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AN ARITHMETIC EQUIVALENCE OF THE RIEMANN HYPOTHESIS

MARC DELÉGLISE✉ and JEAN-LOUIS NICOLAS

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Abstract

Let $h(n)$ denote the largest product of distinct primes whose sum does not exceed n. The main result of this paper is that the property for all $n \geq 1$, we have $\log h(n) < \sqrt{\mathrm{li}^{-1}(n)}$ (where li^{-1} denotes the inverse function of the logarithmic integral) is equivalent to the Riemann hypothesis.

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1. Introduction

If $n \geq 1$ is an integer, let us define $h(n)$ as the greatest product of a family of primes $q_1 < q_2 < \cdots < q_j$ the sum of which does not exceed n. Let ℓ be the additive function such that $\ell(p^\alpha) = p^\alpha$ for p prime and $\alpha \geq 1$. In other words, if the standard factorization of M into primes is $M = q_1^{\alpha_1} q_2^{\alpha_2} \cdots q_j^{\alpha_j}$ we have $\ell(M) = q_1^{\alpha_1} + q_2^{\alpha_2} + \cdots + q_j^{\alpha_j}$ and $\ell(1) = 0$. If μ denotes the Möbius function, $h(n)$ can also be defined by

$$h(n) = \max_{\substack{\ell(M) \leq n \\ \mu(M) \neq 0}} M. \tag{1.1}$$

The above equality implies $h(1) = 1$. Note that

$$\ell(h(n)) \leq n.$$

Landau [16, pages 222–229] introduced the function $g(n)$ as the maximal order of an element in the symmetric group $\mathfrak{S}_n$; he proved that

$$g(n) = \max_{\ell(M) \leq n} M. \tag{1.2}$$

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From (1.1) and (1.2), it follows that

$$h(n) \le g(n), \quad n \ge 1.$$

The sequences $(h(n))_{n\ge 1}$ and $(g(n))_{n\ge 1}$ are sequences A159685 and A000793 in the *On-line Encyclopedia of Integer Sequences*. One can find results about $h(n)$ in [7, 8] and about $g(n)$ in [6, 9, 18, 19]. In the introductions to [6, 9] other references are given. A fast algorithm to compute $h(n)$ and $g(n)$ is described in [7, Section 8] and [9], while in [8, (4.13)] it is proved that

$$\log h(n) \le \log g(n) \le \log h(n) + 5.68(n \log n)^{1/4}, \quad n \ge 1. \tag{1.3}$$

Let li denote the logarithmic integral and li^{-1} its inverse function (see Section 2.2). In [18, Theorem 1(iv)] it is stated that, under the Riemann hypothesis, the inequality

$$\log g(n) < \sqrt{\mathrm{li}^{-1}(n)}$$

holds for n large enough. It is also proved (see [18, Theorem 1(i) and (ii)]) that under the Riemann hypothesis we have

$$\log g(n) = \sqrt{\mathrm{li}^{-1}(n)} + O((n \log n)^{1/4}), \tag{1.4}$$

while if the Riemann hypothesis is not true, there exists $\xi > 0$ such that

$$\log g(n) = \sqrt{\mathrm{li}^{-1}(n)} + (n \log n)^{1/4}\, \Omega_{\pm}((n \log n)^{\xi}). \tag{1.5}$$

With (1.3), (1.4) implies

$$\log h(n) = \sqrt{\mathrm{li}^{-1}(n)} + O((n \log n)^{1/4}), \tag{1.6}$$

while (1.5) yields

$$\log h(n) = \sqrt{\mathrm{li}^{-1}(n)} + (n \log n)^{1/4}\, \Omega_{\pm}((n \log n)^{\xi}). \tag{1.7}$$

From the expansion of $\mathrm{li}(x)$ given below in (2.6), the asymptotic expansion of $\sqrt{\mathrm{li}^{-1}(n)}$ can be obtained by classical methods in asymptotic theory. A nicer method is given in [23]. From (1.4) and (1.6), it turns out that the asymptotic expansions of $\log g(n)$ and $\log h(n)$ do coincide with that of $\sqrt{\mathrm{li}^{-1}(n)}$ (see [18, Corollaire, page 225]):

$$\left.\begin{matrix} \log h(n) \\ \log g(n) \\ \sqrt{\mathrm{li}^{-1}(n)} \end{matrix}\right\} = \sqrt{n \log n}\left(1 + \frac{\log\log n - 1}{2\log n} - \frac{(\log\log n)^2 - 6\log\log n + 9 + o(1)}{8\log^2 n}\right). \tag{1.8}$$

Let us introduce the sequence (b_n) defined by

$$\log h(n) = \sqrt{\mathrm{li}^{-1}(n)} - b_n (n \log n)^{1/4}, \quad \text{i.e. } b_n = \frac{\sqrt{\mathrm{li}^{-1}(n)} - \log h(n)}{(n \log n)^{1/4}}, \quad n \geq 2, \tag{1.9}$$

and the constant

$$c = \sum_{\rho} \frac{1}{|\rho(\rho+1)|} = 0.046\,117\,644\,421\,509\ldots \tag{1.10}$$

where ρ runs over the nontrivial roots of the Riemann ζ function. The computation of the above numerical value is explained below in Section 2.4.2.

The aim of this paper is to make more precise the estimate (1.6) and to prove

Theorem 1.1. *Under the Riemann hypothesis, we have the following.*

(i) $\log h(n) < \sqrt{\mathrm{li}^{-1}(n)}$ *for* $n \geq 1$.

(ii) $b_{17} = 0.497\,95 \cdots \leq b_n \leq b_{1137} = 1.044\,14\ldots$ *for* $n \geq 2$.

(iii) $b_n \geq \frac{2}{3} - c - (0.22\ \log\log n/\log n)$ *for* $n \geq 18$.

(iv) $b_n \leq \frac{2}{3} + c + (0.77\ \log\log n/\log n)$ *for* $n \geq 157\,933\,210$.

(v) $\frac{2}{3} - c = 0.620 \cdots \leq \liminf b_n \leq \limsup b_n \leq \frac{2}{3} + c = 0.712\ldots.$

(vi) *For n tending to infinity,*

$$\Big(\frac{2}{3} - c\Big)\Big(1 + \frac{\log\log n + O(1)}{4\log n}\Big) \leq b_n \leq \Big(\frac{2}{3} + c\Big)\Big(1 + \frac{\log\log n + O(1)}{4\log n}\Big).$$

Under the Riemann hypothesis, Theorem 1.1(iv) shows that, for n large enough, $b_n > 2/3 - c$. We prove (see (5.43) below) that $b_n > 2/3 - c$ holds for $78 \leq n \leq \pi_1(10^{10}) = \sum_{p \leq 10^{10}} p$, and it is reasonnable to think that it holds for all $n \geq 78$. In (iii), we have tried to replace the constant -0.22 by a positive one, but without success.

Corollary 1.2. *Each of the six statements of Theorem 1.1 is equivalent to the Riemann hypothesis.*

Proof. If the Riemann hypothesis fails, (1.7) and (1.9) contradict each statement of Theorem 1.1. □

Corollary 1.3. *Under the Riemann hypothesis,*

$$n \geq 2 \quad \Longrightarrow \quad \sqrt{\mathrm{li}^{-1}(n)} - 1.045(n\log n)^{1/4} \leq \log g(n) \leq \sqrt{\mathrm{li}^{-1}(n)} + 5.19\,(n \log n)^{1/4} \tag{1.11}$$

and (1.11) is equivalent to the Riemann hypothesis.

Proof. From (1.9) and Theorem 1.1(ii), for $n \geq 2$,

$$\sqrt{\mathrm{li}^{-1}(n)} - 1.045(n\log n)^{1/4} \leq \log h(n) \leq \sqrt{\mathrm{li}^{-1}(n)} - 0.49\,(n\log n)^{1/4}$$

which, with (1.3), proves (1.11). If the Riemann hypothesis is not true, (1.5) contradicts (1.11). □

1.1. Notation.

- $\pi_r(x) = \sum_{p \le x} p^r$. For $r = 0$, $\pi_0(x) = \pi(x) = \sum_{p \le x} 1$ is the prime counting function.
- $\Pi_r(x) = \sum_{p^k \le x} (p^{rk}/k) = \sum_{k=1}^{\kappa} (\pi_{rk}(x^{1/k})/k)$ with $\kappa = \lfloor \log x / \log 2 \rfloor$.
- $\theta(x) = \sum_{p \le x} \log p$ and $\psi(x) = \sum_{p^k \le x} \log p = \sum_{k=1}^{\kappa} \theta(x^{1/k})$ are the Chebyshev functions.
- $\Lambda(x) = \begin{cases} \log p & \text{if } x = p^k, \\ 0 & \text{otherwise.} \end{cases}$ is the von Mangoldt function,
- $(p_n)_{n \ge 1}$ is the sequence of prime numbers, where $p_1 = 2$.
- $\mathrm{li}(x)$ denotes the logarithmic integral of x (see Section 2.2), and li^{-1} the inverse function.
- $\gamma_0 = 0.577\,215\,66\ldots$ is the Euler constant. The coefficients γ_m and δ_m are defined in Section 2.4.
- $\sum_\rho f(\rho) = \lim_{T\to\infty} \sum_{|\Im(\rho)| \le T} f(\rho)$ where $f : \mathbb{C} \to \mathbb{C}$ is a complex function and ρ runs over the nontrivial roots of the Riemann ζ function.
- If $\lim_{n\to\infty} u_n = +\infty$, $v_n = \Omega_\pm(u_n)$ is equivalent to
$$\limsup_{n\to\infty} \frac{v_n}{u_n} > 0 \quad \text{and} \quad \liminf_{n\to\infty} \frac{v_n}{u_n} < 0.$$
- We use the following constants:
$$x_0 = 10^{10} + 19 \text{ is the smallest prime exceeding } 10^{10};$$
$$n_0 = \pi_1(x_0) = 2\,220\,822\,442\,581\,729\,257$$
$$L_0 = \log n_0 = 42.244\,409\,270\,801\,490\ldots;$$
$$\lambda_0 = \log L_0 = 3.743\,472\,020\,096\,020\ldots, \; \nu_0 = \lambda_0/L_0 = 0.088\,614\ldots.$$
- Let us write $\sigma_0 = 0$, $N_0 = 1$, and, for $j \ge 1$,
$$N_j = p_1 p_2 \cdots p_j \quad \text{and} \quad \sigma_j = p_1 + p_2 + \cdots + p_j = \ell(N_j). \tag{1.12}$$
- For $n \ge 0$, let $k = k(n)$ denote the integer $k \ge 0$ such that
$$\sigma_k = p_1 + p_2 + \cdots + p_k \le n < p_1 + p_2 + \cdots + p_{k+1} = \sigma_{k+1}. \tag{1.13}$$

In [7, Proposition 3.1], for $j \ge 1$, it is proved that
$$h(\sigma_j) = N_j. \tag{1.14}$$

We often implicitly use the following result: for u and v positive and w real, the function
$$t \mapsto \frac{(\log t - w)^u}{t^v} \text{ is decreasing for } t > \exp\Big(w + \frac{u}{v}\Big).$$

1.2. Plan of the paper. In Section 2 we recall several results and state some lemmas that are used in the proof of Theorem 1.1. Section 2.1 is devoted to effective estimates in prime number theory, Section 2.2 deals with the logarithmic integral, while Section 2.3 give effective estimates for $\pi_r(x) = \sum_{p \le x} p^r$ and especially for $\pi_1(x)$.

