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THE EXACT SECOND-ORDER TERM IN RAMANUJAN'S BOUND FOR $\sigma(n)/n$

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ABSTRACT. Let $\sigma(n)$ be the sum of the divisors of n, and assume the Riemann hypothesis. Ramanujan showed that

$$\sigma(n)/n \le e^{\gamma}\big(\log\log n - 2(\sqrt{2}-1)/\sqrt{\log n} + S_1(\log n) + O(1/(\sqrt{\log n}\,\log\log n))\big),$$

where S_1 is a sum over the zeros of ζ. Nicolas recently made this effective. He placed the coefficient of $1/(\sqrt{\log n}\log\log n)$ in [0.9567, 3.789] at colossally abundant numbers, and asked for its exact asymptotic value.

We show that this coefficient is

$$\kappa + W_2(\log n), \qquad \kappa = \sqrt{2}\,(2+\log 2) - 2 = 1.80868\ldots,$$

where $W_2(x) = -\sum_\rho x^{i\Im\rho}/(1-\rho)^2$ oscillates in $[-\beta,\beta]$ with $\beta = 2+\gamma-\log 4\pi$. In particular the rescaled residual studied numerically by Leshchiner, Musin and Thompson does not converge, and it exceeds $3/2$ at every colossally abundant number with parameter $\xi \ge 4.4\cdot 10^{15}$; this answers their Questions 3 and 4 (the second in the negative). The next coefficient is the constant $c_0 = 8 - \sqrt{2}\,(8 + 4\log 2 + \frac{3}{4}\log^2 2) = -7.7443\ldots$, up to an oscillation of amplitude at most 0.0066.

We also prove explicit two-sided bounds for the remainder at every colossally abundant number above Nicolas's threshold $N^{(0)}$, which has $\log N^{(0)} \approx 10^9$. The proof is computer-assisted: rigorous interval arithmetic covers every real parameter $\xi \in [10^9, e^{300}]$, and an analytic argument covers $\xi > e^{300}$. Corollaries:

- $\sigma(n)/n \le e^{\gamma}(\log\log n - 0.699/\sqrt{\log n})$ for all $n \ge N^{(0)}$;
- Ramanujan's lim sup is approached from above, at every colossally abundant number with $\xi \ge 10^9$;
- an explicit window for the lim inf;
- the analogue for odd integers, refining a criterion of Washington and Yang.

The proof reads colossally abundant numbers as ground states of a free gas of prime modes. In that picture the constant κ separates into a deficit term, a shell-energy term and a prime-square term. Every enclosure is checked against exact values computed from a sieve to 10^{10}.

1. Introduction and main results

1.1. **Background.** Gronwall proved that $\limsup \sigma(n)/(n\log\log n) = e^{\gamma}$. Robin [9] proved that the Riemann hypothesis (RH) is equivalent to

$$\sigma(n) < e^{\gamma} n \log\log n \quad (n > 5040).$$

Long before, in the part of *Highly composite numbers* that was suppressed in 1915 and published in 1997 [8], Ramanujan had shown under RH that

$$(1)\quad \frac{\sigma(n)}{n} \le e^{\gamma}\Big(\log\log n - \frac{2(\sqrt{2}-1)}{\sqrt{\log n}} + S_1(\log n) + \frac{O(1)}{\sqrt{\log n}\,\log\log n}\Big), \qquad S_1(x) = \sum_\rho \frac{x^{\rho-1}}{\rho(1-\rho)}.$$

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Nicolas [6, Thm. 1.1] made (1) effective. Write $L = \log n$ and $\lambda = \log\log n$. Under RH he proved that, for all $n \geq 2$,

$$\frac{\sigma(n)}{n} \leq e^{\gamma}\Big(\lambda - \tfrac{2(\sqrt{2}-1)}{\sqrt{L}} + S_1(L) + \tfrac{3.789}{\sqrt{L}\,\lambda} + \tfrac{0.026\,\lambda}{L^{2/3}}\Big).$$

He also proved a matching lower bound, with 0.9567 and -0.48 in place of 3.789 and 0.026, at every colossally abundant number $N \geq N^{(0)}$ [6, Prop. 5.1]. As the first open question of [6, §7] he asks for the exact asymptotic coefficient of $1/(\sqrt{L}\lambda)$ in (1), remarking that this probably requires a sharper estimate of $\prod_{p\leq x}(1-1/p)$; Lemma 9 below supplies it.

1.2. **Notation.** Let $\rho = \frac{1}{2} + i\gamma_\rho$ run over the nontrivial zeros of ζ; RH is assumed throughout. Put

$$\beta = \sum_{\rho} \frac{1}{\rho(1-\rho)} = 2 + \gamma - \log 4\pi = 0.046191\ldots,$$

$$W(x) = \sum_{\rho} \frac{x^{i\gamma_\rho}}{\rho(1-\rho)}, \qquad W_2(x) = -\sum_{\rho} \frac{x^{i\gamma_\rho}}{(1-\rho)^2}.$$

Under RH, $\rho(1-\rho) = |\rho|^2 = |1-\rho|^2$, so $|W(x)|, |W_2(x)| \leq \beta$.

Colossally abundant (CA) numbers are parametrized as follows. For real $x > 1$ and $k \geq 1$ put

$$F(x,k) = \frac{\log\big(1 + 1/(x + x^2 + \cdots + x^k)\big)}{\log x}.$$

For real $\xi > 1$ let $\varepsilon = F(\xi, 1)$, let $\xi_k = \xi_k(\xi)$ be the root of $F(\xi_k, k) = \varepsilon$ (so $\xi_1 = \xi$), and set

$$N(\xi) = \prod_{k\geq 1} \prod_{p \leq \xi_k} p.$$

This is Nicolas's parametrization [6, Def. 4.3]: his $\xi(N)$, defined by $F(\xi,1) = \varepsilon_i$ for the largest parameter ε_i of N, is one admissible value. Every CA number is $N(\xi)$ for some real ξ in $[P, P')$, where P is its largest prime factor and P' the next prime (see Remark 6 for the boundary case). All statements below hold for every such ξ. Write $t = \log\xi$ and $s = 1/t$. Following Nicolas, define $\alpha(n)$ by

$$\frac{\sigma(n)}{n} = e^{\gamma}\Big(\log\log n - \frac{\alpha(n)}{\sqrt{\log n}}\Big),$$

and set

$$c_\sigma(n) = -e^{\gamma}\alpha(n) = \Big(\frac{\sigma(n)}{n} - e^{\gamma}\log\log n\Big)\sqrt{\log n}.$$

1.3. **The answer to Nicolas's question.**

Theorem 1. *Assume RH. As $N \to \infty$ through colossally abundant numbers,*

$$\frac{c_\sigma(N)}{e^{\gamma}} = 2 - 2\sqrt{2} + W(\xi) + \frac{\kappa + W_2(\xi)}{\log\xi} + O\Big(\frac{1}{\log^2\xi}\Big), \qquad \kappa = \sqrt{2}\,(2 + \log 2) - 2.$$

Equivalently, with $L = \log N$ and $\lambda = \log\log N$,

$$\frac{\sigma(N)}{N} = e^{\gamma}\Big(\lambda - \frac{2(\sqrt{2}-1)}{\sqrt{L}} + S_1(L) + \frac{\kappa + W_2(L)}{\sqrt{L}\,\lambda} + O\Big(\frac{1}{\sqrt{L}\,\lambda^2}\Big)\Big).$$

More precisely, the $O(\log^{-2}\xi)$ term equals $(c_0 + \omega(\xi))/\log^2\xi + O(\log^{-3}\xi)$, where

$$c_0 = 8 - \sqrt{2}\big(8 + 4\log 2 + \tfrac{3}{4}\log^2 2\big) = -7.74433\ldots, \qquad |\omega(\xi)| \leq 2\beta/\gamma_1 < 0.0066,$$

with $\gamma_1 = 14.1347\ldots$ the ordinate of the first zero.

