured that every derivative of the Jacobi theta kernel $\Phi$, whose cosine transform is the Riemann $\Xi$-function, is strictly log-concave on the real line: $J_n = (\Phi^{(n)})^2 - \Phi^{(n-1)}\Phi^{(n+1)} > 0$ for every $n \geq 1$. Sra (2026) disproved this at order nine and recorded the orders up to eight as unverified. We prove $J_n > 0$ on the whole line for $n = 1, \dots, 8$, so the conjecture holds for the first eight derivatives. We determine exactly which orders up to one hundred satisfy the inequality: it fails for precisely 29 orders, the smallest being 9, 16, 23, 29, 30, 31, 38, 39 and 40, and holds for the other 71. The proofs combine an exact integer-polynomial formula for the derivatives, an analytic estimate reducing large arguments to coefficient signs of explicit polynomials, and outward-rounded interval arithmetic with Taylor remainders on a compact range. Finally, we prove that the inequality fails for infinitely many orders: $J_n(0) \leq 0$ for infinitely many odd $n$. The proof compares the Taylor coefficients of $\Phi$ at the origin with the behaviour of $\Phi$ near the cusp $\tau = -1$ of the theta function, where $\Phi$ stays bounded on the imaginary axis but is unbounded on the disc of convergence. Moreover, the even moments of $\Xi$ on the positive half-line take both signs infinitely often.

**Keywords.** Jacobi theta kernel; Riemann $\Xi$-function; Turán inequalities; log-concavity; Coffey–Csordas conjecture; interval arithmetic; computer-assisted proof.
**MSC 2020.** Primary 26D15; Secondary 11M26, 11F27, 30D15, 65G30.

## 1 Introduction

### 1.1 The question

Throughout, $\Phi$ denotes the Jacobi theta kernel in the normalization of Csordas [2, (4.2)],

$$\Phi(t) = \sum_{m=1}^{\infty} \pi m^2 \bigl(2\pi m^2 e^{4t} - 3\bigr) \exp\bigl(5t - \pi m^2 e^{4t}\bigr), \qquad t \in \mathbb{R}, \tag{1}$$

so that $\frac{1}{8}\,\Xi(x/2) = \int_0^\infty \Phi(t)\cos(xt)\,dt$, where $\Xi(z) = \xi(\frac{1}{2} + iz)$ is the Riemann $\Xi$-function [2, (4.1)]. For $n \geq 1$ put

$$J_n(t) = \bigl(\Phi^{(n)}(t)\bigr)^2 - \Phi^{(n-1)}(t)\,\Phi^{(n+1)}(t). \tag{2}$$

The function $\Phi$ is even, positive, and analytic in the strip $|\operatorname{Im} z| < \pi/8$; see [2, Theorem 4.1], which collects these classical facts from Pólya [6] and Csordas, Norfolk and Varga [3]. Differentiating $\Phi(-t) = \Phi(t)$ gives $\Phi^{(k)}(-t) = (-1)^k \Phi^{(k)}(t)$, hence $J_n(-t) = J_n(t)$. The quantity $J_n$ is homogeneous of degree two in $\Phi$, so its sign is the same for every positive normalizing constant in (1); it is also unchanged under a rescaling $t \mapsto ct$ with $c > 0$, since $J_n[\Phi(c\,\cdot)](t) = c^{2n} J_n[\Phi](ct)$.

**Conjecture 1.1** (Coffey–Csordas [1, Conjecture 2.5], as restated by Csordas [2, Open Problem 4.13])**.** *The derivatives of $\Phi$ are strictly log-concave on $\mathbb{R}$: for each $n \in \mathbb{N}$, $J_n(t) > 0$ for all $t \in \mathbb{R}$.*

The case $n = 1$ is the log-concavity of $\Phi$ itself. It follows from the strict concavity of $\log \Phi(\sqrt{t})$ on $t > 0$, due to Csordas and Varga [4] (see [2, Theorem 4.2(b) and Remarks 4.3]), together with $\Phi' < 0$ on $(0, \infty)$ [2, Theorem 4.1(v)] and $\Phi''(0) < 0$; Coffey and Csordas [1] gave a new proof. Sra [9, Theorem 5.2] proved by a computer-assisted interval computation that $J_9(1/50) < 0$, which disproves Conjecture 1.1. In [9, Remark 5.3] he reports AI-assisted proofs for $n = 2$ and $n = 3$, which are not reproduced in that paper, and records the orders $n \le 8$ as unverified. This leaves three questions. We answer (Q1) and (Q3) completely and (Q2) for every order $n \le 100$.

(Q1) Does Conjecture 1.1 hold for the orders $n \le 8$ below Sra's counterexample?

(Q2) For which orders $n$ does $J_n > 0$ hold on $\mathbb{R}$?

(Q3) Is the order $n = 9$ an isolated exception, or does the conjecture fail for infinitely many $n$?

## 1.2 Main results

**Theorem 1.2.** *For $n = 1, 2, \dots, 8$ one has $J_n(t) > 0$ for every $t \in \mathbb{R}$.*

Theorem 1.2 answers (Q1) affirmatively: Conjecture 1.1 holds for the first eight derivatives, so $n = 9$ is the smallest counterexample. The second theorem answers (Q2) exactly for every order up to one hundred.