Section 2.4 recalls two explicit formulas (see (2.37) and (2.38)) of prime number theory, some results about the roots of the Riemann ζ function, and explains the computation of the constant c (see (1.10)).

The computation of $h(n)$ plays an important role in the proof of our results. The algorithm described in [7] is briefly recorded in Section 3.

In Section 4, in preparation for the proof of Theorem 1.1, four lemmas about b_n (defined in (1.9)) are given.

The proof of Theorem 1.1 is given in Section 5. It follows the lines of the proof of [18, Theorem 1] about the asymptotic estimate, under the Riemann hypothesis, of $\log g(n)$, starting from the explicit formula for $\Pi_1(x)$. But here we deal with effective estimates. The positive integers are split into three classes: the small ones (up to and including $n_0 = \pi_1(10^{10} + 19)$) that are mainly treated by computation, the large ones (greater than n_0) and, to prove statement (vi), those tending to infinity. In each class, the ns belonging to the interval $[\sigma_k, \sigma_{k+1}]$ (where σ_k is defined by (1.13)) are considered globally because, from (1.14), $h(\sigma_k)$ is easy to evaluate, and, for $n \in [\sigma_k, \sigma_{k+1}]$, $h(n)$ remains close to $h(\sigma_k)$.

Effective estimates are more technical to get than asymptotic ones. This was why Landau introduced his famous '$\mathcal{O}$' and 'o' notation. But fortunately nowadays computer algebra systems can help us.

A Maple sheet on the website [27] explains the algebraic and numerical computations. The extensive computations described in Section 3.2 have been done in C^{++}.

2. Useful results

2.1. Effective estimates. Platt and Trudgian [21] have shown by computation that

$$\theta(x) < (1+\epsilon)\,x \quad \text{for } x \geq 2, \text{ with } \epsilon = 7.5 \times 10^{-7}, \tag{2.1}$$

thus improving on results of Schoenfeld [24].

Without any hypothesis, we know that

$$|\theta(x) - x| < \frac{\alpha\, x}{\log^3 x} \quad \text{for } x \geq x_1 = x_1(\alpha), \tag{2.2}$$

with

$$\alpha = \begin{cases} 1 & \text{and} \quad x_1 = 89\,967\,803 \text{ (see [12, Theorem 4.2])}, \\ 0.5 & \text{and} \quad x_1 = 767\,135\,587 \text{ (see [12, Theorem 4.2])}, \\ 0.15 & \text{and} \quad x_1 = 19\,035\,709\,163 \text{ (see [3, Theorem 1.1])}. \end{cases}$$

Under the Riemann hypothesis, for $x \geq 599$, we shall use the upper bounds (see [24, (6.3)])

$$|\psi(x) - x| \leq \frac{1}{8\pi}\sqrt{x}\log^2 x \quad \text{and} \quad |\theta(x) - x| \leq \frac{1}{8\pi}\sqrt{x}\log^2 x. \tag{2.3}$$

Lemma 2.1. *Under the Riemann hypothesis, for* $x \geq 1$,

$$\psi(x) - \sqrt{x} - \tfrac{4}{3}x^{1/3} \leq \theta(x) \leq \psi(x) - \sqrt{x} + 2.14.$$

Proof. In [20, Lemma 2.4] or in [22, Lemma 3], the above lower bound is given and $\theta(x) \leq \psi(x) - \sqrt{x}$ is proved for $x \geq 121$. It remains to check that, for $1 \leq x \leq 121$, $\theta(x) - \psi(x) + \sqrt{x} < \sqrt{8} - \log 2 = 2.1352\ldots$ holds. □

2.2. The logarithmic integral. For real x greater than 1, we define $\mathrm{li}(x)$ as (see [1, page 228])

$$\mathrm{li}(x) = \int_0^x \frac{dt}{\log t} = \lim_{\varepsilon \to 0^+}\Big(\int_0^{1-\varepsilon} + \int_{1+\varepsilon}^x \frac{dt}{\log t}\Big) = \int_2^x \frac{dt}{\log t} + \mathrm{li}(2).$$

We have the following values:

x	1	$1.451\,36\ldots$	$1.969\,04\ldots$	2	e^2
$\mathrm{li}(x)$	$-\infty$	0	1	$1.045\,16\ldots$	$4.954\,23\ldots$

From the definition of $\mathrm{li}(x)$, it follows that

$$\frac{d}{dx}\,\mathrm{li}(x) = \frac{1}{\log x} \quad \text{and} \quad \frac{d^2}{dx^2}\,\mathrm{li}(x) = -\frac{1}{x\log^2 x}. \tag{2.4}$$

The function $t \mapsto \mathrm{li}(t)$ is an increasing bijection from $(1, +\infty)$ onto $(-\infty, +\infty)$. We denote by $\mathrm{li}^{-1}(y)$ its inverse function, which is defined and increasing for all $y \in \mathbb{R}$. Note that $\mathrm{li}^{-1}(y) > 1$ holds for all $y \in \mathbb{R}$.

To compute numerical values of $\mathrm{li}(x)$, we used the following formula, due to Ramanujan (see [4, pages 126–131]):

$$\mathrm{li}(x) = \gamma_0 + \log\log x + \sqrt{x}\sum_{n=1}^{\infty} a_n (\log x)^n \quad \text{with } a_n = \frac{(-1)^{n-1}}{n!\,2^{n-1}} \sum_{m=0}^{\lfloor n-1/2 \rfloor} \frac{1}{2m+1}.$$

Let N be a positive integer and $s \geq 1$ a real number. Then

$$\int \frac{t^{s-1}}{\log^N t}\,dt = \frac{1}{(N-1)!}\Big(s^{N-1}\,\mathrm{li}(t^s) - \sum_{k=1}^{N-1} \frac{(k-1)!\,s^{N-1-k}\,t^s}{\log^k t}\Big) \tag{2.5}$$

and, for $x \to \infty$,

$$\mathrm{li}(x) = \sum_{k=1}^{N} \frac{(k-1)!\,x}{(\log x)^k} + O\Big(\frac{x}{(\log x)^{N+1}}\Big). \tag{2.6}$$

We shall need the following lemmas that give bounds for the logarithmic integral.

Lemma 2.2. *For* $t > 4$,

$$\mathrm{li}(t) > \frac{t}{\log t}. \tag{2.7}$$

For $t > 1$,

$$\mathrm{li}(t) < t - 0.82 < t, \tag{2.8}$$

$$\mathrm{li}(t) < 1.49 \frac{t}{\log t}. \tag{2.9}$$

For $t \geq 10^{10}$,

$$\mathrm{li}(t) < \frac{t}{\log t} + 1.101 \frac{t}{\log^2 t}. \tag{2.10}$$

Proof.

- For $t > 1$, the function $t \mapsto \mathrm{li}(t) - t/\log t$ is increasing and vanishes for $t = 3.846\ldots$.
- The function $t \mapsto t - \mathrm{li}(t)$ is minimal for $t = e$ and $e - \mathrm{li}(e) = 0.823\ldots$.
- The maximum of $t \mapsto \mathrm{li}(t) - 1.49\, t/\log t$, obtained for $t = \exp(1.49/0.49)$, is $-0.04\ldots$.
- The function $t \mapsto \mathrm{li}(t) - t/\log t - 1.101\, t/\log^2 t$ is decreasing for $t > 2.95 \times 10^9$ and its value for $t = 10^{10}$ is $-5015.15 \cdots < 0$. □

Lemma 2.3. *For* $t > 77$,

$$\mathrm{li}(t) > \frac{t}{\log t} + \frac{t}{\log^2 t} + \frac{2t}{\log^3 t} + \frac{6t}{\log^4 t}, \tag{2.11}$$

for $t > 4.96 \times 10^{12}$,

$$\mathrm{li}(t) < \frac{t}{\log t} + \frac{t}{\log^2 t} + \frac{2t}{\log^3 t} + \frac{7t}{\log^4 t}, \tag{2.12}$$

and for $t > 1$,

$$\mathrm{li}(t) < \frac{t}{\log t} + \frac{t}{\log^2 t} + \frac{2t}{\log^3 t} + \frac{40}{3} \frac{t}{\log^4 t}. \tag{2.13}$$

Proof. For $u \in \{6, 7, 40/3\}$, we set

$$f = \mathrm{li}(t) - \frac{t}{\log t} - \frac{t}{\log^2 t} - \frac{2t}{\log^3 t} - u \frac{t}{\log^4 t}.$$

From (2.4), we obtain

$$\frac{df}{dt} = \frac{(6-u)\log t + 4u}{\log^5 t}.$$

- For $u = 6$, f is increasing and vanishes for $t = 76.54\ldots$ which proves (2.11).
- For $u = 7$, f is increasing for $t < t_0 = \exp(28) = 1.446 \cdots \times 10^{12}$ and decreasing for $t > t_0$. One computes $f(4.96 \times 10^{12}) = -259.07\ldots < 0$ and (2.12) follows.
- For $u = 40/3$, f is increasing for $t < t_1 = \exp(80/11) = 1440.47\cdots$ and decreasing for $t > t_1$. Therefore, (2.13) results from the negativity of $f(t_1) = -0.0033\ldots$. □

LEMMA 2.4. *For $t \ge 3.28$,*

$$\mathrm{li}^{-1}(t) < t(\log t + \log\log t), \tag{2.14}$$

for $t > 41$,

$$\mathrm{li}^{-1}(t) > t\log t, \tag{2.15}$$

and for $t > 12\,218$,

$$\mathrm{li}^{-1}(t) > t(\log t + \log\log t - 1). \tag{2.16}$$

PROOF.