The coefficient Nicolas asks for is therefore $\kappa+W_2(\log N)+o(1)$. It oscillates in $[\kappa-\beta,\kappa+\beta]=[1.7625,\ 1.8549]$, well inside his window $[0.9567, 3.789]$.

Three contributions add up to κ:

- the second-order term of Mertens' product at primorials, which gives -2 (prime squares);
- the saturation deficit of the doubly occupied primes, which gives $\sqrt{2}(2+\frac{1}{2}\log 2)$;
- the shift of $\log N$ caused by the squared primes, which gives $\frac{1}{2}\sqrt{2}\log 2$.

Robin already isolated the combination $\sqrt{2}(\log 2+2)=3.808$ in the remark following his Lemma 6 [9]. The zeros enter at this order only through W_2. At the next order, c_0 is the sum of 8 (prime squares) and $-\sqrt{2}(8+4\log 2+\frac{3}{4}\log^2 2)$ (deficit and energy of the second shell; the shell parameter v of Lemma 7 enters both with opposite signs and cancels exactly). The zeros contribute only ω, which is bounded by $2\sum_\rho|1-\rho|^{-3}$.

1.4. **Relation to the numerical study of Leshchiner, Musin and Thompson.** In [4], Leshchiner, Musin and Thompson study the same quantity numerically. Their notation is

$$T(n)=-c_\sigma(n),\qquad R(n)=e^\gamma\big(2\sqrt{2}-2-W(\log n)\big),\qquad Q(n)=e^{-\gamma}\big(R(n)-T(n)\big)\log\log n.$$

By Theorem 1, along CA numbers, with $u=\log\log N$,

$$Q(N)=\kappa+W_2(\log N)+\tfrac{3}{2}\big(1-3^{1/3}\big)\,u\,e^{-u/6}+\frac{c_0+\omega}{u}+O(u^{-2}). \tag{2}$$

In their computed range $14\lesssim u\lesssim 25$, Q rises from about 0.36 to about 1.25, and they ask whether it converges (their Question 3), whether $Q\le 3/2$ eventually (Question 4), and what the higher-order coefficients are (Question 6). Under RH:

(1) *Q does not converge.* The function W_2 is a non-constant almost periodic function of $\log\log N$, and every real ξ is a CA parameter. Hence $\limsup Q=\kappa+\limsup W_2$ and $\liminf Q=\kappa+\liminf W_2$, and both lie in $[\kappa-\beta,\kappa+\beta]=[1.7625,\ 1.8549]$.

(2) *$Q\le 3/2$ fails eventually.* By Theorem 2, $Q(N)>3/2$ for every CA number with $\xi\ge 4.4\cdot 10^{15}$. The certified lower bound is >1.501 on every cell beyond that point and >1.73 for $t\ge 300$. Replacing $W(\xi),W_2(\xi)$ by $W(\log N),W_2(\log N)$ changes Q by less than 10^{-4} there.

(3) *The coefficients.* Constant coefficients do not suffice at first order: A_1 must be replaced by $\kappa+W_2(e^u)$. At second order the coefficient is the constant $c_0=-7.744$, up to an oscillation of size at most 0.0066.

(4) *The observed drift.* The term $\frac{3}{2}(1-3^{1/3})ue^{-u/6}$ is $o(u^{-r})$ for every r, but it dominates for $u\lesssim 40$ and explains the drift. With the value $t^2\mathcal{E}\approx -6.5$ observed in Section 5, (2) gives $Q\approx 0.44$ at $u=14$ and $Q\approx 1.29$ at $u=25$. This agrees with their curves, within their truncation error and sampling.

Their Conjecture 1 asks that $\liminf T=c_1$ and $\limsup T=c_2$ along CA numbers. The first equality follows from Theorem 1: Dirichlet's simultaneous approximation makes $W(\xi)$ approach β for arbitrarily large real ξ. The second is equivalent to $\liminf W=-\beta$, which is open [5].

1.5. **Explicit form.**

Theorem 2 (computer-assisted)**.** *Assume RH, and let $N=N(\xi)$ with real $\xi\ge 10^9$. This includes every CA number $N\ge N^{(0)}$, i.e. with largest prime factor $\ge 10^9+7$. Then*

$$\frac{c_\sigma(N)}{e^\gamma}=2-2\sqrt{2}+W(\xi)+\frac{\kappa+W_2(\xi)}{t}+\tfrac{3}{2}\big(1-3^{1/3}\big)\xi^{-1/6}+\mathcal{E},\qquad -21.28\,t^{-2}\le\mathcal{E}\le 6.18\,t^{-2}.$$

The window shrinks as ξ grows. For $\xi \geq 10^{100}$ it is $[-7.87, -7.42]\,t^{-2}$, and for $t \geq 300$ it is $[-7.87, -7.46]\,t^{-2}$. In the form of Nicolas's question,

$$\frac{0.30}{t} \leq \frac{c_\sigma(N)}{e^\gamma} - \bigl(2 - 2\sqrt{2} + W(\xi)\bigr) \leq \frac{1.855}{t} \qquad (\xi \geq 10^9). \tag{3}$$

The term $\xi^{-1/6}$, which comes from prime cubes and the triply occupied shell, is $o(t^{-2})$. We keep it because at $\xi = 10^9$ it equals 0.021, against $1/t^2 = 0.0023$. The width of the window at $\xi = 10^9$ is due almost entirely to the unconditional error terms of the prime number theorem at the second and fourth shells ($\xi_2 \approx 4.5 \cdot 10^4$, $\xi_4 \approx 250$); these decay like $\xi^{-1/4}t^2$.

Remark 3 (how Theorem 2 is proved). The proof has three parts.

(1) The quantity $t^2\mathcal{E}$ is written exactly as a sum of 18 terms; see (8) in Appendix A. Each term is enclosed by an explicit closed-form inequality. These inequalities involve elementary functions, E_1, and the parameters of Lemmas 7 and 11.
(2) The two terms of size $O(1)$ in $t^2\mathcal{E}$ are rational functions of $s = 1/t$ with interval coefficients. Their exact cancellation at orders s^0 and s^1 is verified symbolically.
(3) The remaining terms are evaluated in ball arithmetic (Arb) on a covering of $t \in [\log 10^9, 300]$ by 30 798 closed cells. A cell is an interval of t, not a grid point, so no monotonicity between grid points is needed. For $t \geq 300$ the $O(1)$ terms $U_1 + M_1 + U_6$ are evaluated on 200 subintervals covering $s \in [0, 1/300]$. Every other term is bounded by an explicit majorant built only from the crude shell bounds of Lemma 7 (Appendix B, item 4). These majorants total at most $5t^2e^{-t/6} + 10t^6e^{-t/4}$, which is decreasing for $t \geq 24$ and below 10^{-15} at $t = 300$.

Appendix B gives the details, and the code is in the ancillary files. Every enclosure was also compared with exact values at 101 CA numbers in $[10^9, 10^{10}]$, with no violation.

1.6. **Corollaries.**

Corollary 4. *Assume RH.*

(1) Approach from above. *Since $\kappa > \beta$, for all sufficiently large CA numbers*

$$c_\sigma(N)/e^\gamma > 2 - 2\sqrt{2} + W(\xi).$$

By Theorem 2 this holds for every CA number with $\xi \geq 10^9$. Along any sequence with $W(\xi) \to \beta$, the limit $\limsup c_\sigma = e^\gamma(2 - 2\sqrt{2} + \beta) = -1.3932\ldots$ (Ramanujan, Nicolas–Robin) is approached from above.