**Theorem 1.3.** *Let $1 \le n \le 100$. Then $J_n(t) > 0$ for all $t \in \mathbb{R}$ if and only if $n \notin \mathcal{E}$, where*

$$\mathcal{E} = \{9, 16, 23, 29, 30, 31, 38, 39, 40, 45, 46, 52, 53, 59, 60,\\ 65, 66, 67, 68, 75, 76, 77, 78, 82, 89, 90, 93, 96, 97\}.$$

*For every $n \in \mathcal{E}$, Table 1 gives a point $t_n$ with a certified enclosure of $J_n(t_n) < 0$.*

In particular Conjecture 1.1 holds for 71 of the first 100 orders and fails for the other 29. Several of the negative windows are narrow. The floating-point scan of Remark 4.6 places the negative set of $J_{39}$ in an interval of length about 0.002 near $t = 0.331$, which contains no point of the grid $0.0025\,\mathbb{Z}$; a floating-point bisection places that of $J_{59}$ in $|t| < 0.00064$. The positivity certificates cover every real $t$, so every order declared positive satisfies $J_n > 0$ on all of $\mathbb{R}$.

Since $\Phi$ is even, $\Phi^{(2k+1)}(0) = 0$, and therefore $J_{2k+1}(0) = b_k b_{k+1}$ with $b_k = (-1)^k \Phi^{(2k)}(0)$. The third theorem answers (Q3).

**Theorem 1.4.** *(a) $b_k > 0$ for infinitely many $k$, and $b_k < 0$ for infinitely many $k$.*

*(b) There are infinitely many odd $n$ with $J_n(0) \le 0$. In particular, Conjecture 1.1 fails for infinitely many orders $n$.*

Section 7 shows that $b_k$ is a positive multiple of $\int_0^\infty s^{2k}\,\Xi(s)\,ds$, which gives the following consequence of Theorem 1.4(a).

**Corollary 1.5.** *The even moments $\int_0^\infty s^{2k}\,\Xi(s)\,ds$, $k = 0, 1, 2, \dots$, are positive for infinitely many $k$ and negative for infinitely many $k$. For $k \le 61$ they are nonzero, and positive exactly for $k \in \{0, \dots, 4\} \cup \{15, \dots, 29\} \cup \{49, \dots, 61\}$.*

For $k \le 60$ the sign of $(b_k)$ changes between $k$ and $k + 1$ exactly for $k = 4, 14, 29, 48$, which produces the failures at $t = 0$ for $n = 9, 29, 59, 97$ in Table 1. Every other member $n$ of $\mathcal{E}$ has $J_n(0) > 0$ and fails at some $t > 0$.

### 1.3 Relation to earlier work and route of the proof

Sra's disproof evaluates $J_9$ at one point. His values of $\Phi^{(8)}$, $\Phi^{(9)}$, $\Phi^{(10)}$ at $1/50$ and the centre $-2.61006208371358922\times10^{19}$ of his enclosure of $J_9(1/50)$ agree with our enclosures in all 18 printed digits (output of `cc_witness.py`). Sra's certificate already uses the derivative polynomials $P_k$ of Section 2 and an outward-rounded summation of the theta series with a geometric tail bound; we use the same two tools. The present paper adds the positive cases (including independent proofs for $n = 2, 3$), the exact classification up to order 100, and a structural proof of infinitely many failures.

The proofs of Theorems 1.2 and 1.3 have three ingredients.

- *Exact derivatives* (Section 2). With $u = \pi m^2 e^{4t}$ every derivative of the $m$-th summand is $\pi m^2 e^{5t} e^{-u} P_k(u)$ for an explicit integer polynomial $P_k$ (Lemma 2.2), as in Sra's proof of [9, Theorem 5.2].
- *Large $t$* (Section 3). For $x = \pi e^{4t}$ large, the term $m = 1$ dominates and $e^{-10t} e^{2x} J_n/\pi^2$ is an exact integer polynomial $Q_n(x)$ plus an explicitly bounded remainder (Lemma 3.1). Positivity on $[x_0, \infty)$ then reduces to coefficient signs of one integer polynomial (Proposition 3.2).
- *Compact range* (Section 4). On $[0, T_0(n)]$ we use a cover by intervals on which $J_n$ is bounded below by a Taylor polynomial with interval coefficients and an explicit Lagrange remainder (Proposition 4.5). All quantities are enclosed in outward-rounded interval arithmetic, including the omitted tail of the theta series.

Certified Taylor covers of theta-type kernels with geometric tail bounds were used in our earlier work on positivity questions for Riemann theta products [8, 7]. The argument below is self-contained.

Theorem 1.4 is proved in Section 6. If $(b_k)$ eventually had one sign, zeros allowed, the Taylor series of $\Phi$ at 0 would be dominated on each circle $|z| = r < \pi/8$ by its value on the imaginary axis, up to a bounded error. Jacobi's transformation at the cusp $\tau = -1$ shows that $\Phi(iy)$ tends to 0 as $y \to \pi/8$, while $\Phi$ is unbounded on the disc $|z| < \pi/8$, along points that approach the cusp tangentially. The same transformation at the same cusp underlies Hardy's proof that $\zeta(s)$ has infinitely many zeros on the critical line (see Titchmarsh [10, Chapter X]); Remark 7.2 makes the connection explicit.

## 2 Exact derivatives and tail bounds

**Definition 2.1.** Let $P_0(u) = 2u - 3$ and $P_{k+1}(u) = 4uP_k'(u) + (5 - 4u)P_k(u)$ for $k \geq 0$. Write $P_k(u) = \sum_i p_{k,i} u^i$, let $\overline{P}_k(u) = \sum_i |p_{k,i}| u^i$, and let $Q_n = P_n^2 - P_{n-1}P_{n+1}$ for $n \geq 1$.

The recursion for $P_k$ and formula (3) below are used by Sra in the proof of [9, Theorem 5.2]; we include the short derivation for completeness.