- For $t \ge e$, let us consider the function $f = \mathrm{li}(t(\log(t) + \log\log t)) - t$. Denoting $\log t$ by L, we have
$$\frac{df}{dt} = \frac{\log t + 1 + \log\log t + 1/\log t}{\log(t(\log t + \log\log t))} - 1 = \frac{L + 1 - L\log(1 + (\log L)/L)}{L^2 + L\log(L + \log L)}.$$
The denominator is greater than or equal to 1 and the numerator is greater than or equal to $L + 1 - \log L \ge L + 1 - (L-1) = 2 > 0$. So f is increasing and its value for $t = 3.28$ is $0.0073\cdots > 0$, which completes the proof of (2.14).
- Now, let us consider $f(t) = \mathrm{li}(t\log t) - t$. We have
$$f'(t) = \frac{\log t + 1}{\log(t\log t)} - 1 = \frac{1 - \log\log t}{\log t + \log\log t} < 0$$
for $t > e^e = 15.15\ldots$, which shows that f is decreasing for $t > e^e$ and, from $f(41) = -0.048\cdots < 0$, we get (2.15).
- Finally, for $t > 1$, we set $f(t) = t(\log t + \log\log t - 1)$. We have $f'(t) = \log t + \log\log t + 1/\log t$ which is positive for $t > e$ so that f is increasing for $t > e$. As $f(t_0) = 1$ for $t_0 = 3.1973\ldots$, we assume $t > t_0$ so that $f(t) > 1$, $L = \log t > 1$ and $\log L > 0$ hold. We set
$$y = t - \mathrm{li}(f(t)) = t - \mathrm{li}(t(\log t + \log\log t - 1))$$
and, using the inequality $\log(1+u) \ge u/(1+u)$ (for $u > -1$), we obtain
$$\begin{aligned} y'\log f(t) &= \log\Big(1 + \frac{\log L - 1}{L}\Big) - \frac{1}{L} \\ &\ge \frac{\log L - 1}{L(1 + (\log L - 1)/L)} - \frac{1}{L} = \frac{(L-1)(\log L - 2) - 1}{L(L + \log L - 1)}. \end{aligned}$$
For $t > e^{e^2} = 1618.17\ldots$, the denominator is positive. The numerator is increasing, and positive for $t = 4678$. Therefore, y is increasing for $t > 4678$. It remains to calculate $y(12218) = 0.00106\cdots > 0$ to prove (2.16). □

LEMMA 2.5. *The function $t \mapsto \sqrt{\mathrm{li}^{-1}(t)}$ is defined and increasing for $t \in \mathbb{R}$.*

- *It is concave for $t > \mathrm{li}(e^2) = 4.954\ldots$.*
- *Let $a \le 1$ be a real number. For $t \ge 31$, the function $t \mapsto \sqrt{\mathrm{li}^{-1}(t)} - a(t(\log t))^{1/4}$ is concave.*

PROOF.

- Let us set $f_1 = \sqrt{\mathrm{li}^{-1}(t)}$, $f_2 = (t(\log t))^{1/4}$, $F = f_1 - af_2$ and $u = \mathrm{li}^{-1}(t)$, that is, $t = \mathrm{li}(u)$. We have

$$\frac{df_1}{dt} = \frac{\log u}{2\sqrt{u}}, \quad \frac{d^2 f_1}{dt^2} = -\frac{\log u(\log u - 2)}{4u^{3/2}}, \quad \frac{d^2 f_2}{dt^2} = -\frac{3\log^2 t + 2\log t + 3}{16(t\log t)^{7/4}}.$$

  Let us assume $t > \mathrm{li}(e^2)$. We have $u > e^2$, $\log u > 2$ and $(d^2 f_1/dt^2) < 0$, so that f_1 is concave.
- Further, $(d^2 f_2/dt^2) < 0$ so that if $a \le 0$ then $F = f_1 - af_2$ is concave. Moreover, from (2.8) and (2.7), we have $u/\log u < t = \mathrm{li}\, u < u$ and

$$0 < -\frac{d^2 f_2}{dt^2} \le \frac{3\log^2 u + 2\log u + 3}{16(u(1 - (\log\log u)/\log u))^{7/4}}.$$

  If $0 < a \le 1$ holds, it suffices to show that $|(d^2 f_2/dt^2)/(d^2 f_1/dt^2)| < 1$. Writing L for $\log u$ leads to

$$\begin{aligned}\left|\frac{d^2 f_2}{dt^2}\Big/\frac{d^2 f_1}{dt^2}\right| &\le \frac{1}{4\,u^{1/4}}\left(1 - \frac{\log L}{L}\right)^{-7/4}\left(\frac{3L^2 + 2L + 3}{L(L-2)}\right)\\ &= \frac{1}{4\,u^{1/4}}\left(1 - \frac{\log L}{L}\right)^{-7/4}\left(3 + \frac{8}{L} + \frac{19}{L(L-2)}\right).\end{aligned} \tag{2.17}$$

The three factors on the right-hand side of (2.17) are positive and decreasing on u so that their product is decreasing, and for $u = 103$, $t = 30.77\ldots$ it is less than 1. □

REMARK 2.6. By using more accurate inequalities, it would be possible to replace the bound $t \ge 31$ by $t \ge 8.42\ldots$.

2.3. Study of $\pi_r(x) = \sum_{p\le x} p^r$. Without any hypothesis, improving on results of Massias and Robin about the bounds of $\pi_r(x) = \sum_{p\le x} p^r$ (see [17, Théorème D]), by using recent improvements on effective estimates of $\theta(x)$, we prove the following proposition.

PROPOSITION 2.7. *Let α, $x_1 = x_1(\alpha)$ be two real numbers such that $0 < \alpha \le 1$, $x_1 \ge 89\,967\,803$ and $|\theta(x) - x| < \alpha x/\log^3 x$ for $x \ge x_1$. Then, for $r \ge 0.6$ and $x \ge x_1$,*

$$\begin{aligned}\pi_r(x) \le C_0 &+ \frac{x^{r+1}}{(r+1)\log x} + \frac{x^{r+1}}{(r+1)^2\log^2 x} + \frac{2x^{r+1}}{(r+1)^3\log^3 x}\\ &+ \frac{(51\alpha r^4 + 176\alpha r^3 + 222\alpha r^2 + 120\alpha r + 23\alpha + 168)x^{r+1}}{24(r+1)^4\log^4 x}\end{aligned} \tag{2.18}$$

with

$$C_0 = \pi_r(x_1) - \frac{x_1^r\theta(x_1)}{\log x_1} - \frac{3\alpha r^4 + 8\alpha r^3 + 6\alpha r^2 + 24 - \alpha}{24}\,\mathrm{li}(x_1^{r+1}) + \frac{(3\alpha r^3 + 5\alpha r^2 + \alpha r + 24 - \alpha)x_1^{r+1}}{24\log x_1} + \frac{\alpha(3r^2 + 2r - 1)x_1^{r+1}}{24\log^2 x_1} + \frac{\alpha(3r-1)x_1^{r+1}}{12\log^3 x_1} - \frac{\alpha x_1^{r+1}}{4\log^4 x_1}. \tag{2.19}$$

Let $r_0(\alpha)$ be the unique positive root of the equation $3r^4 + 8r^3 + 6r^2 - 24\alpha - 1 = 0$. We have $r_0(\alpha) \geq r_0(1) = 1.1445\ldots$. For $0.06 \leq r \leq r_0(\alpha)$ and $x \geq x_1(\alpha)$,

$$\pi_r(x) \geq \widehat{C_0} + \frac{x^{r+1}}{(r+1)\log x} + \frac{x^{r+1}}{(r+1)^2\log^2 x} + \frac{2x^{r+1}}{(r+1)^3\log^3 x} - \frac{(2\alpha r^4 + 7\alpha r^3 + 9\alpha r^2 + 5\alpha r + \alpha - 6)x^{r+1}}{(r+1)^4\log^4 x}, \tag{2.20}$$

while if $r > r_0(\alpha)$ and $x \geq x_1(\alpha)$, we have

$$\pi_r(x) \geq \widehat{C_0} + \frac{x^{r+1}}{(r+1)\log x} + \frac{x^{r+1}}{(r+1)^2\log^2 x} + \frac{2x^{r+1}}{(r+1)^3\log^3 x} - \frac{(51\alpha r^4 + 176\alpha r^3 + 222\alpha r^2 + 120\alpha r + 23\alpha - 168)x^{r+1}}{24(r+1)^4\log^4 x}, \tag{2.21}$$

with

$$\widehat{C_0} = \pi_r(x_1) - \frac{x_1^r\theta(x_1)}{\log x_1} + \frac{3\alpha r^4 + 8\alpha r^3 + 6\alpha r^2 - \alpha - 24}{24}\,\mathrm{li}(x_1^{r+1}) - \frac{(3\alpha r^3 + 5\alpha r^2 + \alpha r - \alpha - 24)x_1^{r+1}}{24\log x_1} - \frac{\alpha(3r^2 + 2r - 1)x_1^{r+1}}{24\log^2 x_1} - \frac{\alpha(3r-1)x_1^{r+1}}{12\log^3 x_1} + \frac{\alpha x_1^{r+1}}{4\log^4 x_1}. \tag{2.22}$$

Proof. It is convenient to set

$$s = r + 1.$$

By Stieltjes integral, we have

$$\pi_r(x) = \sum_{p\leq x} p^r = \pi_{s-1}(x) = \pi_{s-1}(x_1) + \int_{x_1}^{x} \frac{t^{s-1}}{\log t}\, d[\theta(t)]$$

and, by partial integration,

$$\pi_{s-1}(x) = \pi_{s-1}(x_1) + \frac{x^{s-1}\theta(x)}{\log x} - \frac{x_1^{s-1}\theta(x_1)}{\log x_1} - \int_{x_1}^{x}\Big(\frac{(s-1)t^{s-2}}{\log t} - \frac{t^{s-2}}{\log^2 t}\Big)\theta(t)\, dt. \tag{2.23}$$