(2) A sharper Robin margin. *For every integer $n \geq N^{(0)}$, $\alpha(n) \geq 0.699$; that is,*

$$\frac{\sigma(n)}{n} \leq e^\gamma\Bigl(\log\log n - \frac{0.699}{\sqrt{\log n}}\Bigr).$$

This improves Nicolas's $\alpha(n) \geq 0.582$ [6, Cor. 1.2] in this range.

(3) The lim inf. *We have $\liminf_{N \text{ CA}} c_\sigma(N) = e^\gamma\bigl(2 - 2\sqrt{2} + \liminf W\bigr)$. Hence, using $\liminf W \leq -0.00499$ [5],*

$$-1.5578 \;\leq\; \liminf_{N \text{ CA}} c_\sigma(N) \;\leq\; -1.4844.$$

Corollary 5 (odd integers)**.** *Assume RH. Let M be the odd part of a CA number $N = N(\xi)$ with $\xi \geq 10^9$, and put*

$$c_{\text{odd}}(M) = \bigl(\sigma(M)/M - \tfrac{e^\gamma}{2}\log\log M\bigr)\sqrt{\log M}.$$

Then

$$0 < \frac{c_{\text{odd}}(M)}{e^\gamma/2} - \frac{c_\sigma(N)}{e^\gamma} \leq \frac{t + \log t + 0.37}{\sqrt{\xi}}.$$

The constant 0.37 *is sharp to within* 0.004*: the supremum of* $\log\kappa + 1/(2\kappa)$ *over the admissible range is* 0.3665*, and the observed maximum on* $[10^9, 10^{10}]$ *is* 0.3655*. Hence Theorem 1 holds for the odd ground states* M *with* e^γ *replaced by* $e^\gamma/2$*. Theorem 2 also holds for them, with its upper constants increased by* $t^2(t+\log t + 0.37)/\sqrt{\xi}$*. This amount is decreasing in* ξ *and is at most* 0.33 *for* $\xi \geq 10^9$*. This refines Washington and Yang's criterion* [11]*: RH holds if and only if* $\sigma(m) < \frac{e^\gamma}{2} m \log\log m$ *for all large odd* m*.*

1.7. **The ground-state reading.** The proofs are organized around one observation, which goes back in substance to Ramanujan [7] and Alaoglu–Erdős [1]. A CA number of parameter ε is a *ground state* of

$$H_\varepsilon(n) = \varepsilon \log n - \log\frac{\sigma(n)}{n} = \sum_p \sum_{a=1}^{a_p} \big(\varepsilon - \eta(p,a)\big)\log p,$$

where $p^{a_p} \parallel n$ and

$$\eta(p,a) = F(p,a) = \frac{\log\big(1 + 1/(p+\cdots+p^a)\big)}{\log p}.$$

This is a free gas of bosonic modes labelled by primes, with quanta of energy $\log p$ and decreasing "efficiencies" $\eta(p,a)$. The ground state fills every quantum with $\eta \geq \varepsilon$. The result is a Fermi sea of singly occupied primes $p \leq \xi$, together with shells: the primes $p \leq \xi_k$ have exponent $\geq k$, and $\xi_k \approx (k\xi)^{1/k}$.

In this language:

- the reduction of Robin's criterion to CA numbers (Robin's Proposition 1; [6, Lemma 4.15]) is the exact equivalence of the canonical and microcanonical ensembles for a concave target;
- Ramanujan's minimization arguments in [7] is the corresponding Legendre transform for $d(n)$;
- the finite-size correction splits into a fermionic part (the primorial, i.e. Mertens' product) and a bosonic part (the shells).

The leading constant $2-2\sqrt{2}$ is 2 from prime squares in the explicit formula, minus $\sqrt{2}$ of reward lost by the doubly occupied shell (its *saturation deficit*), minus $\sqrt{2}$ of extra energy carried by that shell. Theorem 1 is the next order of the same bookkeeping. Stationarity of the ground state ($\eta = \varepsilon$ at every shell edge) also makes the prime-number-theorem error *at* a shell edge cancel between deficit and shell energy at first order. This is used in the explicit proof (term M_5 in Appendix A).

The shell structure also explains why σ and d behave differently. For $d(n)$ the second shell sits at $X^{\log(3/2)/\log 2}$, far above the RH scale $\sqrt{X}$, so the shells dominate the zeros (cf. [7]). For σ the second shell $\xi_2 \approx \sqrt{2\xi}$ sits exactly at the RH scale, so shells and zeros enter at the same order.

2. Structure of colossally abundant numbers

Since $F(\cdot,k)$ is decreasing and $\varepsilon = F(\xi,1)$ is decreasing in ξ, each $\xi_k(\xi)$ is increasing in ξ, and $\xi_{k+1} < \xi_k$. With $a_p = k$ for $\xi_{k+1} < p \leq \xi_k$,

$$\log N = \sum_{k\geq 1} \theta(\xi_k) = \theta(\xi) + R, \qquad \frac{\sigma(N)}{N} = \prod_{p\leq\xi} \frac{1}{1-1/p}\cdot e^\Lambda, \qquad \Lambda = \sum_{p\leq\xi} \log\big(1 - p^{-a_p-1}\big). \tag{4}$$

These are exact for every real ξ; no correction factor is needed.

Remark 6 (ties). At a critical value of ε, the maximizers of $\sigma(n)/n^{1+\varepsilon}$ are the numbers N' with $N(\xi^-) \mid N' \mid N(\xi)$. Write $\mu = \log(N(\xi)/N')$. Then $\log(\sigma/N)$ drops by exactly $\varepsilon\mu$ and $\log N$ by μ. Since $\varepsilon \log N(\xi)\, e^{\log(\sigma/N)-\gamma} = 1 + O(\xi^{-1/2}t)$, the first-order change of c_σ/e^γ cancels. One finds $|\Delta(c_\sigma/e^\gamma)| \le (t^2/(8\pi) + 3.5)\,\mu/\xi$ for $\mu \le \sqrt{\xi}$, and $\le 1.1\,\mu/\xi$ when $\xi \le 10^{19}$. By a result of Siegel quoted in [1, p. 455] (a case of the six exponentials theorem [3]), at most two primes share a critical value, so $\mu \le 2t$. The effect is at most $(t^3/(4\pi) + 7t)/\xi$, far below every constant stated here.

Lemma 7 (shells)**.** *For every $k \ge 2$ and real $\xi > 1$, $\xi^{1/k} \le \xi_k \le (k\xi)^{1/k}$. For every real $\xi \ge 10^9$,*

$$\xi_2 = \sqrt{2\xi}\Big(1 - \frac{\log 2}{2t} + \frac{v}{t^2}\Big) \qquad \textit{with} \qquad 0.47 \le v \le 0.55.$$

As $\xi \to \infty$, $v \to (\log 2 + \frac{3}{4}\log^2 2)/2 = 0.52674$, in agreement with the coefficient $a/2 + 3a^2/8$ ($a = \log 2$) in Nicolas's expansion [6, (4.27)]*. The true value at $\xi = 10^9$ is $v = 0.48105$. The crude bounds are* [6, (4.26)]*; we include the short proof for completeness.*

Proof. Crude bounds. Put $z = \xi^{1/k}$ and $S = z + \cdots + z^k \le k\xi$. Then $(1+1/S)^k \ge 1 + k/S \ge 1 + 1/\xi$, so $F(z,k) \ge \varepsilon$ and $\xi_k \ge z$. Now put $z = (k\xi)^{1/k}$, so $S \ge k\xi$. Then $F(z,k) \le k/(S(t + \log k)) \le 1/(\xi(t + \log k)) \le 1/((\xi + \frac{1}{2})t) \le \varepsilon$; the third inequality is $t/2 \le \xi \log k$. Hence $\xi_k \le z$.