**Lemma 2.2.** *For every $k \geq 0$, $P_k \in \mathbb{Z}[u]$ has degree $k+1$ and leading coefficient $2(-4)^k$, and*

$$\Phi^{(k)}(t) = e^{5t} \sum_{m=1}^{\infty} \pi m^2 e^{-u_m} P_k(u_m), \qquad u_m = \pi m^2 e^{4t}, \quad t \in \mathbb{R}. \tag{3}$$

*For $n \geq 1$, $Q_n \in \mathbb{Z}[u]$ has degree $2n+1$ and leading coefficient $4^{2n+1}$, and $Q_n(0) = 0$.*

*Proof.* The $m$-th summand of (1) is $\pi m^2 e^{5t} e^{-u} P_0(u)$ with $u = u_m$. Since $du/dt = 4u$, the derivative of $e^{5t}e^{-u}P(u)$ is $e^{5t}e^{-u}\big(5P - 4uP + 4uP'\big)$, which gives the recursion. The degree and leading coefficient follow by induction, the term $-4uP_k$ raising the degree by one. On a compact interval $|t| \le T$ the $k$-th derivative of the $m$-th summand is bounded by $\pi m^2 e^{5T} \exp(-\pi m^2 e^{-4T}) \overline{P}_k(\pi m^2 e^{4T})$, which is summable in $m$; hence every differentiated series converges uniformly on compact sets and (3) holds. Write $P_k = 2(-4)^k u^{k+1} + (-4)^k d_k u^k + \cdots$. Comparing the coefficients of $u^{k+1}$ in the recursion gives $d_{k+1} = d_k - 2k - \frac{9}{2}$ with $d_0 = -3$, so $d_k = -3 - \frac{7}{2}k - k^2$. In $Q_n$ the terms of degree $2n+2$ cancel, because $4 \cdot 16^n - 2(-4)^{n-1} \cdot 2(-4)^{n+1} = 0$, and the coefficient of $u^{2n+1}$ is $16^n(4d_n - 2d_{n-1} - 2d_{n+1}) = -2 \cdot 16^n (d_{n+1} - 2d_n + d_{n-1}) = 4^{2n+1}$. Finally $P_k(0) = -3 \cdot 5^k$, so $Q_n(0) = 9 \cdot 25^n - 9 \cdot 25^n = 0$. □

Every statement about $Q_n$ below is checked on its exact integer coefficients; the leading coefficient shows the behaviour for large $u$.

**Lemma 2.3.** *For $u \ge 0$ and $\lambda \ge 1$ one has $|P_k(u)| \le \overline{P}_k(u)$, $\overline{P}_k$ is nondecreasing on $[0,\infty)$, and $\overline{P}_k(\lambda u) \le \lambda^{k+1} \overline{P}_k(u)$.*

*Proof.* The coefficients of $\overline{P}_k$ are nonnegative and its degree is $k+1$. □

**Lemma 2.4** (geometric tail)**.** *Let $a \ge 0$, $\alpha > 0$ and $M \ge 1$, and suppose $r = \big(\frac{M+2}{M+1}\big)^a e^{-\alpha(2M+3)} < 1$. Then*

$$S_M(a,\alpha) := \sum_{m > M} m^a e^{-\alpha m^2} \le \frac{(M+1)^a e^{-\alpha(M+1)^2}}{1-r}.$$

*Proof.* The ratio of consecutive terms, $\big(\frac{m+1}{m}\big)^a e^{-\alpha(2m+1)}$, is nonincreasing in $m$, so it is at most $r$ for $m \ge M+1$. Compare with a geometric series. □

## 3 The large-argument range

Put $x = \pi e^{4t}$. Then $u_m = m^2 x$, and (3) gives $e^{-5t}\Phi^{(k)}(t) = \pi \sum_m m^2 e^{-m^2 x} P_k(m^2 x)$.

**Lemma 3.1.** *Let $n \ge 1$ and $x_0 > 0$ satisfy $(3/2)^{2n+6} e^{-5x_0} \le \frac{1}{2}$. Put*

$$W_n = 2^{2n+6}\,\overline{P}_n^{\,2} + 17 \cdot 2^{2n+3}\,\overline{P}_{n-1}\overline{P}_{n+1}, \qquad V_n = \overline{P}_n^{\,2} + \overline{P}_{n-1}\overline{P}_{n+1}.$$

*Then for every $t$ with $x = \pi e^{4t} \ge x_0$,*

$$\frac{e^{2x-10t}}{\pi^2}\, J_n(t) \;\ge\; Q_n(x) - e^{-3x} W_n(x) - e^{-6x}\, 2^{4n+10}\, V_n(x).$$

*Proof.* Write $A_k = P_k(x)$ and $\sigma_k = \sum_{m \ge 2} m^2 e^{-m^2 x} P_k(m^2 x)$, so that $e^{-5t}\Phi^{(k)}(t) = \pi(e^{-x} A_k + \sigma_k)$. Expanding (2),

$$\frac{e^{-10t}}{\pi^2} J_n = e^{-2x} Q_n(x) + 2e^{-x} A_n \sigma_n + \sigma_n^2 - e^{-x} A_{n-1}\sigma_{n+1} - e^{-x} A_{n+1}\sigma_{n-1} - \sigma_{n-1}\sigma_{n+1}.$$

By Lemma 2.3, $|A_k| \le \overline{P}_k(x)$ and $|P_k(m^2 x)| \le m^{2k+2} \overline{P}_k(x)$, so $|\sigma_k| \le \overline{P}_k(x)\, S_1(2k+4, x)$. For $k \le n+1$ the ratio in Lemma 2.4 with $M = 1$ is $(3/2)^{2k+4} e^{-5x} \le (3/2)^{2n+6} e^{-5x_0} \le \frac{1}{2}$, hence $|\sigma_k| \le 2^{2k+5} e^{-4x} \overline{P}_k(x)$. Inserting these bounds,

$$2e^{-x}|A_n \sigma_n| \le 2^{2n+6} e^{-5x} \overline{P}_n^{\,2}, \qquad e^{-x}\big(|A_{n-1}\sigma_{n+1}| + |A_{n+1}\sigma_{n-1}|\big) \le (2^{2n+7} + 2^{2n+3}) e^{-5x} \overline{P}_{n-1}\overline{P}_{n+1},$$

and $\sigma_n^2 + |\sigma_{n-1}\sigma_{n+1}| \le 2^{4n+10} e^{-8x} V_n(x)$. Since $2^{2n+7} + 2^{2n+3} = 17 \cdot 2^{2n+3}$, multiplying by $e^{2x}$ gives the claim. □