Since $x \ge x_1(\alpha)$ holds, in (2.23), from our assumption, we have $\theta(x) \le x + \alpha x/\log^3 x$. Under the integral sign, as $s \ge 1 + 1/\log x_1(\alpha) \ge 1 + 1/\log(89\,967\,803) = 1.054\ldots$, the expression in parentheses is positive and $\theta(t) \ge t - \alpha t/\log^3 t$, which implies

$$\pi_{s-1}(x) \le \pi_{s-1}(x_1) - \frac{x_1^{s-1}\theta(x_1)}{\log x_1} + \frac{x^s}{L} + \frac{\alpha x^s}{L^4} - (s-1)I_1 + I_2 + (s-1)\alpha I_4 - \alpha I_5, \quad (2.24)$$

with $L = \log x$ and, for $i \ge 1$, $I_i = \int_{x_1}^{x} (t^{s-1}/\log^i t)\, dt = f_i(x) - f_i(x_1)$ with $f_i(t) = \int (t^{s-1}/\log^i t)$. By (2.5), we obtain

$$f_1 = \mathrm{li}(t^s), \quad f_2 = s\,\mathrm{li}(t^s) - \frac{t^s}{\log t}, \quad f_3 = \frac{s^2}{2}\,\mathrm{li}(t^s) - \frac{s\,t^s}{2\log t} - \frac{t^s}{2\log^2 t},$$
$$f_4 = \frac{s^3\,\mathrm{li}(t^s)}{6} - \frac{s^2 t^s}{6\log t} - \frac{s\,t^s}{6\log^2 t} - \frac{t^s}{3\log^3 t},$$
$$f_5 = \frac{s^4\,\mathrm{li}(t^s)}{24} - \frac{s^3 t^s}{24\log t} - \frac{s^2 t^s}{24\log^2 t} - \frac{s\,t^s}{12\log^3 t} - \frac{t^s}{4\log^4 t}.$$

Let us set

$$\begin{aligned} f(t) &= -(s-1)f_1 + f_2 + (s-1)\alpha f_4 - \alpha f_5 \\ &= \frac{3\alpha s^4 - 4\alpha s^3 + 24}{24}\,\mathrm{li}(t^s) - \frac{(3\alpha s^3 - 4\alpha s^2 + 24)t^s}{24\log t} \\ &\quad - \frac{\alpha s(3s-4)t^s}{24\log^2 t} - \frac{\alpha(3s-4)t^s}{12\log^3 t} + \frac{\alpha t^s}{4\log^4 t}. \end{aligned} \quad (2.25)$$

From (2.24), we have

$$\pi_{s-1}(x) \le C_0 + \frac{x^s}{L} + \frac{\alpha x^s}{L^4} + f(x) \quad \text{with } C_0 = \pi_{s-1}(x_1) - \frac{x_1^{s-1}\theta(x_1)}{\log x_1} - f(x_1).$$

Now, we have $s = r + 1 \ge 1.6$, $x^s \ge x_1(\alpha)^{1.6} > 89\,967\,803^{1.6} > 4.96 \cdot 10^{12}$, and we may use the upper bound (2.12) of $\mathrm{li}(x^s)$ in (2.25) to get

$$\pi_{s-1}(x) \le C_0 + \frac{x^s}{sL} + \frac{x^s}{s^2L^2} + \frac{2x^s}{s^3L^3} + \frac{(51\alpha s^4 - 28\alpha s^3 + 168)x^s}{24s^4L^4}$$

which, by substituting $r + 1$ for s, proves (2.18) and (2.19).

To get a lower bound for $\pi_{s-1}(x)$, in (2.23), we use the inequalities $\theta(x) \ge x - \alpha x/L^3$ and $\theta(t) \le t + \alpha t/\log^3 t$. We obtain

$$\begin{aligned} \widehat{f}(t) &= -(s-1)f_1 + f_2 - (s-1)\alpha f_4 + \alpha f_5 \\ &= \frac{-3\alpha s^4 + 4\alpha s^3 + 24}{24}\,\mathrm{li}(t^s) + \frac{(3\alpha s^3 - 4\alpha s^2 - 24)t^s}{24\log t} \\ &\quad + \frac{\alpha s(3s-4)t^s}{24\log^2 t} + \frac{\alpha(3s-4)t^s}{12\log^3 t} - \frac{\alpha t^s}{4\log^4 t} \end{aligned}$$

(note that $\widehat{f}(t)$ is obtained by substituting $-\alpha$ for α in (2.25)) and

$$\pi_{s-1}(x) \geq \widehat{C_0} + \frac{x^s}{L} - \frac{\alpha x^s}{L^4} + \widehat{f}(x) \quad \text{with } \widehat{C_0} = \pi_{s-1}(x_1) - \frac{x_1^{s-1}\theta(x_1)}{\log x_1} - \widehat{f}(x_1).$$

Let us set $\varphi(r) = 3r^4 + 8r^3 + 6r^2 - 24/\alpha - 1$. We have $\varphi'(r) = 12r(r+1)^2$; φ is minimal and negative for $r = 0$ and has one negative and one positive root, $r_0(\alpha)$. Note that $r_0(\alpha)$ is decreasing on α. We compute $r_0(1) = 1.1445\ldots$, $r_0(0.5) = 1.4377\ldots$ and $r_0(0.15) = 2.1086\ldots$.

The coefficient of $\mathrm{li}(x^s)$ in $\widehat{f}(x)$ is

$$\frac{-3\alpha s^4 + 4\alpha s^3 + 24}{24} = \frac{-3\alpha r^4 - 8\alpha r^3 - 6\alpha r^2 + \alpha + 24}{24} = -\frac{\alpha\varphi(r)}{24}$$

and changes sign for $r = r_0(\alpha)$. For $0.06 \leq r \leq r_0(\alpha)$ we have $x^s \geq x_1^s \geq x_1^{1.06} > 77$ and we use the lower bound (2.11) of $\mathrm{li}(x^s)$ in $\widehat{f}(x)$ to get (2.20), while for $r > r_0(\alpha)$, $x^s \geq x_1(\alpha)^{2.14} > 89\,967\,803^{2.14} > 4.96 \times 10^{12}$ and we use (2.12) to get (2.21). □

Corollary 2.8. *For $x \geq 110\,117\,910$,*

$$\pi_1(x) \leq \frac{x^2}{2\log x} + \frac{x^2}{4\log^2 x} + \frac{x^2}{4\log^3 x} + \frac{107\, x^2}{160\log^4 x} \tag{2.26}$$

and, for $x \geq 905\,238\,547$,

$$\pi_1(x) \geq \frac{x^2}{2\log x} + \frac{x^2}{4\log^2 x} + \frac{x^2}{4\log^3 x} + \frac{3\, x^2}{20\log^4 x}. \tag{2.27}$$

Proof. We choose $r = 1$, $\alpha = 0.15$, $x_1 = 19\,035\,709\,163$ and, from (2.2), we apply (2.18). By computation we get $\pi_1(x_1) = 7\,823\,414\,443\,039\,054\,263$,

$$\theta(x_1) = 19\,035\,493\,858.482\,419\,137\ldots, \qquad f(x_1) = -7.485\,421\,258\cdots \times 10^{18}$$

and C_0, defined by (2.19) with $r = 1$, is equal to $-1.586\cdots \times 10^{13} < 0$ so that (2.26) follows from (2.18) for $x \geq x_1$ and, by computation, for $110\,117\,909 \leq x < x_1$.

Similarly, $\widehat{C_0}$, defined by (2.22), is equal to $1.655\cdots \times 10^{14} > 0$ which implies (2.27) from (2.20) for $x \geq x_1$ and by computation for $905\,238\,546 \leq x < x_1$. □

Remark 2.9. In [2, Theorem 6.7 and Proposition 6.9], Axler gives similar estimates for $\pi_1(x)$.

Lemma 2.10. *Let us assume that $x \geq x_0 = 10^{10} + 19$ and $n = \pi_1(x)$ hold. Then x satisfies*

$$\sqrt{n\log n}\left(1 + 0.365\,\frac{\log\log n}{\log n}\right) \leq x \leq \sqrt{n\log n}\left(1 + \frac{\log\log n}{2\log n}\right). \tag{2.28}$$

Proof. When $x \to \infty$, from the formula $n = \pi_1(x) = \mathrm{li}(x^2) + O(x^2\exp(-a\log x))$ with $a > 0$ (see [18, Lemme B]), we can see that the asymptotic expansion of x is given by (1.8). In particular, we have

$$x = \sqrt{n\log n}\left(1 + \frac{\log\log n - 1 + o(1)}{2\log n}\right), \qquad n \to \infty. \tag{2.29}$$

Now we have to prove the effective bounds (2.28) of x. For convenience, we write L for $\log n$ and λ for $\log\log n$. We suppose $x \geq x_0 = 10^{10} + 19$. We have $n \geq n_0 = \pi_1(x_0) = 2.22 \times \cdots 10^{18}$, $L = \log n > 42.24$ and $\lambda = \log\log n > 3.74$.

The upper bound. Let us note $f(n) = \sqrt{nL}(1 + \lambda/2L)$. Since $(t^2/2\log t)(1 + (1/2\log t))$ is increasing as a function of t for $t > e$, the inequality $x \leq f(n)$ is equivalent to

$$\frac{x^2}{2\log x}\Big(1 + \frac{1}{2\log x}\Big) \leq \frac{f(n)^2}{2\log f(n)}\Big(1 + \frac{1}{2\log f(n)}\Big). \tag{2.30}$$

From (2.27), for $x \geq x_0$, we have $(x^2/2\log x)(1 + (1/2\log x)) \leq \pi_1(x) = n$. Note that this result has been proved in [3, Corollary 6.10] for $x \geq 302\,971$. Thus to ensure (2.30) it suffices to prove

$$n < \frac{f(n)^2}{2\log f(n)}\Big(1 + \frac{1}{2\log f(n)}\Big).$$

As we have $2\log f(n) = L + \lambda + 2\log(1 + \lambda/(2L)) \leq L + \lambda + \lambda/L$, it suffices to show that

$$nL\frac{(1 + \lambda/(2L))^2}{L + \lambda + \lambda/L}\Big(1 + \frac{1}{L + \lambda + \lambda/L}\Big) > n$$

or, equivalently, that

$$L(1 + \lambda/(2L))^2(L + \lambda + \lambda/L + 1) - (L + \lambda + \lambda/L)^2 > 0.$$

But the left-hand side above is equal to

$$L + \frac{\lambda^2}{4}\Big(1 - \frac{3}{L} - \frac{4}{L^2}\Big) + \frac{\lambda^3}{4L}\Big(1 + \frac{1}{L}\Big),$$

which is positive for $L \geq 4$, that is, for $n \geq e^4$.