Second shell. Write $z = \sqrt{2\xi}(1 + w)$ with $w = -\frac{\log 2}{2}s + vs^2$. Using $\log(1+y) \le y$ and $\log(1 + 1/\xi) \ge 1/(\xi + \frac{1}{2})$, a sufficient condition for $\xi_2 \le z$ is $(z + z^2)\log z \ge (\xi + \frac{1}{2})t$. With $\log(1+w) \ge w/(1+w)$ this follows from

$$P_{\mathrm{up}}(s) := (1+w)^2(1 + s\log 2) + 2ws(1+w) - 1 \;\ge\; \tfrac{1}{2}e^{-1/s}.$$

Using $\log(1+y) \ge y/(1 + y/2)$ and $\log(1 + 1/\xi) \le 1/\xi$, a sufficient condition for $\xi_2 \ge z$ is $(z^2 + z + \frac{1}{2})\log z \le \xi t$. With $\log(1+w) \le w$ this follows from

$$P_{\mathrm{lo}}(s) := 1 - (1+w)^2(1 + s\log 2 + 2ws) \;\ge\; \delta\,(1 + s\log 2 + 2ws),$$

where

$$\delta = \tfrac{1}{2}\big(\sqrt{2}(1+w)e^{-1/(2s)} + \tfrac{1}{2}e^{-1/s}\big).$$

Both P_{up} and P_{lo} are polynomials in s that vanish to second order at $s = 0$, with

$$P_{\mathrm{up}}/s^2 \to 2v - \log 2 - \tfrac{3}{4}\log^2 2 \qquad \text{and} \qquad P_{\mathrm{lo}}/s^2 \to -2v + \log 2 + \tfrac{3}{4}\log^2 2.$$

We checked the two inequalities after division by s^2, with $v = 0.55$ and $v = 0.47$ respectively, in ball arithmetic on 4000 cells covering $s \in (0, 1/\log 10^9]$. The right-hand sides divided by s^2 are increasing in s, so on each cell they were bounded by their value at the right endpoint. The minimal margins are 0.0465 and 0.0184. □

Remark 8. A previous draft claimed $v \ge 0.48$ with margin 0.0022. The value $v(10^9) = 0.48105$ shows that 0.48 is true. However, the sufficient inequality above has margin below $3 \cdot 10^{-5}$ at $\xi = 10^9$ when $v = 0.48$, so it does not certify that value. We therefore use 0.47. Because v cancels at leading order in $t^2\mathcal{E}$, this costs nothing visible.

3. Proof of Theorem 1

Write $U = \sqrt{\xi}\,t$, and put

$$u = -\log f(\xi), \quad f(x) = e^\gamma \log\theta(x) \prod_{p \le x}(1 - 1/p); \qquad A = -\Lambda.$$

By (4),

$$\frac{c_\sigma(N)}{e^\gamma} = \sqrt{\log N}\,\Big[\log\theta(\xi)\big(e^{u-A} - 1\big) - \log\Big(1 + \frac{R}{\theta(\xi)}\Big)\Big]. \tag{5}$$

The primorial piece.

Lemma 9. *Under RH,*

$$U\,u = 2 + W(\xi) + \frac{W_2(\xi) - 2}{t} + \tfrac{3}{2}\,\xi^{-1/6} + \frac{8 + \omega_u(\xi)}{t^2} + O(t^{-3}), \qquad |\omega_u| \le \frac{2\beta}{\gamma_1}.$$

Proof. Start from Stieltjes integration of $\sum_{p\le x} 1/p$ against θ and Mertens' identity $B = \gamma + \sum_p(\log(1-1/p) + 1/p)$. With $E(s) = \theta(s) - s$ and $w(s) = (1 + \log s)/(s^2 \log^2 s)$ this gives the exact identity

$$\log f(x) = K(x) + \mathrm{Br}(x) + T(x), \qquad K(x) = \int_x^\infty E(s)\, w(s)\, ds,$$

$$\mathrm{Br}(x) = \log\log\theta(x) - \log\log x - \frac{E(x)}{x\log x}, \qquad T(x) = -\sum_{p>x}\Big(\log\big(1 - \tfrac{1}{p}\big) + \tfrac{1}{p}\Big).$$

Under RH, $\mathrm{Br} = O(\log^3 x/x)$ and $0 < T \le 1/(2(x-1))$, both negligible.

Decompose

$$E(s) = (\psi(s) - s) - \sum_{k\ge 2}\theta(s^{1/k}), \qquad \psi(s) - s = -\sum_\rho \frac{s^\rho}{\rho} - \log 2\pi - \tfrac{1}{2}\log(1 - s^{-2}).$$

Note that $\int_x^\infty w = 1/(x\log x)$, so the constants contribute $-\log(2\pi)/(xt) + O(x^{-3})$.

Zeros. Integrate the zero sum termwise; this is justified as in [6, Lemma 3.1]. Integrating by parts twice,

$$\frac{1}{\rho}\int_x^\infty s^{\rho-2}\Big(\frac{1}{\log s} + \frac{1}{\log^2 s}\Big)ds = \frac{x^{\rho-1}}{\rho(1-\rho)t} - \frac{x^{\rho-1}}{(1-\rho)^2 t^2} + \frac{2}{(1-\rho)^2}\int_x^\infty \frac{s^{\rho-2}}{\log^3 s}\, ds.$$

One more integration by parts gives $\big|\int_x^\infty s^{\rho-2}\log^{-3} s\, ds\big| \le x^{-1/2}t^{-3}(1 + 6/t)/|1-\rho|$. Since $\sum|1-\rho|^{-3} \le \beta/\gamma_1$, the last terms contribute at most $2\beta(1+6/t)/(\gamma_1\sqrt{x}\,t^3)$ in absolute value. Summing over ρ, the zeros contribute

$$-\frac{W(x)}{\sqrt{x}\,t} - \frac{W_2(x)}{\sqrt{x}\,t^2} + r_z, \qquad |U r_z| \le \frac{2\beta(1+6/t)}{\gamma_1 t^2}$$

to K.

Prime powers. Put $J_b(x) = \int_x^\infty s^b w(s)\, ds$. The substitution $s = e^v$ gives

$$U J_b(x) = e^{-t(1/2-b)}\Big[1 + \frac{b}{1-b}\,Q\big((1-b)t\big)\Big], \qquad Q(z) = ze^z E_1(z). \tag{6}$$

Here $Q(z) = \sum_{k<n}(-1)^k k!\, z^{-k} + R_n$, where R_n lies between 0 and $(-1)^n n! z^{-n}$. For $b = \frac{1}{2}$ this gives $UJ_{1/2} = 1 + Q(t/2) = 2 - 2/t + 8/t^2 - 48/t^3 + \cdots$. That is the prime-square term $2 - 2/t$ of the lemma together with the $8/t^2$. The term $\theta(s^{1/3})$ gives $UJ_{1/3} = \frac{3}{2}\xi^{-1/6}(1 + O(1/t))$. The remaining prime-power terms and the error $\theta(y) - y$ in $\theta(s^{1/k})$ are $O(\xi^{-1/4}t^2)$.

Collecting terms and multiplying by $-U$ proves the lemma. □

The saturation deficit and the shell energy.