**Proposition 3.2.** *Let $n \ge 1$, let $x_0, L, \ell$ be positive integers with $L \le e^{3x_0}$ and $(3/2)^{2n+6}e^{-5x_0} \le \frac{1}{2}$, and put $E_\ell(y) = \sum_{j=0}^{\ell}(3y)^j/j!$. Suppose that the polynomial*

$$C_n(y) = L^2\, Q_n(x_0+y)\, E_\ell(y) - L\, W_n(x_0+y) - 2^{4n+10}\, V_n(x_0+y)$$

*has nonnegative coefficients and $C_n(0) > 0$. Then $J_n(t) > 0$ for every $t$ with $\pi e^{4t} \ge x_0$.*

*Proof.* Let $x = x_0 + y$ with $y \ge 0$. Then $C_n(y) \ge C_n(0) > 0$. Because $W_n, V_n \ge 0$ on $[0,\infty)$ and $E_\ell > 0$, this forces $Q_n(x) > 0$. Moreover $e^{3y} \ge E_\ell(y)$, $e^{-3x} \le L^{-1}e^{-3y}$ and $e^{-6x} \le L^{-2}e^{-3y}$. Hence

$$e^{-3x}W_n(x) + e^{-6x}2^{4n+10}V_n(x) \le \frac{e^{-3y}}{L^2}\big(LW_n(x) + 2^{4n+10}V_n(x)\big) < e^{-3y}E_\ell(y)\,Q_n(x) \le Q_n(x),$$

and Lemma 3.1 gives $J_n(t) > 0$. □

All hypotheses of Proposition 3.2 are finite integer computations once $x_0$ is fixed: we take $\ell = 6$, $L = \lfloor \sum_{j<9x_0+80}(3x_0)^j/j! \rfloor$, check $2\cdot 3^{2n+6} \le 2^{2n+6}L_5$ with $L_5 \le e^{5x_0}$ obtained in the same way, and compute $C_n$ (multiplied by $\ell!$) exactly. We then choose $T_0(n) \in \frac{1}{1000}\mathbb{Z}$ with $\pi e^{4T_0(n)} \ge x_0$, verified with $\pi > 314159/10^5$ and a partial sum of $e^{4T_0}$.

**Lemma 3.3.** *For each $1 \le n \le 100$ the hypotheses of Proposition 3.2 hold with the integer $x_0(n)$ listed in the verification output; consequently $J_n(t) > 0$ for $|t| \ge T_0(n)$. For $n \le 8$ the values are*

| $n$ | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
|---|---|---|---|---|---|---|---|---|
| $x_0(n)$ | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 |
| $T_0(n)$ | 0.061 | 0.117 | 0.162 | 0.201 | 0.234 | 0.264 | 0.290 | 0.314 |

*and in general $x_0(n)$ grows linearly, from $x_0(64) = 117$, $T_0(64) = 0.905$, to $x_0(100) = 195$, $T_0(100) = 1.033$.*

*Proof.* This is the output of `cc_large_t.py` (exact integer arithmetic); evenness of $J_n$ covers $t \le -T_0(n)$. □

## 4 The compact range

On $[0, T_0(n)]$ several terms of the theta series matter and the individual terms cancel strongly, so we use enclosures with rigorous error terms.

**Lemma 4.1** (point enclosure)**.** *Let $t \ge 0$, $k \ge 0$, $M \ge 1$ and $\alpha = \pi e^{4t}$. Then*

$$\Big|\Phi^{(k)}(t) - e^{5t}\sum_{m=1}^{M}\pi m^2 e^{-u_m}P_k(u_m)\Big| \le \pi e^{5t}\sum_i |p_{k,i}|\,\alpha^i\, S_M(2i+2,\alpha),$$

*and the right side is bounded by Lemma 2.4 whenever its ratio condition holds.*

*Proof.* For $m > M$, $|P_k(\alpha m^2)| \le \sum_i |p_{k,i}|\alpha^i m^{2i}$; sum over $m > M$ and interchange the finite sum over $i$. □

**Lemma 4.2** (uniform bound)**.** *Let $0 \le a \le b$, $M \ge 1$, $\alpha = \pi e^{4a}$ and $\beta = \pi e^{4b}$. For every $\xi \in [a,b]$,*

$$|\Phi^{(k)}(\xi)| \le e^{5b}\Big(\sum_{m=1}^{M}\pi m^2 e^{-\alpha m^2}\overline{P}_k(\beta m^2) + \pi\sum_i |p_{k,i}|\,\beta^i\, S_M(2i+2,\alpha)\Big).$$

*Proof.* For $\xi \in [a,b]$ we have $\alpha m^2 \le u_m(\xi) \le \beta m^2$. Bound $e^{5\xi} \le e^{5b}$, $e^{-u_m} \le e^{-\alpha m^2}$ and, by Lemma 2.3, $|P_k(u_m)| \le \overline{P}_k(\beta m^2)$; the tail is treated as in Lemma 4.1. □