The lower bound. First, from (2.26), for $x \geq x_0$, we have

$$n = \pi_1(x) \leq \frac{x^2}{2\log x} + \frac{x^2}{4\log^2 x}\Big(1 + \frac{1}{\log x_0} + \frac{107}{40\log^2 x_0}\Big) \leq \frac{x^2}{2\log x}\Big(1 + \frac{a}{2\log x}\Big) \tag{2.31}$$

with $a = 1.049$. This time, we set $f(n) = \sqrt{nL}(1 + b\lambda/L)$ with $b = 0.365$. We have $2\log f(n) = L + \lambda + 2\log(1 + b\lambda/L)$. Using the inequality $\log(1 + u) \geq u/(1 + u_0)$ valid for $0 \leq u \leq u_0$, we have

$$2\log f(n) \geq L + \lambda + c_0\lambda/L \quad \text{with } c_0 = 0.7 < 2b/(1 + b\lambda_0/L_0) = 0.707\ldots. \tag{2.32}$$

We have to prove that $x \geq f(n)$ holds for $n \geq n_0$. From the increasingness of the mapping $t \mapsto (t^2/2\log t)(1 + (a/2\log t))$, it suffices to show that

$$\frac{x^2}{2\log x}\Big(1 + \frac{a}{2\log x}\Big) \geq \frac{f(n)^2}{2\log f(n)}\Big(1 + \frac{a}{2\log f(n)}\Big). \tag{2.33}$$

From (2.31) and (2.32), to prove (2.33), it suffices to prove

$$n \geq \frac{nL(1+b\lambda/L)^2}{L+\lambda+c_0\lambda/L}\Big(1+\frac{a}{L+\lambda+c_0\lambda/L}\Big),$$

that is,

$$L\Big(1+\frac{b\lambda}{L}\Big)^2\Big(L+\lambda+\frac{c_0\lambda}{L}+a\Big)-\Big(L+\lambda+\frac{c_0\lambda}{L}\Big)^2 \leq 0 \tag{2.34}$$

and, equivalently, by expanding (2.34) and dividing by λL, that

$$2b-1+\frac{a}{\lambda}+\frac{(b^2+2b-1)\lambda+2ab}{L}+\frac{b^2\lambda^2+ab^2\lambda}{L^2} + c_0\Big(-\frac{1}{L}+\frac{2\lambda(b-1)}{L^2}+\frac{b^2\lambda^2}{L^3}\Big)-\frac{c_0^2\lambda}{L^3} \leq 0. \tag{2.35}$$

The coefficient of c_0 in (2.35) satisfies

$$c_0\Big(-\frac{1}{L}+\frac{2\lambda(b-1)}{L^2}+\frac{b^2\lambda^2}{L^3}\Big) \leq -\frac{c_0}{L}+\frac{c_0\lambda}{L^2}\Big(2b+\frac{b^2\lambda_0}{L_0}-2\Big) \leq -\frac{c_0}{L}-\frac{d\lambda}{L^2}$$

with $d = 0.88 < c_0(2-2b-b^2\lambda_0/L_0) = 0.8807\ldots$, so that it suffices to show that

$$B = 2b-1+\frac{a}{\lambda}+\frac{(b^2+2b-1)\lambda+2ab}{L}+\frac{b^2\lambda^2+(ab^2-d)\lambda}{L^2}-\frac{c_0}{L} \leq 0,$$

for $L = \exp(\lambda)$ and $\lambda \geq \lambda_0$. For that, we write $c_0 = c_1+c_2+c_3$ with $c_1 = 0.44$ and $c_2+c_3 = 0.26$. We have

$$B = \Big[2b-1+\frac{a}{\lambda}-\frac{c_1}{L}\Big]+\frac{(b^2+2b-1)\lambda+2ab-c_2}{L}+\frac{b^2\lambda^2+(ab^2-d)\lambda-c_3L}{L^2}. \tag{2.36}$$

It is easy to see that $a/\lambda - c_1/L = 1.049/\lambda - 0.44e^{-\lambda}$ is decreasing for $\lambda > 0$ and its value for $\lambda = \lambda_0$ is $0.2698\ldots$, so that the term in square brackets in (2.36) is negative.

For $\lambda_0 \leq \lambda \leq 4.3$ we choose $c_2 = 0.26$, $c_3 = 0$, and we have

$$(b^2+2b-1)\lambda+2ab-c_2 \leq (b^2+2b-1)\lambda_0+2ab-c_2 = -0.0062\cdots < 0$$

and $b^2\lambda+(ab^2-d) \leq 4.3b^2+(ab^2-d) = -0.167\ldots$, so that B is negative.

For $\lambda > 4.3$, we choose $c_2 = 0.18$, $c_3 = 0.08$, and we have

$$(b^2+2b-1)\lambda+2ab-c_2 < 4.3(b^2+2b-1)+2ab-c_2 = -0.0023\cdots < 0.$$

The inequality $\lambda^2 \leq 4e^{\lambda-2} = 4L/e^2$ implies $b^2\lambda^2 - c_3L \leq (4b^2e^{-2}-c_3)\ L = -0.0078\ldots L < 0$ and, as we also have $ab^2-d = -0.74\cdots < 0$, we conclude that B is still negative, which completes the proof of Lemma 2.10. □

2.4. The Riemann ζ function and explicit formulas for ψ and Π_1.

2.4.1. Explicit formulas. We shall use the two explicit formulas

$$\psi(x) = x + \frac{\Lambda(x)}{2} - \sum_\rho \frac{x^\rho}{\rho} - \log(2\pi) - \frac{1}{2}\log\Big(1 - \frac{1}{x^2}\Big) \quad x > 1, \tag{2.37}$$

(see [16, pages 334 and 353] with $r = 0$ and $\zeta'(0)/\zeta(0) = \log(2\pi)$), and

$$\Pi_1(x) = \mathrm{li}(x^2) + \frac{x\Lambda(x)}{2\log x} - \sum_\rho \int_{-1}^{\infty} \frac{x^{\rho-t}}{\rho - t}\, dt - \log 12 + \int_x^\infty \frac{dt}{(t^2-1)\log t}, \quad x > 1 \tag{2.38}$$

(see [16, pages 360 and 361], with $R = 1$ and $\zeta(-1) = -1/12$).

In connection with (2.37) we shall use the following lemma (cf. [15, page 169 Théorème 5.8(b)] or [14, page 162 Theorem 5.8(b)]):

Lemma 2.11. *If a, b are fixed real numbers satisfying $1 \le a < b < \infty$, and g any function with a continuous derivative on the interval $[a, b]$, then*

$$\int_a^b g(t)\psi(t)\, dt = \int_a^b g(t)\Big[t - \log(2\pi) - \frac{1}{2}\log\Big(1 - \frac{1}{t^2}\Big)\Big]\, dt - \sum_\rho \int_a^b g(t)\frac{t^\rho}{\rho}\, dt. \tag{2.39}$$

We also have (see [13, page 67] or [5, page 272])

$$\sum_\rho \frac{1}{\rho} = 1 + \frac{\gamma_0}{2} - \frac{1}{2}\log\pi - \log 2 = 0.023\,095\,708\,966\,121\,033\ldots$$

and

$$\sum_\rho \frac{1}{\rho(1-\rho)} = \sum_\rho \Big(\frac{1}{\rho} + \frac{1}{1-\rho}\Big) = 2\sum_\rho \frac{1}{\rho} = 0.046\,191\,417\,932\,2420\ldots. \tag{2.40}$$

The coefficients γ_m are defined by the Laurent expansion of $\zeta(s)$ around 1 (cf. [5, Section 10.3.5]):

$$\zeta(s) = \frac{1}{s-1} + \sum_{m=0}^{\infty} \frac{\gamma_m}{m!}(s-1)^m.$$

We have

$m =$	0	1	2	3	4
$\gamma_m =$	0.57721 ...	−0.07281 ...	−0.00969 ...	0.00205 ...	0.00232 ...

The coefficients δ_m are defined by $\delta_1 = \gamma_0$, $\delta_2 = 2\gamma_1 + \gamma_0^2$, and, for $m \ge 1$,

$$\delta_{m+1} = (m+1)\frac{\gamma_m}{m!} + \sum_{j=0}^{m-1} \frac{\gamma_j \delta_{m-j}}{j!}.$$

These coefficients allow us to compute the sums $\sum_\rho (1/\rho^m)$ (see [5, pages 207 and 272]):

$$\sum_\rho \frac{1}{\rho^m} = 1 + \delta_m - \zeta(m)\Big(1 - \frac{1}{2^m}\Big), \quad m \geq 2. \tag{2.41}$$

For $m = 2$, we get

$$\sum_\rho \frac{1}{\rho^2} = 1 - \frac{\pi^2}{8} + 2\gamma_1 + \gamma_0^2 = -0.046\,154\,317\,295\,804\,6\ldots.$$

2.4.2. *Computation of* $\sum_\rho 1/|\rho(1+\rho)|$ *and* $\sum_\rho 1/|\Im\rho|^2$. It is known (see [28]) that every nontrivial root ρ of ζ satisfies

$$|\Im(\rho)| > 14.134\,725\,141\,734\,693\,79. \tag{2.42}$$

LEMMA 2.12. *Under the Riemann hypothesis, for* $k \geq 2$,

$$\sum_\rho \frac{1}{|\rho|^k} \leq \frac{10}{14^k}. \tag{2.43}$$

PROOF. Under the Riemann hypothesis, we have $\overline{\rho} = 1 - \rho$, and from (2.40),

$$\sum_\rho \frac{1}{|\rho|^2} = \sum_\rho \frac{1}{\rho(1-\rho)} = 0.046\,191\,41\cdots \leq \frac{1}{20}. \tag{2.44}$$

Using (2.42), we may write

$$\sum_\rho \frac{1}{|\rho|^k} \leq \frac{1}{14^{k-2}} \sum_\rho \frac{1}{|\rho|^2} \leq \frac{196}{20 \times 14^k},$$

which proves (2.43). □

LEMMA 2.13. *Let t be a complex number satisfying $|t| < 1/2$. Then*

$$f(t) = ((1-t^2)(1-2t))^{-1/2} = \sum_{n=0}^{\infty} c_n t^n \quad \textit{with } 0 \leq c_n \leq \frac{4}{3}\, 2^n, \tag{2.45}$$

and, if $|t| \leq 1/6$,

$$\Re(f(t)) \geq \tfrac{1}{3} \quad \textit{and} \quad |\Im(f(t))| \leq \tfrac{2}{3}.$$

PROOF. We have $(1-t)^{-1/2} = \sum_{n\geq 0} a_n t^n$ with

$$0 \leq a_n = (-1)^n \frac{(-\frac{1}{2})(-\frac{3}{2})\cdots(-\frac{2n-1}{2})}{n!} = \frac{1}{2^{2n}}\binom{2n}{n} \leq 1.$$