Lemma 10. *Write* $B = \sqrt{\log N}\,\log(1 + R/\theta(\xi))$. *Then*

$$U\,A = \sqrt{2} - \frac{\sqrt{2}\,(2 + \frac{1}{2}\log 2)}{t} + \frac{3^{1/3}}{2}\,\xi^{-1/6} + \frac{P_2(s)}{t^2} + O(\xi^{-1/4}t^2),$$

$$B = \sqrt{2} - \frac{\sqrt{2}\log 2}{2t} + 3^{1/3}\xi^{-1/6} + \frac{\sqrt{2}\,v}{t^2} + O(\xi^{-1/4}t^2),$$

where $P_2(0) = \sqrt{2}(8 + 4\log 2 + \frac{3}{4}\log^2 2 - v)$*, and each* $O(\xi^{-1/4}t^2)$ *is to be read as* $O(\xi^{-1/4}t^2 + \xi^{-1/6}t^{-1})$*. Both estimates use RH, through the bound* $E(y) = O(\sqrt{y}\log^2 y)$ *at* $y = \xi, \xi_2, \xi_3$ *and on* $(\xi_2, \xi]$*; unconditionally the error terms are only* $O(e^{-c\sqrt{t}})$ *relative to the main terms.*

Proof. Primes $\xi_2 < p \le \xi$ have $a_p = 1$ and lose $-\log(1 - p^{-2})$. Primes $\xi_3 < p \le \xi_2$ lose $-\log(1 - p^{-3})$. For $g_m(s) = s^{-m}/\log s$, Stieltjes integration gives the exact identity

$$\sum_{y<p\le z} p^{-m} = E_1\big((m-1)\log y\big) - E_1\big((m-1)\log z\big) + g_m(z)E(z) - g_m(y)E(y) + \int_y^z E(s)\,\big(-g_m'(s)\big)\,ds. \tag{7}$$

For $m = 2$, $y = \xi_2$, the main term is $E_1(\log \xi_2)$, and

$$UE_1(\log\xi_2) = \frac{\sqrt{2}\,Q(\log\xi_2)}{(1+w)D}, \qquad D = 1 + s\log 2 + 2s\log(1+w), \qquad \frac{1}{\log\xi_2} = \frac{2s}{D},$$

with w as in Lemma 7. Expanding in s gives the first two terms and P_2; the exact cancellations are verified symbolically. For B write $\sqrt{\log N} = \sqrt{\xi}\,(1 + O(\xi^{-1/2}))$ and $R = \xi_2 + \theta(\xi_3) + O(\xi^{1/4}) + E(\xi_2)$. Then use $\xi_2/\sqrt{\xi} = \sqrt{2}(1+w)$. The cube terms come from $UE_1(2\log\xi_3)$ and $\xi_3/\sqrt{\xi}$, with $\xi_3 = (3\xi)^{1/3}(1 + O(1/t))$. The boundary terms in $E(\xi_2)$ cancel between UA and B at first order (stationarity). The remaining errors are $O(\xi^{-1/4}t^2)$, plus $O(\xi^{-1/6}/t)$ from $\nu_3 = \xi_3/(3\xi)^{1/3} = 1 - \log 3/(3t) + O(t^{-2})$. □

Assembly. By Lemmas 9 and 10, $u - A = O(1/U)$, so $e^{u-A} - 1 = (u - A) + O(U^{-2})$. Under RH,

$$\sqrt{\log N}\,\log\theta(\xi) = U\big(1 + O(t^2\xi^{-1/2})\big).$$

Substituting into (5),

$$\frac{c_\sigma(N)}{e^\gamma} = 2 + W + \frac{W_2 - 2}{t} - \Big[\sqrt{2} - \frac{\sqrt{2}(2 + \frac{1}{2}\log 2)}{t}\Big] - \Big[\sqrt{2} - \frac{\sqrt{2}\log 2}{2t}\Big] + \frac{8 + \omega_u - P_2(0) - \sqrt{2}v}{t^2} + O(t^{-3}),$$

where the three $\xi^{-1/6}$ contributions, which total $\frac{3}{2}(1 - 3^{1/3})\xi^{-1/6}$, are $o(t^{-3})$. The t^{-1} coefficient is κ, since

$$-2 + \sqrt{2}\big(2 + \tfrac{1}{2}\log 2\big) + \tfrac{1}{2}\sqrt{2}\log 2 = \kappa,$$

and the t^{-2} coefficient is $8 - \sqrt{2}(8 + 4\log 2 + \frac{3}{4}\log^2 2) + \omega_u = c_0 + \omega$, with v cancelling. This proves the first formula of Theorem 1 and its refinement.

For the second formula, note that $\lambda = \log\log N = t + O(\xi^{-1/2}t^2)$ and $\log N/\xi = 1 + O(\xi^{-1/2}t^2)$. Write $\delta = |\log\log N - t|$. Then

$$|W(\log N) - W(\xi)| \;\le\; \sum_\rho \frac{\min(2,\ |\gamma_\rho|\,\delta)}{|\rho|^2} = O\big(\delta\log(1/\delta)\big) = O\big(\xi^{-1/2}t^3\big),$$

splitting the sum at $|\gamma_\rho| = 1/\delta$; similarly for W_2. Finally divide by $\sqrt{\log N}$. □

4. Explicit bounds, and the proofs of the corollaries

4.1. **Inputs.** Write $E(y) = \theta(y) - y$ and $Y = 10^{19}$. We use:

- Büthe [2, Thm. 2, (1.6), (1.7)]: $0.05\sqrt{y} < y - \theta(y) \le 1.95\sqrt{y}$ for $1423 \le y \le 10^{19}$, and $y - \theta(y) > 0$ for $1 \le y \le 10^{19}$. These bounds are unconditional.
- A direct computation over the primes below 1423, in the ancillary file `cconst.py`, gives $\sup_{0<y\le 1423}(y - \theta(y))/\sqrt{y} = 2.05282$, attained as $y \to 1423^-$. Hence

$$-C\sqrt{y} \le E(y) < 0 \qquad (0 < y \le 10^{19}), \qquad C = 2.0529.$$

- Schoenfeld's RH bound $|E(y)| \le \frac{1}{8\pi}\sqrt{y}\log^2 y$ for $y \ge 599$ [10]. Consequently $\theta(y) \le (1 + 10^{-7})y$ for all $y > 0$.
- Lemma 7, the crude shell bounds, and certified roots for $\xi_3, \dots, \xi_6$ at cell endpoints (Lemma 11).
- $\sum_\rho |\rho|^{-2} = \beta$ and $|\rho| \ge \gamma_1 > 14.1347$.

Nicolas [6, (2.2)] quotes Büthe's lower bound as $\theta(x) > x - 1.94\sqrt{x}$ for $1427 < x \le 10^{19}$, while the arXiv version of [2, Thm. 2] states $1.95\sqrt{x}$ from $x \ge 1423$. Our argument uses only $C = 2.0529$, which dominates both forms: the supremum of $(y - \theta(y))/\sqrt{y}$ over $(0, 1427]$, computed directly, is 2.0528, attained just below 1423.

Lemma 11 (certified shell roots)**.** *Since $\xi_k(\xi)$ is increasing in ξ, on a cell $\xi \in [e^{t_a}, e^{t_b}]$ we have $\xi_k \in [z^-, z^+]$ whenever $F(z^-, k) \ge F(e^{t_a}, 1)$ and $F(z^+, k) \le F(e^{t_b}, 1)$. These two inequalities are checked in ball arithmetic for $k = 3, \dots, 6$ at every cell endpoint. For $k \ge 7$ the crude bounds of Lemma 7 are used.*

4.2. **The explicit theorem.** Theorem 2 follows from the exact decomposition (8) and the enclosures of Appendix A, evaluated as described in Appendix B. The constants are the extremes over all cells:

range of ξ	$t^2\mathcal{E} \in$	$t\big(c_\sigma/e^\gamma - (2 - 2\sqrt{2} + W)\big) \in$
$\xi \ge 10^9$	$[-21.28,\ 6.18]$	$[0.301,\ 1.855)$
$\xi \ge 10^{10}$	$[-15.24,\ 1.39]$	$[0.772,\ 1.855)$
$\xi \ge 10^{12}$	$[-9.72,\ -3.37]$	$[1.228,\ 1.855)$
$\xi \ge 10^{15}$	$[-7.87,\ -5.74]$	$[1.474,\ 1.855)$
$\xi \ge 10^{20}$	$[-7.87,\ -6.64]$	$[1.595,\ 1.855)$
$\xi \ge 10^{50}$	$[-7.87,\ -7.23]$	$[1.698,\ 1.855)$
$\xi \ge 10^{100}$	$[-7.87,\ -7.42]$	$[1.729,\ 1.855)$
$t \ge 300$	$[-7.87,\ -7.46]$	$[1.736,\ 1.855)$
$t \to \infty$	$c_0 \pm 0.0066 = [-7.751,\ -7.737]$	$\to [\kappa - \beta, \kappa + \beta]$

The weaker constants of the previous draft, $[-58.6, 17.0]$ for $t^2\mathcal{E}$ and $[-1.50, 2.24]$ in (3), are therefore also proved.