**Lemma 4.3** (Taylor model)**.** *Let $n \ge 1$, $c \in \mathbb{R}$, $h > 0$ and $K \ge 1$. For $j \in \{n-1, n, n+1\}$ let $T_j(\tau) = \sum_{i<K} \Phi^{(j+i)}(c)\,\tau^i/i!$, let $B_{j+K} \ge \sup_{|\xi-c|\le h} |\Phi^{(j+K)}(\xi)|$, $R_j = B_{j+K}h^K/K!$, and $\rho_j \ge \sup_{|\tau|\le h} |T_j(\tau)|$. Then for $|\tau| \le h$,*

$$\left|J_n(c+\tau) - \left(T_n(\tau)^2 - T_{n-1}(\tau)T_{n+1}(\tau)\right)\right| \le 2\rho_n R_n + R_n^2 + \rho_{n-1}R_{n+1} + \rho_{n+1}R_{n-1} + R_{n-1}R_{n+1}.$$

*Proof.* By Taylor's theorem with Lagrange remainder, $\Phi^{(j)}(c+\tau) = T_j(\tau) + r_j(\tau)$ with $|r_j(\tau)| \le R_j$. Substitute into (2) and bound each cross term. □

**Lemma 4.4** (polynomial lower bound)**.** *Let $p$ be a real polynomial, $\sigma \in \mathbb{R}$, $\delta > 0$, and write $p(\sigma+\nu) = \sum_i d_i \nu^i$. Then $p(\sigma+\nu) \ge d_0 - \sum_{i\ge 1} |d_i|\delta^i$ for $|\nu| \le \delta$.*

*Proof.* For $|\nu| \le \delta$ each term satisfies $d_i\nu^i \ge -|d_i|\delta^i$. □

**Proposition 4.5** (certified cover)**.** *Let $[c-h, c+h] \subset [0,\infty)$. Suppose that interval enclosures of $\Phi^{(k)}(c)$, $k \le n+K$, are computed from Lemma 4.1, the bounds $B_{j+K}$ from Lemma 4.2, and that, after splitting $[-h,h]$ into pieces of radius $\delta$ and applying Lemma 4.4 to $p = T_n^2 - T_{n-1}T_{n+1}$ on each piece, the smallest lower bound exceeds the error bound of Lemma 4.3. Then $J_n > 0$ on $[c-h, c+h]$.*

*Proof.* Lemmas 4.3 and 4.4; every quantity is enclosed in outward-rounded interval arithmetic, so the inequalities hold for the exact values. □

**Implementation.** The program `cc_run.py` covers $[0, T_0(n)]$ by consecutive intervals $[c-h, c+h]$ with dyadic endpoints, starting at 0, with radius $h = \min\{h_0,\, 0.4/(4\pi e^{4a})\}$ at the left end $a$, rounded down to a multiple of $2^{-20}$. It uses the interval arithmetic of `mpmath` [5] (outward rounding for the field operations, exp and $\pi$), truncates the theta series after $M = \max\{3, \lceil (N/(\pi e^{4a}))^{1/2} \rceil\}$ terms, where $k_{\max}$ is the largest derivative order enclosed, $N = \max\{6(k_{\max}+2), 5(d+40)\}$ and $d$ is the number of decimal digits, and adds the tail bound of Lemma 4.1 as a symmetric interval. Pieces are refined by factors of four up to 64 pieces, and an interval that is still not certified is bisected, up to seven times. An interval whose enclosure of $J_n(c)$ lies below zero is reported as a certified negative value. The parameters are:

| run | orders | $K$ | digits | $h_0$ | intervals | time (14 cores) |
|---|---|---|---|---|---|---|
| A | $1 \le n \le 9$ | 24 | 80 | 0.002 | 85 | 25 s |
| B | $1 \le n \le 64$ | 30 | 100 | 0.002 | 257 | 2 min |
| C | $65 \le n \le 100$ | 40 | 130 | 0.0015 | 416 | 5 min |

*Remark* 4.6. The program `cc_jet_scan.py` recomputes $\Phi^{(k)}$ independently, by power-series arithmetic for $\exp(-ue^{4\tau})$ instead of the polynomials $P_k$, and scans $J_n$ on $[0, 1.1]$ with step 0.0005. It finds negative values exactly for the orders in $\mathcal{E}$. This floating-point scan is an independent consistency check of the certified classification.

## 5 Proof of Theorems 1.2 and 1.3

*Proof of Theorem 1.2.* Fix $n \le 8$. By Lemma 3.3, $J_n(t) > 0$ for $|t| \ge T_0(n)$. Run A certifies, by Proposition 4.5, every interval of a cover of $[0, T_0(n)]$ (the mesh reaches 0.339975). On each interval $[c-h, c+h]$ the certified lower bound of $J_n$ is at least 0.33 times $\Phi^{(n)}(c)^2 + |\Phi^{(n-1)}(c)\Phi^{(n+1)}(c)|$; the smallest such ratio, 0.335, occurs for $n = 8$. Evenness gives $J_n > 0$ on $(-T_0(n), 0]$. □

*Proof of Theorem 1.3.* For $n \notin \mathcal{E}$, runs B and C certify $J_n > 0$ on a cover of $[0, T_0(n)]$, and Lemma 3.3 and evenness complete the proof. For $n \in \mathcal{E}$, the program `cc_witness.py` encloses $J_n(t_n)$ at the points of Table 1; the upper end of each enclosure is negative. For odd $n$ with $t_n = 0$ the value is $J_n(0) = -\Phi^{(n-1)}(0)\Phi^{(n+1)}(0)$, because $\Phi^{(n)}(0) = 0$. □

Table 1: Certified negative values. Each $J_n(t_n)$ is enclosed in an interval of relative width below $10^{-80}$, and the displayed values are rounded; the column $r_n$ is $J_n/(\Phi^{(n)2} + |\Phi^{(n-1)}\Phi^{(n+1)}|)$ at $t_n$, rounded. The last column lists the runs of consecutive points of the grid $0.0005\,\mathbb{Z} \cap [0, 1.1]$ at which $J_n < 0$ (floating-point scan of Remark 4.6).