Therefore,

$$0 \leq c_n = \sum_{m=0}^{n/2} a_m (2^{n-2m} a_{n-2m}) \leq 2^n \sum_{m=0}^{\infty} \frac{1}{4^m} = \frac{2^{n+2}}{3},$$

which proves (2.45). If $|t| \le 1/6$, then

$$\Big|\sum_{n=1}^{\infty} c_n t^n\Big| \le \sum_{n=1}^{\infty} \frac{c_n}{6^n} \le \frac{4}{3}\sum_{n=1}^{\infty}\Big(\frac{2}{6}\Big)^n = \frac{2}{3},$$

whence

$$\Re(f(t)) = 1 + \Re\Big(\sum_{n=1}^{\infty} c_n t^n\Big) \ge 1 - \Big|\sum_{n=1}^{\infty} c_n t^n\Big| \ge 1 - \frac{2}{3} = \frac{1}{3}$$

and

$$|\Im(f(t))| = \Big|\Im\Big(\sum_{n=1}^{\infty} c_n t^n\Big)\Big| \le \Big|\sum_{n=1}^{\infty} c_n t^n\Big| \le \frac{2}{3},$$

which completes the proof of Lemma 2.13. □

Lemma 2.14. *Under the Riemann hypothesis, in the notation of (2.45), we have*

$$\sum_{\rho} \frac{1}{|\rho(1+\rho)|} = -\sum_{n=0}^{\infty} c_n \sum_{\rho} \frac{1}{\rho^{n+2}}. \tag{2.46}$$

Proof. Let $\rho = 1/2 + \imath\gamma$ be a nontrivial root of $\zeta(s)$ under the Riemann hypothesis. First we observe that f defined by (2.45) satisfies

$$\Big(-\frac{1}{\rho^2} f\Big(\frac{1}{\rho}\Big)\Big)^2 = \frac{1}{\rho^4(1-1/\rho^2)(1-2/\rho)} = \frac{1}{\rho(1-\rho)(\rho+1)(2-\rho)} = \frac{1}{|\rho(1+\rho)|^2} \tag{2.47}$$

so that $-f(1/\rho)/\rho^2$ is real. Let us write

$$f\Big(\frac{1}{\rho}\Big) = a + b\imath.$$

As, by (2.42), $|1/\rho| < 1/14$, Lemma 2.13 gives $a \ge 1/3$, $|b| \le 2/3$ and

$$-\frac{1}{\rho^2} f\Big(\frac{1}{\rho}\Big) = -\frac{a+b\imath}{(1/2+\imath\gamma)^2} = \frac{(\gamma^2 - 1/4 + \imath\gamma)(a+b\imath)}{(1/4+\gamma^2)^2}.$$

Thus the sign of $-f(1/\rho)/\rho^2$ is the sign of $a(\gamma^2 - 1/4) - b\gamma$. As

$$a(\gamma^2 - 1/4) - b\gamma \ge \frac{1}{3}\Big(\gamma^2 - \frac{1}{4}\Big) - \frac{2}{3}|\gamma| = \frac{1}{3}\Big(|\gamma| - \frac{2+\sqrt{5}}{2}\Big)\Big(|\gamma| - \frac{2-\sqrt{5}}{2}\Big) > 0$$

we have $-f(1/\rho)/\rho^2 > 0$, which, with (2.47), shows that

$$\frac{1}{|\rho(1+\rho)|} = -\frac{1}{\rho^2} f\Big(\frac{1}{\rho}\Big).$$

Therefore, from Lemma 2.13, we get

$$\sum_{\rho} \frac{1}{|\rho(1+\rho)|} = -\sum_{\rho} \frac{1}{\rho^2}\Big(\sum_{n=0}^{\infty} \frac{c_n}{\rho^n}\Big) \tag{2.48}$$

and, since from Lemmas 2.12 and 2.13 the sum $\sum_{\rho,n} (c_n/|\rho|^{n+2})$ is finite, we may permute the summations in (2.48), which yields (2.46). □

By using Lemmas 2.12–2.14 together with formula (2.41), it is possible to compute c defined in (1.10) with great precision.

LEMMA 2.15. *Under the Riemann hypothesis,* $\sum_\rho (1/\Im(\rho)^2) \le 0.046\,249\,3$.

PROOF. Let us set $\rho = 1/2 + \imath\gamma$. From (2.42) we have $|\gamma| \ge 14.134$, and from (2.44) we have

$$\sum_\rho \frac{1}{\gamma^2} = \sum_\rho \frac{1 + 1/(4\gamma^2)}{1/4 + \gamma^2} \le \sum_\rho \frac{1 + \frac{1}{4\times 14.134^2}}{1/4+\gamma^2}$$
$$= \Big(1 + \frac{1}{4\times 14.134^2}\Big)\sum_\rho \frac{1}{|\rho|^2} \le 0.046\,249\,3.$$

A more precise estimate can be obtained by writing $\gamma^2 = -(\rho - 1/2)^2$:

$$\sum_\rho \frac{1}{\gamma^2} = \sum_\rho -\frac{(1-1/(2\rho))^{-2}}{\rho^2} = -\sum_{m=0}^{\infty} \frac{m+1}{2^m}\Big(\sum_\rho \frac{1}{\rho^{m+2}}\Big).$$

To calculate the above series, choose some $M > 0$. For $m \le M$, use (2.41), and for $m > M$, use Lemma 2.12 to get an upper bound for the remainder. □

3. Computation of $h(n)$

For n small, a table of $h(n)$ for $n \le 10^6$ has been precomputed by the naive algorithm described in [7, Section 1.4].

For the computation of $h(n)$ for n large, the algorithm described in [7] is used. Let us recall some points about it.

3.1. Computing an isolated value of $h(n)$ or $\log h(n)$ for n possibly large.

- *The factorization of* $h(n)$. Let $k = k(n)$ be defined above by (1.13). The value $h(n)$ may be written as the product (see [7, Section 8])

  $$h(n) = N_k \cdot G(p_k, n - \sigma_k), \tag{3.1}$$

  where $G(p, m)$ is defined in [9] by

  $$G(p,m) = \max \frac{Q_1 Q_2 \cdots Q_s}{q_1 q_2 \cdots q_s},$$

  the maximum being taken over the primes $Q_1, Q_2, \ldots, Q_s, q_1, q_2, \ldots, q_s$, $s \ge 0$, satisfying

  $$2 \le q_s < q_{s-1} < \cdots < q_1 \le p_k < Q_1 < Q_2 < \cdots < Q_s \quad \text{and} \quad \sum_{i=1}^{s} (Q_i - q_i) \le m.$$

  Of course, $h(n)$ is an integer, and equation (3.1) says that the prime factors of $h(n)$ are

  $$(\{p_1, p_2, \ldots, p_k\} \setminus \{q_1, q_2, \ldots, q_s\}) \cup \{Q_1, Q_2, \ldots, Q_s\}. \tag{3.2}$$

Thus the computation of p_k and $G(p_k, n-\sigma_k)$ gives the factorization of $h(n)$. We remark that, for large values of n, say $n \geq 10^{30}$, this factorization is not really effective because we are not able to enumerate the primes $p_1, p_2, \ldots, p_k$.

- *Computing* $G(p_k, n-\sigma_k)$. The execution of the algorithm described in [9, Section 9] is relatively fast and shows that s is small and that, with the exception of the smallest one, q_s, all primes of $\{q_1, q_2, \ldots, q_s\} \cup \{Q_1, Q_2, \ldots, Q_s\}$ are very close to p_k. But we are unable to prove this fact, nor evaluate the complexity of this algorithm, nor even its termination. The time for computing 1000 values $G(p_k, n-\sigma_k)$ for n close to 10^8 is about 4 seconds.
- *Computing* p_k *and* σ_k. For small values of n, say $n \leq 10^{18}$, the trivial method may be used: we add the first j primes until the sum σ_j exceeds n. If n is very large, say $n > 10^{24}$, this is impracticable. But the Lagarias–Miller–Odlysko algorithm for computing $\pi(x)$, improved by Deléglise and Rivat to cost $O(x^{2/3}/\log^2 x)$ operations (see [10]), may be adapted to compute at the same cost sums of the form $S_f(x) = \sum_{p\leq x} f(p)$ where f is a completely multiplicative function. Choosing $f(x) = x$, we are able to compute $\pi_1(x) = \sum_{p\leq x} p$ with the same complexity, and also to compute p_k and s_k in time $O(n^{1/3}/(\log n)^{5/3})$ (see [7, Section 8] for more details).
- *Computing* $\log(h(n))$. Once p_k, s_k and $G(p_k, n-s_k)$ are computed, from the prime factors (3.2) of $h(n)$ we get

$$\log h(n) = \theta(p_k) + \sum_{1\leq j\leq s} \log(Q_j) - \sum_{1\leq j\leq s} \log(q_j).$$

  The last two terms of this sum are obtained by computing a small number of log values, the $(\log q_i)_{1\leq i\leq s}$ and $(\log Q_i)_{1\leq i\leq s}$. It remains to compute $\theta(p_k)$. If p_k is small, say $p_k \leq 10^{10}$, we may use the naive algorithm, enumerate the primes up to p_k and add their logarithms. If p_k is large, the naive algorithm is too slow.
  To compute $\theta(x)$ more efficiently, we first compute $\psi(x)$ in $O(x^{2/3+\epsilon})$, using the algorithm given in [11], and then add the difference $\psi(x) - \theta(x)$ which is easily computed in time $O(x^{1/2+\epsilon})$ by the naive algorithm (see [25]). Some values of $\theta(x)$ for x up to 10^{18} are given in [26]. Table 1 shows, for $2 \leq n \leq 18$, the largest prime $p_k < 10^n$, $\theta(p_k) = \log h(\sigma_k)$ and b_{σ_k}.

3.2. The computations we did for this work.

Computation of all the b_{σ_k} *for* $p_k \leq 10\,000\,000\,019$. For the proof of (5.42) and (5.43) in Proposition 5.11 we need to compute b_{σ_k} for all the primes $p_k \leq 10^{10} + 19$. The sophisticated method presented in [25] to compute $\theta(p_k)$ is useless because each value $\theta(p_k)$ we need is obtained at once from the previous one $\theta(p_{k-1})$ by adding $\log p_k$.

We enumerate the 455 052 512 primes up to $p_{455\,052\,712} = 10\,000\,000\,019$, computing for each of them σ_k, $\log h(\sigma_k) = \theta(p_k)$ and b_{σ_k}. This was the most expensive computation we did. It took about 7 hours.

Computation of isolated values of $h(n)$. For the proof of (5.44) in Proposition 5.11 we compute isolated values of b_n for $n \leq n_1 = 305\,926\,023$. Here also, for these small

TABLE 1. Values of p_k, $\theta(p_k)$, b_{σ_k}, where p_k is the largest prime less than 10^n.