4.3. **Proof of Corollary 4.** *(1)* By Theorem 1 the difference $c_\sigma/e^\gamma - (2 - 2\sqrt{2} + W)$ equals $(\kappa + W_2)/t + O(t^{-2}) \ge (\kappa - \beta)/t + O(t^{-2})$, which is positive for large ξ. The explicit threshold is the left end of the last cell on which the certified lower bound $(\kappa - \beta)/t + \frac{3}{2}(1 - 3^{1/3})\xi^{-1/6} + \min_{\text{cell}} \mathcal{E}$ is ≤ 0. Beyond it, the bound is positive on every cell up to $t = 300$, and it is positive for $t \ge 300$ by the tail window, since $\kappa - \beta - 7.87/300 > 0$.

(2) At CA numbers with $\xi \ge 10^9$, Theorem 2 with $W, W_2 \le \beta$ gives, on every cell,

$$c_\sigma/e^\gamma \le 2 - 2\sqrt{2} + \beta + \frac{\kappa + \beta}{t} + \tfrac{3}{2}(1 - 3^{1/3})\xi^{-1/6} + \max_{\text{cell}} \mathcal{E} \le -0.699.$$

The maximum over all cells of the middle expression is -0.69933. Since $t \mapsto e^\gamma(\log t - a/\sqrt{t})$ is increasing and concave, Nicolas's interpolation lemma [6, Lemma 6.1] extends $\alpha \geq 0.699$ from consecutive CA numbers to every n between them.

(3) The leading term in Theorem 1 (Robin, Nicolas) gives $c_\sigma/e^\gamma = 2-2\sqrt{2}+W(\xi)+o(1)$. Every prime is the parameter ξ of some CA number, and W varies by $o(1)$ between consecutive primes. Hence the lim inf equals $e^\gamma(2-2\sqrt{2}+\liminf W)$. Then use $-\beta \leq \liminf W \leq -0.00499$ [5]. □

4.4. **Proof of Corollary 5.** Let $a = v_2(N)$, $L = \log N$, $L' = \log M = L - a\log 2$, and $X = \sigma(N)/(Ne^\gamma) = \log L + c_\sigma/(e^\gamma\sqrt{L})$. Since $\sigma(M)/M = (\sigma(N)/N)/(2(1-2^{-a-1}))$,

$$\frac{c_{\mathrm{odd}}(M)}{e^\gamma/2} - \frac{c_\sigma(N)}{e^\gamma} = \frac{c_\sigma}{e^\gamma}\Big(\sqrt{\tfrac{L'}{L}} - 1\Big) + \sqrt{L'}\,\log\frac{L}{L'} + X\sqrt{L'}\,\frac{2^{-a-1}}{1-2^{-a-1}}.$$

All three terms are positive, because $c_\sigma < 0$; this proves the left inequality. A previous draft bounded the third term by λ/ξ, which is wrong: that term is of size $(0.69\text{–}1.39)/\sqrt{\xi}$.

For the right inequality, write $2^a = \kappa_a \xi t$. From $\xi_a \geq 2$, i.e. $F(2,a) \geq \varepsilon$, together with $\log(1+y) \leq y$ and $\varepsilon \geq 1/((\xi+\frac{1}{2})t)$, we get $\kappa_a \leq (1+\xi^{-1})/(2\log 2)$. From $\xi_{a+1} < 2$, together with $\log(1+y) \geq y/(1+y/2)$ and $\varepsilon \leq 1/(\xi t)$, we get $\kappa_a > 1/(4\log 2)$. Then:

- the second term is $\leq a\log 2/(\sqrt{L}(1 - a\log 2/L))$;
- the first term is $\leq 0.9\, a\log 2/L$, using $|c_\sigma/e^\gamma| \leq 0.9$ and $1-\sqrt{1-y} \leq y$;
- the third term is $\leq \log L\,\sqrt{L}/(2\kappa_a\xi t)\,(1+2^{-a})$.

Now use $a\log 2 = t + \log t + \log\kappa_a$, $L/\xi \in [1-2.06\,\xi^{-1/2},\ 1+1.5\,\xi^{-1/2}]$ (from C and $R \leq 1.42\sqrt{\xi}$), and $|\log L - t| \leq 2\xi^{-1/2}$. At $\xi = 10^9$ these corrections total $\leq 1.5\cdot 10^{-3}$, they decrease with ξ, and the factor $(1+1/\xi)$ in κ_a adds $< 10^{-8}$. We obtain

$$\sqrt{\xi}\Big(\frac{c_{\mathrm{odd}}}{e^\gamma/2} - \frac{c_\sigma}{e^\gamma}\Big) \leq t + \log t + \max_{\kappa\in[1/(4\log 2),\,1/(2\log 2)]}\Big(\log\kappa + \frac{1}{2\kappa}\Big) + 0.003.$$

The function $\log\kappa + 1/(2\kappa)$ is convex, and it takes the same value $\log 2 - \log(2\log 2) = 0.36651$ at both endpoints. This gives the stated bound. □

5. Numerical verification

We ran a segmented sieve up to 10^{10}. Accumulators were held in binary128, and the sieve outputs θ, $\sum\log(1-1/p)$ and $\sum\log(1-p^{-2})$ at 401 log-spaced points. It reproduces $\pi(10^{10}) = 455\,052\,511$ and $\theta(10^{10}) = 9\,999\,939\,830.66$. At each point ξ we built $N(\xi)$ exactly from the shell rule. W and W_2 were summed over the first 1942 zeros. The truncation error of each is at most $\tau = \beta - \sum_{n\leq 1942} 2/(\frac{1}{4}+\gamma_n^2) \leq 9.1\cdot 10^{-4}$; this uses only that the list of zeros is complete.

ξ	$t^2\mathcal{E}$ (exact)	enclosure	$\sum U_i$ (exact)	enclosure	$\sum M_i$ (exact)	enclosure
1.00×10^9	-6.579	$[-21.26,\ 6.16]$	6.698	$[2.44,\ 13.29]$	-13.280	$[-23.69,\ -7.14]$
3.16×10^9	-6.459	$[-17.82,\ 3.48]$	6.724	$[3.21,\ 11.74]$	-13.184	$[-21.03,\ -8.27]$
1.00×10^{10}	-6.526	$[-15.23,\ 1.37]$	6.579	$[3.84,\ 10.55]$	-13.106	$[-19.06,\ -9.18]$

At all 101 checkpoints each exact value lies inside its enclosure; the exact $t^2\mathcal{E}$ ranges over $[-6.71, -6.44]$. The exact values are near the centre of the enclosures; the width at 10^9 comes from the unconditional range $-C\sqrt{y} \leq E(y) < 0$ at $y \approx \xi_2$ and $y \approx \xi_4$ (terms U_3, U_5, M_2, M_6, M_7). Using the explicit formula for E inside these integrals, as is done for K, would shrink the window further. For odd ground states the offset $\sqrt{\xi}\,(c_{\mathrm{odd}}/(e^\gamma/2) - c_\sigma/e^\gamma) - (t+\log t)$ has maximum 0.3655 over the checkpoints, against the proved 0.37.