| $n$ | $t_n$ | $J_n(t_n)$ | $r_n$ | grid negative set in $[0, 1.1]$ |
|---|---|---|---|---|
| 9 | 0 | $-7.8376 \times 10^{19}$ | $-1.000$ | $[0.0000, 0.0245]$ |
| | 0.02 | $-2.6101 \times 10^{19}$ | $-0.279$ | |
| 16 | 0.13 | $-3.2076 \times 10^{41}$ | $-1.000$ | $[0.1150, 0.1470]$ |
| 23 | 0.21 | $-1.4366 \times 10^{65}$ | $-0.981$ | $[0.2065, 0.2270]$ |
| 29 | 0 | $-5.0213 \times 10^{87}$ | $-1.000$ | $[0.0000, 0.0070]$ |
| 30 | 0.28 | $-5.5449 \times 10^{90}$ | $-0.685$ | $[0.2750, 0.2860]$ |
| 31 | 0.27 | $-2.1177 \times 10^{94}$ | $-0.325$ | $[0.2675, 0.2790]$ |
| 38 | 0.33 | $-1.8087 \times 10^{121}$ | $-0.987$ | $[0.3190, 0.3310]$ |
| 39 | 0.331 | $-2.3436 \times 10^{124}$ | $-0.595$ | $[0.3305, 0.3320]$ |
| 40 | 0.085 | $-4.6787 \times 10^{130}$ | $-0.980$ | $[0.0805, 0.0895]$ |
| 45 | 0.37 | $-6.2301 \times 10^{149}$ | $-0.463$ | $[0.3635, 0.3720]$ |
| 46 | 0.373 | $-1.4794 \times 10^{154}$ | $-1.000$ | $[0.3690, 0.3775]$ |
| 52 | 0.404 | $-2.5995 \times 10^{178}$ | $-0.080$ | $[0.4025, 0.4055]$ |
| 53 | 0.148 | $-1.3463 \times 10^{185}$ | $-0.998$ | $[0.1430, 0.1530]$, $[0.4045, 0.4135]$ |
| | 0.408 | $-3.4950 \times 10^{183}$ | $-0.999$ | |
| 59 | 0 | $-3.2667 \times 10^{209}$ | $-1.000$ | $[0.0000, 0.0005]$ |
| 60 | 0.44 | $-3.5113 \times 10^{213}$ | $-0.798$ | $[0.4365, 0.4445]$ |
| 65 | 0.196 | $-2.2259 \times 10^{236}$ | $-0.130$ | $[0.1940, 0.1970]$ |
| 66 | 0.198 | $-4.5331 \times 10^{241}$ | $-0.861$ | $[0.1960, 0.2015]$ |
| 67 | 0.468 | $-8.0114 \times 10^{243}$ | $-0.311$ | $[0.4660, 0.4710]$ |
| 68 | 0.465 | $-5.5178 \times 10^{248}$ | $-0.992$ | $[0.4620, 0.4680]$ |
| 75 | 0.491 | $-2.0921 \times 10^{280}$ | $-0.998$ | $[0.4870, 0.4940]$ |
| 76 | 0.063 | $-1.4850 \times 10^{287}$ | $-0.987$ | $[0.0610, 0.0655]$ |
| 77 | 0.24 | $-2.7481 \times 10^{291}$ | $-0.883$ | $[0.2385, 0.2430]$ |
| 78 | 0.238 | $-2.8354 \times 10^{295}$ | $-1.000$ | $[0.2360, 0.2395]$ |
| 82 | 0.514 | $-2.0398 \times 10^{312}$ | $-0.972$ | $[0.5105, 0.5170]$ |
| 89 | 0.536 | $-3.4691 \times 10^{344}$ | $-0.995$ | $[0.5325, 0.5370]$ |
| 90 | 0.276 | $-1.7223 \times 10^{352}$ | $-0.999$ | $[0.2735, 0.2795]$ |
| 93 | 0.1135 | $-7.8056 \times 10^{366}$ | $-1.000$ | $[0.1110, 0.1160]$ |
| 96 | 0.554 | $-1.1294 \times 10^{377}$ | $-0.928$ | $[0.5530, 0.5555]$ |
| 97 | 0 | $-1.2033 \times 10^{386}$ | $-1.000$ | $[0.0000, 0.0025]$, $[0.5550, 0.5570]$ |
| | 0.556 | $-1.4210 \times 10^{381}$ | $-0.839$ | |

## 6 Infinitely many failures

For $\operatorname{Re} w > 0$ let $\theta(w) = \sum_{m\in\mathbb{Z}} e^{-\pi m^2 w}$, and for $\operatorname{Re} s > 0$ let $\Lambda(s) = \sum_{m\in\mathbb{Z}} e^{-\pi(m+1/2)^2 s}$. Let $\mathcal{S} = \{z : |\operatorname{Im} z| < \pi/8\}$; for $z \in \mathcal{S}$ we have $\operatorname{Re} e^{4z} = e^{4\operatorname{Re} z}\cos(4\operatorname{Im} z) > 0$.

**Lemma 6.1.** *(a) For $z \in \mathcal{S}$ and $w = e^{4z}$, the series* (1) *converges locally uniformly and*

$$\Phi(z) = e^{5z}\Big(w\,\theta''(w) + \tfrac{3}{2}\,\theta'(w)\Big).$$

*(b) For $\operatorname{Re} v > 0$, $\theta(i+v) = v^{-1/2}\Lambda(1/v)$ with the principal branch of $v^{-1/2}$.*

*(c) For $\operatorname{Re} v > 0$, with $\Lambda$ and its derivatives evaluated at $1/v$,*

$$\theta'(i+v) = -\tfrac{1}{2}v^{-3/2}\Lambda - v^{-5/2}\Lambda', \qquad \theta''(i+v) = \tfrac{3}{4}v^{-5/2}\Lambda + 3v^{-7/2}\Lambda' + v^{-9/2}\Lambda''.$$