10^n	p_k	$\theta(10^n) = \theta(p_k) = \log(h(\sigma_k))$	b_{σ_k}
10^2	97	83.7283903990639229450269228	0.7971418778
10^3	997	956.245265120058867812401516	0.8664331562
10^4	9 973	9895.99137915698731266894967	0.8251657523
10^5	99 991	99685.3892686125508366238513	0.7737525640
10^6	999 983	998484.175025634292133973037	0.7367904834
10^7	9 999 991	9.99517931785631189684434575e6	0.7143942804
10^8	99 999 989	9.99877300180220043832124342e7	0.7140806334
10^9	999 999 937	9.99968978577566144799126238e8	0.7031135733
10^{10}	9 999 999 967	9.99993983065775738415922199e9	0.6775769607
10^{11}	99 999 999 977	9.99997376531074446948519125e10	0.6722402061
10^{12}	999 999 999 989	9.99999030333096224636996079e11	0.6691580533
10^{13}	9 999 999 999 971	9.99999698829303419965318214e12	0.6701952673
10^{14}	99 999 999 999 973	9.99999905732469785384070303e13	0.6750588408
10^{15}	999 999 999 999 989	9.99999965752660939840767064e14	0.6751612720
10^{16}	9 999 999 999 999 937	9.99999988771710403489939845e15	0.6632601747
10^{17}	99 999 999 999 999 997	9.99999997065823724523710638e16	0.6521858401
10^{18}	999 999 999 999 999 989	9.99999999144115634512109067e17	0.6693675714

values of n we do not need the method presented in [25] to speed up the computations of the $\theta(p_k)$ values. We content ourselves with using a precomputed table of (σ_k, θ_k) values. The essential cost of each computation of $h(n)$ is then reduced to the cost of computation of $G(p_k, n - \sigma_k)$.

4. Estimates of b_n

In the proof of Theorem 1.1 we shall use Lemmas 4.1–4.4. The first of these establishes a property of concavity (see Figure 1 which displays the graph of (n, b_n) for $2 \le n \le 100$).

LEMMA 4.1. *Let b_n be defined by (1.9) and $k = k(n)$ by (1.13). For each $n \ge 2$, if* $\min(b_{\sigma_k}, b_{\sigma_{k+1}}) \le 1$, *then*

$$b_n \ge \min(b_{\sigma_k}, b_{\sigma_{k+1}}).$$

PROOF. Computation shows that $b_n \ge \min(b_{\sigma_k}, b_{\sigma_{k+1}})$ is satisfied if $n < 41 = \sigma_6$. Thus we may suppose $n \ge 41$. Let us set $\varepsilon = (\log p_{k+1})/p_{k+1}$. The function $\varphi(t) = \log t - \varepsilon t$ is concave for $t > 1$. For $k \ge 2$, we have $\varphi(2) = \log 2 - 2\log p_{k+1}/p_{k+1} \ge \log 2 - 2\log 5/5 > 0$ and $\varphi(p_{k+1}) = 0$. Let q denote an arbitrary prime number. Thus $\varphi(q)$ is greater than or equal to 0 for $2 \le q \le p_k$ and less than or equal to 0 for $q \ge p_{k+1}$. Then, for each squarefree integer N,

$$\log N - \varepsilon\ell(N) = \sum_{q \mid N} \varphi(q) \le \sum_{q \mid N,\ q \le p_k} \varphi(q) \le \sum_{q \le p_k} \varphi(q)$$
$$= \log N_k - \varepsilon\sigma_k = \log N_{k+1} - \varepsilon\sigma_{k+1}. \tag{4.1}$$

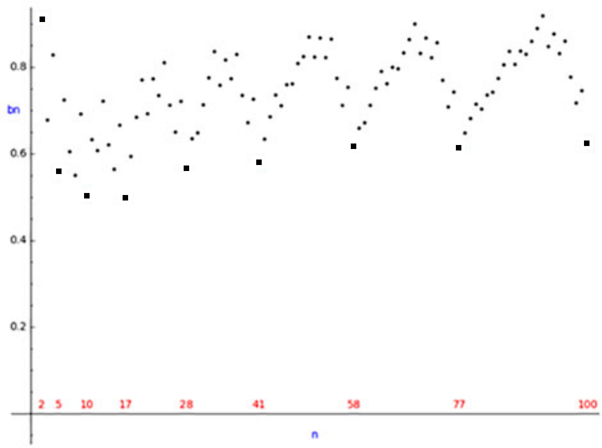

FIGURE 1. Graph of $(n, b_n)_{2\le n\le 100}$. The black squares are the (σ_k, b_{σ_k}) points.

We write

$$n = \alpha\sigma_k + \beta\sigma_{k+1} \quad \text{with } 0 \le \alpha \le 1 \text{ and } \beta = 1 - \alpha. \tag{4.2}$$

From (1.1), $\ell(h(n)) \le n$ holds and applying (4.1) to $N = h(n)$ yields

$$\begin{aligned} \log h(n) &\le \varepsilon\ell(h(n)) + \log N_k - \varepsilon\sigma_k \le \varepsilon n + \log N_k - \varepsilon\sigma_k \\ &= \varepsilon(\alpha\sigma_k + \beta\sigma_{k+1}) + \alpha(\log N_k - \varepsilon\sigma_k) + \beta(\log N_{k+1} - \varepsilon\sigma_{k+1}) \\ &= \alpha \log N_k + \beta \log N_{k+1}. \end{aligned} \tag{4.3}$$

Let us define $\Phi(t)$ on each interval $[\sigma_k, \sigma_{k+1}]$ by

$$\Phi(t) = \sqrt{\mathrm{li}^{-1}(t)} - \min(b_{\sigma_k}, b_{\sigma_{k+1}})(t \log t)^{1/4}. \tag{4.4}$$

Since $\min(b_{\sigma_k}, b_{\sigma_{k+1}}) \le 1$ and $\sigma_k \ge 31$ are assumed, from Lemma 2.5, Φ is concave on $[\sigma_k, \sigma_{k+1}]$. Moreover, from the definition of b_{σ_k} and $b_{\sigma_{k+1}}$, we have $\log N_k = \log h(\sigma_k) = \sqrt{\mathrm{li}^{-1}(\sigma_k)} - b_{\sigma_k}(\sigma_k \log \sigma_k)^{1/4} \le \Phi(\sigma_k)$ and $\log N_{k+1} = \log h(\sigma_{k+1}) \le \Phi(\sigma_{k+1})$, which, from (4.3) and (4.2), implies

$$\log h(n) \le \alpha \log N_k + \beta \log N_{k+1} \le \alpha\, \Phi(\sigma_k) + \beta\, \Phi(\sigma_{k+1}) \le \Phi(\alpha\sigma_k + \beta\sigma_{k+1}) = \Phi(n).$$

With (1.9) defining b_n and (4.4), this gives $b_n \ge \min(b_{\sigma_k}, b_{\sigma_{k+1}})$. □

LEMMA 4.2. *Let n_1, n_2 be integers such that $2 \le n_1 < n_2$. If $\sqrt{\mathrm{li}^{-1}(n_2)} \ge \log h(n_1)$ then, for $n_1 \le n \le n_2$,*

$$b_n \le \frac{\sqrt{\mathrm{li}^{-1}(n_2)} - \log h(n_1)}{(n_1 \log n_1)^{1/4}}.$$

PROOF. This results from formula (1.9), defining b_n, and from the nondecreasingness of $\sqrt{\mathrm{li}^{-1}}$, $\log h$ and $n\log n$. □

LEMMA 4.3. *Let $\mu > 0$, n_1, n_2 be integers such that $16 \le n_1 < n_2$ and*

$$\frac{\sqrt{\mathrm{li}^{-1}(n_2)} - \log h(n_1)}{(n_1\log n_1)^{1/4}} \le \frac{2}{3} + c + \mu\frac{\log\log n_2}{\log n_2}. \tag{4.5}$$

Then

$$b_n < \frac{2}{3} + c + \mu\,\frac{\log\log n}{\log n} \tag{4.6}$$

holds for each $n \in [n_1, n_2]$.

PROOF. We have $b_n \le (\sqrt{\mathrm{li}^{-1}(n_2)} - \log h(n_1)/(n\log n)^{1/4})$. If $\sqrt{\mathrm{li}^{-1}(n_2)} - \log h(n_1) \le 0$, then $b_n \le 0$ and (4.6) holds. If $\sqrt{\mathrm{li}^{-1}(n_2)} - \log h(n_1) > 0$, (4.6) results from (4.5) and the decreasingness of $c + 2/3 + \mu\log\log n/\log n$ for $n \ge 16$. □

LEMMA 4.4. *Let p_k satisfy $p_k \ge x_0 = 10^{10} + 19$, $\sigma_k = \sum_{p\le p_k} p \ge n_0 = \pi_1(x_0)$, and n be an integer such that $\sigma_k \le n \le \sigma_{k+1}$. Then*

$$\frac{1}{\log\sigma_k} \ge \frac{1}{\log n} > \frac{1}{(1 + 3\times 10^{-10})\log\sigma_k} \tag{4.7}$$

and

$$\sqrt{\mathrm{li}^{-1}(n)} - \sqrt{\mathrm{li}^{-1}(\sigma_k)} \le 1.14\log\sigma_k. \tag{4.8}$$

PROOF. First, from Bertrand's postulate, we have $p_{k+1} < 2p_k$ and

$$n - \sigma_k \le \sigma_{k+1} - \sigma_k = p_{k+1} < 2p_k.$$

From Lemma 2.10, as $\sigma_k = \pi_1(p_k)$ holds, we have

$$\begin{aligned} p_k &\le \sqrt{\sigma_k\log\sigma_k}\Big(1 + \frac{\log\log\sigma_k}{2\log\sigma_k}\Big) \le \Big(1 + \frac{\log\log n_0}{2\log n_0}\Big)\sqrt{\sigma_k\log\sigma_k} \\ &< 1.045\sqrt{\sigma_k\log\sigma_k}, \end{aligned}$$

so that

$$n \le \sigma_{k+1} < \sigma_k + 2p_k < \sigma_k + 2.09\sqrt{\sigma_k\log\sigma_k} = \sigma_k\Big(1 + 2.09\sqrt{\frac{\log\sigma_k}{\sigma_k}}\Big) \tag{4.9}$$

holds. Furthermore, we obtain

$$\begin{aligned} \log n &\le \log\sigma_k + 2.09\sqrt{\frac{\log\sigma_k}{\sigma_k}} = \log\sigma_k\Big(1 + \frac{2.09}{\sqrt{\sigma_k\log\sigma_k}}\Big) \\ &\le \log\sigma_k\Big(1 + \frac{2.09}{\sqrt{n_0\log n_0}}\Big) < (1 + 3\times 10^{-10})\log\sigma_k, \end{aligned}$$

which implies (4.7).