6. Remarks

(1) The same method applies to Ramanujan's σ_{-s}, $0 < s < 1$, which Nicolas raises in [6, §7]. Only the efficiencies η and the shell positions change.

(2) In the ground-state picture, the RH-sensitive part of Robin's inequality is a finite-size correction. Every zero contributes a mode damped like $e^{-(1-\Re\rho)\log\xi}$. Under RH the non-oscillating amplitude $2\sqrt{2}-2$ exceeds the whole zero sum β by a factor of about 18, and Theorem 1 shows that the next order adds the positive amount $(\kappa \pm \beta)/\log\xi$. At the order after that, the zeros contribute less than $0.0066/\log^2\xi$ against the constant $c_0 = -7.744$. In this sense the RH-sensitive information sits in the damping exponent rather than in these amplitudes; this is an interpretation, not a theorem.

Appendix A. The explicit enclosures

Throughout, $\xi \geq 10^9$ is real and $t = \log\xi$, $s = 1/t$, $U = \sqrt{\xi}\,t$. Let $E(y) = \theta(y) - y$. For a ball y, $E(y) \in [-\eta_L(y)\sqrt{y},\ \eta_U(y)\sqrt{y}]$ with $(\eta_L, \eta_U) = (C, 0)$ if $y \leq Y$ and $(\mathcal{S}, \mathcal{S})$ if $y > Y$, where $\mathcal{S}(y) = \log^2 y/(8\pi)$. Also $w(s) = (1+\log s)/(s^2\log^2 s)$, $Q(z) = ze^z E_1(z)$, and J_b is as in (6). Put

$$\mathrm{Sch}_{b,k}(X_0) = \int_{X_0}^{\infty} s^b \frac{(\log s/k)^2}{8\pi} w(s)\,ds = \frac{X_0^{b-1}}{8\pi k^2}\Big[\frac{\log X_0}{1-b} + \frac{1}{(1-b)^2} + \frac{1}{1-b}\Big].$$

This bounds the contribution of Schoenfeld's range $s^{1/k} > Y$; it is used with $X_0 = \max(\xi, Y^k)$.

Exact decomposition. Let $\xi_2 = \sqrt{2\xi}(1+w)$ with $w = -\frac{\log 2}{2}s + vs^2$ (Lemma 7). Let $\nu_3 = \xi_3/(3\xi)^{1/3}$, $L_k = \log\xi_k$, $R_4 = \sum_{k\geq 4}\theta(\xi_k)$, $R_0 = \xi_2 + \xi_3 + R_4$, $E_2 = E(\xi_2)$, $E_3 = E(\xi_3)$, and $g_m(s) = s^{-m}/\log s$. With u, A, R as in (5), write $1 + d = \sqrt{\log N}\log\theta(\xi)/U$ and $Y_* = W + W_2/t + UG - UA$, where $UG := Uu - W - W_2/t$. Put $y_* = Y_*/U$ and $q = e^{y_*} - 1 - y_*$. Then (5) is the identity

$$\frac{c_\sigma}{e^\gamma} = (1+d)\,Y_* + U(1+d)\,q - B, \qquad B = \sqrt{\log N}\log\big(1 + R/\theta(\xi)\big),$$

and

$$t^2\mathcal{E} = \sum_{i=1}^{9} U_i + \sum_{i=1}^{7} M_i + A_1 + A_2. \tag{8}$$

The terms are listed below, each with its enclosure; all are exact identities or inequalities, and κ_n denotes an unknown number in $[0,1]$.

Primorial piece ($t^2(UG - 2 + 2s - \frac{3}{2}\xi^{-1/6}) = \sum U_i$).

$U_1 = t^2\big(Q(t/2) - 1 + 2s\big) = \sum_{k=2}^{7}(-1)^k k!\,2^k s^{k-2} + \kappa_8\,8!\,2^8 s^6$, a polynomial in s.

$U_2 = \frac{1}{2}t^2 e^{-t/6}\big(Q(2t/3) - 1\big)$, with Q given by six terms of its enveloping series.

$U_3 = t^2U\int_\xi^\infty E(\sqrt{s})w \in \big[-Ct^2UJ_{1/4} - t^2U\mathrm{Sch}_{1/4,2},\ t^2U\mathrm{Sch}_{1/4,2}\big]$; the C-part is present only if $\xi < Y^2$.

U_4 is the same with $s^{1/3}$, $J_{1/6}$, $\mathrm{Sch}_{1/6,3}$.

$U_5 = t^2U\int_\xi^\infty \sum_{k\geq 4}\theta(s^{1/k})w$. The upper bound is $\sum_{k=4}^{M}(UJ_{1/k} + U\mathrm{Sch}_{1/(2k),k})$ plus the tail $U(1{+}10^{-7})(1{+}1/\ell_0)e^{(b-1)\ell_0}/((1{-}b)\log 2)$. Here $M = \max(60, \lceil 2t/\log 2\rceil)$, $b = 1/(M{+}1)$, $\ell_0 = (M+1)\log 2$, and the tail uses that $\theta(s^{1/k}) = 0$ unless $s \geq 2^k$. The lower bound is $\max\big(0, \sum_{k=4}^{14}(UJ_{1/k} - CUJ_{1/(2k)} - U\mathrm{Sch}_{1/(2k),k})\big)$.

$U_6 = -t^2Ur_z \in [-1,1]\cdot 2\beta(1+6s)/\gamma_1$.

$U_7 = -t^2UK_{\mathrm{const}} \in t^2\big[\log(2\pi)e^{-t/2} - e^{-5t/2},\ \log(2\pi)e^{-t/2}\big]$.

$U_8 = -t^2 U\,\mathrm{Br} \in \big[0,\ t^2U(2a^2/t + 8a^2/t^2)\big]$, with $a \ge |E(\xi)|/\xi$. Here $h(e) = \log(1+\log(1+e)/t) - e/t$ is concave with maximum $h(0) = 0$. For $|e| \le a \le \frac12$ with $2a/t \le \frac12$, the inequalities $\log(1+y) \ge y - y^2/(1+y)$ $(-1 < y \le 0)$, $\log(1+y) \ge y - y^2/2$ $(y \ge 0)$ and $|\log(1+e)| \le a/(1-a)$ give $h(e) \ge -2a^2/t - 8a^2/t^2$. At $\xi \ge 10^9$, $a \le 7\cdot 10^{-5}$.

$U_9 = -t^2 UT \in \big[-t^2 \cdot \frac12(1+\frac{1}{\xi-1})(1+10^{-7})e^{-t/2}(2+s),\ 0\big]$.

Deficit and shell energy $(-t^2[UA - \sqrt2 + \sqrt2(2+\frac12\log 2)s - \frac{3^{1/3}}{2}\xi^{-1/6}] - t^2[B - \sqrt2 + \frac{\sqrt2\log 2}{2}s - 3^{1/3}\xi^{-1/6}] = \sum M_i)$.

$M_1 = -P_2(s) - \sqrt2 v$, where $P_2(s) = t^2\big(\sqrt2 Q(L_2)/((1+w)D) - \sqrt2 + \sqrt2(2+\frac12\log 2)s\big)$. Here $Q(L_2)$ is given by eight terms of its series in $1/L_2 = 2s/D$, and $\log(1+w) = w + \mu s^2$ with $\mu \in [-(\frac{\log 2}{2} - vs)^2/(2(1+w)^2),\ -(\frac{\log 2}{2} - vs)^2/2]$. The numerator of P_2 vanishes to order s^2 (verified symbolically), and M_1 is evaluated as an explicit rational function of (s, v, μ, κ_8).