*(d) $\Lambda(s+2i) = -i\,\Lambda(s)$ for $\operatorname{Re} s > 0$, and the same holds for $\Lambda'$ and $\Lambda''$.*

*Proof.* (a) With $F(w) = \sum_{m\ge1} e^{-\pi m^2 w} = (\theta(w)-1)/2$ we have $\sum_{m\ge1}\pi m^2(2\pi m^2 w - 3)e^{-\pi m^2 w} = 2wF''(w)+3F'(w)$, and $e^{5z}e^{-\pi m^2 e^{4z}}$ is the $m$-th exponential in (1). Local uniform convergence on $\mathcal{S}$ follows from $\operatorname{Re} w > 0$. (b) Since $e^{-i\pi m^2} = (-1)^m$, $\theta(i+v) = \sum_m (-1)^m e^{-\pi m^2 v}$. For $v > 0$, Poisson summation applied to $x \mapsto e^{-\pi x^2 v + i\pi x}$, whose Fourier transform is $\xi \mapsto v^{-1/2}e^{-\pi(\xi-1/2)^2/v}$, gives $\sum_m (-1)^m e^{-\pi m^2 v} = v^{-1/2}\sum_k e^{-\pi(k-1/2)^2/v}$; both sides are analytic in $\operatorname{Re} v > 0$. (c) Differentiate (b) twice in $v$. (d) $e^{-2\pi i(m+1/2)^2} = e^{-2\pi i(m^2+m)}e^{-\pi i/2} = -i$ for every integer $m$. □

For $\sigma > 0$ and $j \ge 0$ put $\Lambda_j(\sigma) = \sum_{m\in\mathbb{Z}}(\pi(m+\frac12)^2)^j e^{-\pi(m+1/2)^2\sigma}$, so that $|\Lambda^{(j)}(s)| \le \Lambda_j(\operatorname{Re} s)$, with equality for real $s$.

**Lemma 6.2** (the imaginary axis)**.** $\sup_{0\le y<\pi/8}|\Phi(iy)| < \infty$.

*Proof.* Since $\Phi$ is continuous on $[0,\pi/8)i$, it suffices to show $\Phi(iy) \to 0$ as $y \to \pi/8$. Write $4y = \pi/2 - \alpha$ with $0 < \alpha \le \pi/4$. Then $w = e^{4iy} = \sin\alpha + i\cos\alpha$ and $v = w - i$ satisfies $\operatorname{Re} v = \sin\alpha > 0$, $|v| = 2\sin(\alpha/2) \ge 2\alpha/\pi$, and $\operatorname{Re}(1/v) = \frac12\cot(\alpha/2) \ge \pi/(4\alpha) \ge 1$. For $\sigma \ge 1$, $\Lambda_j(\sigma) \le c_j e^{-\pi\sigma/4}$ with $c_j = \Lambda_j(1)e^{\pi/4}$, because $e^{-\pi(m+1/2)^2\sigma} \le e^{-\pi\sigma/4}e^{-\pi((m+1/2)^2-1/4)}$. By Lemma 6.1(a),(c), and $|w| = 1$,

$$|\Phi(iy)| \le \Big(\tfrac34|v|^{-5/2}c_0 + 3|v|^{-7/2}c_1 + |v|^{-9/2}c_2 + \tfrac34|v|^{-3/2}c_0 + \tfrac32|v|^{-5/2}c_1\Big)e^{-\pi^2/(16\alpha)},$$

where each power satisfies $|v|^{-q} \le (\pi/(2\alpha))^q$. The right side tends to 0 as $\alpha \to 0$. □

**Lemma 6.3** (unboundedness on the disc)**.** *For $j \ge 1$ let $v_j = 1/(1+2ij)$, $w_j = i + v_j$ and $z_j = \frac14\operatorname{Log} w_j$. Then $z_j \in \mathcal{S}$, $|z_j| < \pi/8$ for all large $j$, and $|\Phi(z_j)| \to \infty$.*

*Proof.* We have $v_j = (1-2ij)/(1+4j^2)$, so $\operatorname{Re} w_j = \operatorname{Re} v_j > 0$ and $\operatorname{Im} w_j = 1 - 2j/(1+4j^2) > 0$; thus $\operatorname{Arg} w_j \in (0,\pi/2)$ and $z_j \in \mathcal{S}$ with $e^{4z_j} = w_j$. Next, $|w_j|^2 = 1 - a_j$ with $a_j = (4j-1)/(1+4j^2)$, and $\operatorname{Arg} w_j = \pi/2 - \arctan(\varepsilon_j)$ with $\varepsilon_j = \operatorname{Re} w_j/\operatorname{Im} w_j = 1/(4j^2-2j+1)$. As $j\to\infty$, $\log|w_j| = -\frac12 a_j + O(j^{-2}) = -\frac{1}{2j} + O(j^{-2})$ and $\operatorname{Arg} w_j = \frac{\pi}{2} - \frac{1}{4j^2} + O(j^{-3})$, so

$$|4z_j|^2 = (\log|w_j|)^2 + (\operatorname{Arg} w_j)^2 = \frac{\pi^2}{4} - \frac{\pi-1}{4j^2} + O(j^{-3}) < \frac{\pi^2}{4}$$

for all large $j$. For the size of $\Phi(z_j)$, note $1/v_j = 1 + 2ij$, so by Lemma 6.1(d) the numbers $|\Lambda^{(q)}(1/v_j)|$ equal $\Lambda_q(1) > 0$ for $q = 0, 1, 2$. By Lemma 6.1(a),(c),

$$|\Phi(z_j)| \geq |w_j|^{5/4}\Big(|w_j||v_j|^{-9/2}\Lambda_2(1) - |w_j|(\tfrac{3}{4}|v_j|^{-5/2}\Lambda_0(1) + 3|v_j|^{-7/2}\Lambda_1(1)) \\ - \tfrac{3}{4}|v_j|^{-3/2}\Lambda_0(1) - \tfrac{3}{2}|v_j|^{-5/2}\Lambda_1(1)\Big).$$