$M_2 = t^2\Big\{\frac{3^{1/3}}{2}e^{-t/6}\big[1 - Q(2L_3)/(\nu_3^2 D_3)\big] - 3^{1/3}e^{-t/6}(\nu_3\Psi - 1) - \xi^{-1/2}R_4\Psi - \sqrt2(1+w)(\Psi - 1)\Big\}$. Here $D_3 = 1 + s\log 3 + 3s\log\nu_3$, $\Psi = \sqrt{1+e+r_0}\,\varphi(r_0/(1+e))/(1+e)$, $r_0 = R_0/\xi$, $e = E(\xi)/\xi$, and $\varphi(q) = \log(1+q)/q \in [1 - q/2, 1 - q/2 + q^2/3]$.

$M_3 = t^2U\big(E_1(t) + E_1(2L_2)\big)$.

$M_4 = -t^2 U g_2(\xi)E(\xi)$.

$M_5 = t^2E_2\big(Ug_2(\xi_2) - Ug_3(\xi_2) - B'(R_*)\big)$
$\quad + t^2E_3\big(Ug_3(\xi_3) - B'(R_*)\big)$. Here $B'(R) = (1 + \frac12\log(1 + R/\theta))/\sqrt{\theta + R}$ and $R_* \in R_0 + [E_2 + E_3]$; this is the mean-value form of B in R. The two coefficients are $O(s^2\xi^{-1/2})$ (stationarity).

$M_6 = -t^2U\big[\int_{\xi_2}^{\xi} E(-g_2') + \int_{\xi_3}^{\xi_2} E(-g_3')\big]$. These are bounded with $\int_y^z \sqrt{s}(-g_m')$ and $\int_y^z \sqrt{s}\log^2 s\,(-g_m')$, both in closed form via E_1.

$M_7 = -t^2U(A_{2x} + A_{3x} + A_{4+})$, where:

- $A_{2x} \le \sum_{p>\xi_2} p^{-4}/(1-\xi_2^{-2})$ and $A_{3x} \le \sum_{p>\xi_3} p^{-6}/(1-\xi_3^{-3})$, with $\sum_{p>y} p^{-m} \le (1+10^{-7})y^{1-m}\big(\frac{m}{(m-1)\log y} + \frac{1}{(m-1)\log^2 y}\big)$;
- A_{4+} consists of the prime sums (7) over $(\xi_{k+1}, \xi_k]$ with exponent $k+1$, for $k = 3, \dots, 7$; their upper bounds are multiplied by $1/(1-\xi_{k+1}^{-(k+1)})$, using $-\log(1-y) \le y/(1-y)$. To these are added the primes $p \le \xi_8$;
- for those small primes, stationarity ($p > \xi_{a_p+1}$, i.e. $F(p, a_p+1) < \varepsilon$) and $-\log(1 - p^{-a-1}) \le \frac{p}{p-1}F(p, a+1)\log p \cdot (1-p^{-a-1})^{-1}$ give loss $\le \frac{64}{63}\,\varepsilon\, p\log p/(p-1)$. Since $\sum_{p\le x}\log p/(p-1) < \log x + 0.76$, their total is $\le \frac{64}{63}\varepsilon(\theta(\xi_8) + \log\xi_8 + 0.76)$. The factor $\frac{64}{63}$ is conservative.

Assembly.

$A_1 = t^2 dY_*$, with $1 + d = \sqrt{1+e+R/\xi}\,(1 + \log(1+e)/t)$ and $|W|, |W_2| \le \beta$ inside Y_*.

$A_2 = t^2U(1+d)q \in \big[0,\ t^2U(1+d)\,y_*^2 e^{|y_*|}/2\big]$.

Appendix B. Verification

(1) `symbolic.py` (sympy, exact arithmetic) checks the following, and exports U_1, P_2 and the polynomials of Lemma 7 with exact coefficients in $\mathbb{Q}(\log 2, \sqrt2)$:

- the numerator of P_2 vanishes at orders s^0 and s^1;
- $M_1(0) = -\sqrt2(8 + 4\log 2 + \frac34\log^2 2)$, independently of v;
- $U_1(0) = 8$.

(2) `lemma_shell2.py` proves Lemma 7; `cconst.py` computes C.
(3) `engine.py` (python-flint/Arb, 160-bit balls) evaluates (8) on a closed cell $t \in [t_a, t_b]$. Every function is applied to balls, so the result encloses all values on the cell. The cell widths Δt grow from $4 \cdot 10^{-4}$ at $t = \log 10^9$ to 0.05; `cover.py` covers $[\log 10^9, 300]$ with 30 798 cells.
(4) `tail2.py` evaluates $U_1 + M_1 + U_6$ on 200 subintervals covering $s \in [0, 1/300]$, giving $[-7.865, -7.469]$. For $t \geq 300$ we have $\xi > Y^6$, so only Schoenfeld's bound and the crude shell bounds $\xi^{1/k} \leq \xi_k \leq (k\xi)^{1/k}$ are needed. From the formulas of Appendix A these give:
   - $|U_2| \leq \frac{3}{4} t e^{-t/6}$;
   - $|U_3|, |U_4| \leq t^4 e^{-t/4}/50$;
   - $|U_5| \leq t^6 e^{-t/4}$;
   - $|U_7| + |U_8| + |U_9| + |M_3| + |M_4| + |A_1| + |A_2| \leq t^6 e^{-t/2}$;
   - $|M_2| \leq 4t^2 e^{-t/6} + 3t^3 e^{-t/4} + t^4 e^{-t/2}$, using $\nu_3 \in [3^{-1/3}, 1]$, $D_3 \geq 1$, $Q \leq 1$ and $R_4 \leq 2t(4\xi)^{1/4}$;
   - $|M_5| + |M_6| + |M_7| \leq 3t^4 e^{-t/4}$.

   These sum to at most $5t^2 e^{-t/6} + 10t^6 e^{-t/4}$, which is decreasing for $t \geq 24$ and $< 10^{-15}$ at $t = 300$. As a consistency check, `tail.py` evaluates the engine on point cells at $t = 300, 600, \ldots, 4800$; it finds sums $\leq 10^{-19}$, at the level of rounding.
(5) `validate.py` compares every group of terms with exact values from the sieve, and `oddcheck.py` checks Corollary 5.
(6) The covering was run with a frozen `engine.py` (SHA-256 `5f56e4db...f371d53f`). An independent check by a separate AI instance, working only from this appendix and the code, re-derived the decomposition (8) by hand. The referee checked it numerically to 10^{-52} at 11 sieve checkpoints, checked each enclosure term by term against exact values, and compared `engine.py` with this appendix line by line; the corrections it raised are incorporated in this version. This is not a substitute for human refereeing.

Data and code. All files named above, together with the sieve (`sieve_build.py`, which writes and compiles the C source), a file list with reproduction steps (`manifest.yaml`), the per-cell output (`cells.csv`, one row per cell with its t-interval and enclosures, rounded outward) and the validation output, are included as ancillary files (directory `anc/`).

Use of AI. This paper was produced with substantial assistance from Claude, an AI model by Anthropic. Claude drafted the text, derived the explicit enclosures, wrote and ran the verification code (the sieve, the zero computation, the interval-arithmetic covering and the symbolic checks), and carried out the literature checks. An independent check of Appendix A and of `engine.py` was performed by a separate instance of the same model working only from the written appendix and the code; its findings are incorporated. No human referee has checked the proofs. The contributor takes responsibility for the submission. All code, the per-cell output and the validation logs are in the ancillary files, so that every computational claim can be re-run.

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