Since $|w_j| \to 1$ and $|v_j| = (1 + 4j^2)^{-1/2} \to 0$, the right side is $\Lambda_2(1)|v_j|^{-9/2}(1 + o(1)) \to \infty$. □

*Proof of Theorem 1.4.* Since $\Phi$ is even and analytic on the disc $|z| < \pi/8$, which lies in $\mathcal{S}$, its Taylor series $\Phi(z) = \sum_k \Phi^{(2k)}(0)z^{2k}/(2k)!$ converges there, and $\Phi(iy) = \sum_k b_k y^{2k}/(2k)!$ with $b_k = (-1)^k\Phi^{(2k)}(0)$. (a) Suppose that there are $k_0$ and $\epsilon \in \{\pm 1\}$ with $\epsilon b_k \geq 0$ for all $k \geq k_0$. Then $|b_k| = \epsilon b_k$ for $k \geq k_0$, and for $|z| = r < \pi/8$,

$$|\Phi(z)| \leq \sum_k |b_k|\frac{r^{2k}}{(2k)!} = \sum_{k<k_0}\big(|b_k| - \epsilon b_k\big)\frac{r^{2k}}{(2k)!} + \epsilon\,\Phi(ir) \leq C + \sup_{0\leq y<\pi/8}|\Phi(iy)|,$$

with $C = 2\sum_{k<k_0}|b_k|(\pi/8)^{2k}/(2k)!$. By Lemma 6.2 the right side is finite, so $\Phi$ is bounded on the disc, which contradicts Lemma 6.3. Hence neither sign is eventually excluded: $b_k > 0$ for infinitely many $k$ and $b_k < 0$ for infinitely many $k$.

(b) Let $k$ satisfy $b_k > 0$. By (a) there is $l > k$ with $b_l < 0$; let $i$ be the largest index in $[k, l)$ with $b_i > 0$. Then $b_{i+1} \leq 0$, so $b_i b_{i+1} \leq 0$ with $i \geq k$. Since $k$ can be taken arbitrarily large, this gives infinitely many such $i$. Finally $\Phi^{(2i+1)}(0) = 0$ gives $J_{2i+1}(0) = -\Phi^{(2i)}(0)\Phi^{(2i+2)}(0) = b_i b_{i+1} \leq 0$. □

## 7 Moments of the Riemann Ξ-function

*Proof of Corollary 1.5.* Let $H(x) = \int_0^\infty \Phi(t)\cos(xt)\,dt = \frac{1}{2}\int_{\mathbb{R}}\Phi(t)e^{ixt}\,dt$, so $H(x) = \frac{1}{8}\Xi(x/2)$ [2, (4.1)]. Fix $0 < y < \pi/8$. On the closed strip $|\operatorname{Im} z| \leq y$, $|\Phi(z)|$ decays faster than any exponential as $\operatorname{Re} z \to +\infty$, by the bound $|e^{-\pi m^2 e^{4z}}| = e^{-\pi m^2 e^{4\operatorname{Re} z}\cos(4\operatorname{Im} z)}$, and as $\operatorname{Re} z \to -\infty$ by evenness. Shifting the line of integration to $\operatorname{Im} t = \pm y$ gives $|H(x)| \leq C_y e^{-y|x|}$. Hence Fourier inversion gives $\Phi(t) = \frac{2}{\pi}\int_0^\infty H(x)\cos(xt)\,dx$, differentiation under the integral is allowed, and

$$b_k = (-1)^k\Phi^{(2k)}(0) = \frac{2}{\pi}\int_0^\infty x^{2k}H(x)\,dx = \frac{2^{2k-1}}{\pi}\int_0^\infty s^{2k}\,\Xi(s)\,ds.$$

Theorem 1.4(a) shows that $b_k > 0$ for infinitely many $k$ and $b_k < 0$ for infinitely many $k$. The signs for $k \leq 61$ are certified by `cc_taylor0.py`, which encloses $\Phi^{(2k)}(0)$ for $k \leq 61$. □

*Remark* 7.1. The first four sign blocks of $(b_k)$ have lengths $5, 10, 15, 19$, and $b_k > 0$ for $49 \leq k \leq 61$; these block lengths are certified by `cc_taylor0.py`. The elements of $\mathcal{E}$, certified by Theorem 1.3, recur with gaps close to 7.

*Remark* 7.2. The bound $|H(x)| \leq C_y e^{-y|x|}$ for every $y < \pi/8$ makes both sides of $\Phi(t) = \frac{1}{2\pi}\int_0^\infty \Xi(s)\cos(2st)\,ds$ analytic in $|\operatorname{Im} t| < \pi/8$, so $\Phi(iy) = \frac{1}{2\pi}\int_0^\infty \Xi(s)\cosh(2sy)\,ds$ for $0 \leq y < \pi/8$. The proof of Lemma 6.2 therefore shows that these integrals tend to 0 as $2y \to \pi/4$. This is the analogue for $\Phi$ of the cusp behaviour of the theta function that drives Hardy's proof that $\zeta(s)$ has infinitely many zeros on the critical line; see Titchmarsh [10, Chapter X].

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**Data and code availability.** The verification scripts cited in the text are included with this article, together with their outputs:

- `ccpoly.py`: the exact polynomials $P_k$ and $Q_n$;
- `cc_large_t.py`: Lemma 3.3;
- `cc_compact.py` and `cc_run.py`: Proposition 4.5 and runs A–C;
- `cc_witness.py`: Table 1;
- `cc_taylor0.py`: Corollary 1.5;
- `cc_jet_scan.py`: Remark 4.6.

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