Let us set $f(t) = \sqrt{\mathrm{li}^{-1}(t)}$. From Lemma 2.5, we know that $f'(t) = (\log \mathrm{li}^{-1}(t)/2\sqrt{\mathrm{li}^{-1}(t)})$ is positive and decreasing for $\mathrm{li}^{-1}(t) > e^2$. By the mean value theorem, we have $f(n) - f(\sigma_k) \le (n-\sigma_k) f'(\sigma_k)$ and, from (4.9) and (2.15),

$$\begin{aligned}\sqrt{\mathrm{li}^{-1}(n)} - \sqrt{\mathrm{li}^{-1}(\sigma_k)} &\le (n-\sigma_k)\frac{\log \mathrm{li}^{-1}(\sigma_k)}{2\sqrt{\mathrm{li}^{-1}(\sigma_k)}} \le 2.09\sqrt{\sigma_k \log \sigma_k}\,\frac{\log(\sigma_k \log \sigma_k)}{2\sqrt{\sigma_k \log \sigma_k}}\\ &= 1.045 \log \sigma_k \Big(1 + \frac{\log\log \sigma_k}{\log \sigma_k}\Big)\\ &\le 1.045\Big(1+\frac{\log\log n_0}{\log n_0}\Big)\log \sigma_k = 1.1376\ldots \log \sigma_k,\end{aligned}$$

which proves (4.8). □

5. Proof of Theorem 1.1

Let x satisfy $p_k \le x < p_{k+1}$. Then, from (1.12) and (1.14),

$$\sigma_k = \pi_1(x), \qquad \log h(\sigma_k) = \log N_k = \theta(x)$$

and, from (1.9),

$$b_{\sigma_k} = \frac{\sqrt{\mathrm{li}^{-1}(\pi_1(x))} - \theta(x)}{(\pi_1(x)\log \pi_1(x))^{1/4}}.$$

The aim of Sections 5.1–5.4 is to obtain, under the Riemann hypothesis, an effective estimate of the numerator of b_{σ_k}.

5.1. Estimate of li($\theta^2(x)$).

Lemma 5.1. *Under the Riemann hypothesis, for* $x \ge x_0 = 10^{10} + 19$,

$$\mathrm{li}(\theta^2(x)) = \mathrm{li}(x^2) + \frac{x}{\log x}(\theta(x) - x) + K_1(x) \tag{5.1}$$

with $0 \le K_1(x) \le 0.0008 x \log^3 x$.

Proof. Let us assume that $x \ge x_0$ holds. Applying Taylor's formula to the function $t \mapsto \mathrm{li}(t^2)$ yields

$$\mathrm{li}(\theta^2(x)) = \mathrm{li}(x^2) + \frac{x}{\log x}(\theta(x) - x) + K_1(x)$$

with

$$K_1(x) = \Big(\frac{1}{\log v} - \frac{1}{\log^2 v}\Big)\frac{(\theta(x)-x)^2}{2}, \tag{5.2}$$

where v satisfies $v \ge \min(x, \theta(x))$. From (2.3), we get

$$\frac{\theta(x)}{x} \ge 1 - \frac{\log^2 x}{8\pi\sqrt{x}} \ge 1 - \frac{\log^2 x_0}{8\pi\sqrt{x_0}} \ge 0.9997$$

and $v \geq 0.9997x$ holds. Setting $\varepsilon = -\log 0.9997$ yields $\log v \geq \log x - \varepsilon$ and

$$0 < \frac{1}{\log v} - \frac{1}{\log^2 v} < \frac{1}{\log v} \leq \frac{1}{\log x - \varepsilon} = \frac{1}{\log x}\Big(1 + \frac{\varepsilon}{\log x - \varepsilon}\Big)$$
$$\leq \frac{1}{\log x}\Big(1 + \frac{\varepsilon}{\log x_0 - \varepsilon}\Big) \leq \frac{1.000\,014}{\log x}.$$

Finally, (2.3) and (5.2) imply $0 \leq K_1(x) \leq (1.000\,014/2\log x)((1/8\pi)\sqrt{x}\log^2 x)^2 \leq 0.000\,792\, x \log^3 x$, which completes the proof of (5.1). □

5.2. Estimate of $\Pi_1(x) - \pi_1(x)$.

Lemma 5.2. *Under the Riemann hypothesis, for $x \geq x_0 = 10^{10} + 19$,*

$$\Pi_1(x) = \sum_{p^m \leq x} \frac{p^m}{m} = \mathrm{li}(x^2) - \sum_\rho \frac{x^{\rho+1}}{(\rho+1)\log x} + \frac{x\Lambda(x)}{2\log x} + K_2(x) \tag{5.3}$$

with $|K_2(x)| \leq 0.04625(x^{3/2}/\log^2 x)$.

Proof. In view of (2.38), we first consider the integral $\int_{-1}^{\infty}(x^{\rho-t}/\rho - t)\,dt$ where ρ is a nontrivial zero of ζ. Partial integration yields

$$\int_{-1}^{\infty} \frac{x^{\rho-t}}{\rho - t}\,dt = \frac{x^{\rho+1}}{(\rho+1)\log x} + J_\rho(x) \quad \text{with } J_\rho(x) = \frac{x^\rho}{\log x}\int_{-1}^{\infty}\frac{e^{-t\log x}}{(\rho - t)^2}\,dt,$$

and, since $\Re(\rho) = 1/2$,

$$|J_\rho(x)| \leq \frac{\sqrt{x}}{\log x}\int_{-1}^{\infty}\frac{e^{-t\log x}}{\Im(\rho)^2}\,dt = \frac{x^{3/2}}{(\log^2 x)\Im(\rho)^2}.$$

Let us set $J(x) = \sum_\rho J_\rho(x)$. Applying Lemma 2.15 yields

$$|J(x)| = \Big|\sum_\rho J_\rho(x)\Big| \leq \frac{x^{3/2}}{\log^2 x}\sum_\rho \frac{1}{\Im(\rho)^2} \leq 0.046\,249\,3\frac{x^{3/2}}{\log^2 x},$$

and (2.38) implies

$$\Pi_1(x) = \mathrm{li}(x^2) + \frac{x\Lambda(x)}{2\log x} - \sum_\rho \frac{x^{\rho+1}}{(\rho+1)\log x} + K_2(x) \tag{5.4}$$

with

$$K_2(x) = -\log 12 - J(x) + \int_x^{\infty}\frac{dt}{(t^2-1)\log t}.$$

For $t \geq x \geq 2$, we have $(1/(t^2-1)\log t) \leq (4/3t^2\log x)$ and

$$\int_x^{\infty}\frac{dt}{(t^2-1)\log t} \leq \frac{4}{3\log x}\int_x^{\infty}\frac{dt}{t^2} = \frac{4}{3\,x\log x}$$

so that

$$|K_2(x)| \le \frac{x^{3/2}}{\log^2 x}\Big(0.046\,249\,3 + \frac{4\log x}{3x^{5/2}} + \frac{(\log 12)\log^2 x}{x^{3/2}}\Big). \tag{5.5}$$

In (5.5), the expression in parentheses is decreasing for $x \ge x_0$ and its value for $x = x_0$ is less than 0.04625, which, together with (5.4), completes the proof of (5.3). □

LEMMA 5.3. *For $x \ge 2$,*

$$\Pi_1(x) - \pi_1(x) = \frac{x}{\log x}(\psi(x) - \theta(x)) - \sum_{k=2}^{\kappa} B_k, \quad \text{with } \kappa = \Big\lfloor \frac{\log x}{\log 2} \Big\rfloor, \tag{5.6}$$

and

$$B_k = \frac{1}{k}\int_2^{x^{1/k}} \frac{t^{k-1}}{\log^2 t}(k\log t - 1)\theta(t)\,dt. \tag{5.7}$$

PROOF. From the definition of Π_1,

$$\Pi_1(x) - \pi_1(x) = \sum_{k=2}^{\kappa} \sum_{p \le x^{1/k}} \frac{p^k}{k} = \sum_{k=2}^{\kappa} \frac{\pi_k(x^{1/k})}{k},$$

and, by Stieltjes integral,

$$\pi_k(y) = \int_{2^-}^{y} \frac{t^k}{\log t}\,d[\theta(t)] = \frac{\theta(y)y^k}{\log y} - \int_2^y \frac{t^{k-1}}{\log^2 t}(k\log t - 1)\theta(t)\,dt,$$

so that

$$\begin{aligned}\Pi_1(x) - \pi_1(x) &= \sum_{k=2}^{\kappa} \frac{\theta(x^{1/k})x}{k(\log x)/k} - \sum_{k=2}^{\kappa} \frac{1}{k}\int_2^{x^{1/k}} \frac{t^{k-1}}{\log^2 t}(k\log t - 1)\theta(t)\,dt \\ &= \frac{x}{\log x}(\psi(x) - \theta(x)) - \sum_{k=2}^{\kappa} B_k.\end{aligned}$$

□

5.3. Bounding $\sum_{k=2}^{+\infty} B_k$.

PROPOSITION 5.4. *Under the Riemann hypothesis, for $x \ge x_0 = 10^{10} + 19$ and $\kappa = \lfloor \log x/\log 2 \rfloor$, B_k defined by (5.7) satisfies*

$$\frac{2x^{3/2}}{3\log x} - 0.327\,\frac{x^{3/2}}{\log^2 x} \le \sum_{k=2}^{\kappa} B_k \le \frac{2x^{3/2}}{3\log x} + 0.31\,\frac{x^{3/2}}{\log^2 x}. \tag{5.8}$$

PROOF. The proof of this proposition is rather technical. We begin by establishing some lemmas. For $k \le \kappa$, we have $x^{1/k} \ge x^{\log 2/\log x} = 2$, and for $t \ge 2$ and $k \ge 2$, we have $k\log t > 1$, so that $B_k > 0$ holds.

LEMMA 5.5. *For $x \ge x_0$, we have the bounds*

$$0 \le \sum_{k=3}^{\kappa} B_k \le 1.066\frac{x^{4/3}}{\log x}. \tag{5.9}$$

PROOF. Using (2.1) and (2.5), we have

$$B_k \le \frac{1+\epsilon}{k}\int_2^{x^{1/k}} \frac{kt^k}{\log t}\,dt = (1+\epsilon)(\mathrm{li}(x^{1+1/k}) - \mathrm{li}(2^{k+1})) \le (1+\epsilon)\,\mathrm{li}(x^{1+1/k}),$$

with $\epsilon = 7.5\times 10^{-7}$. Now, by (2.10),

$$B_k \le (1+\epsilon)\frac{x^{1+1/k}}{\log x^{1+1/k}}\Big(1+\frac{1.101}{\log x_0}\Big) \le \frac{1.05\,x^{1+1/k}}{(1+1/k)\log x}. \tag{5.10}$$

The hypothesis $x \ge x_0$ implies $\kappa \ge 33$. Furthermore,

$$\begin{aligned}\sum_{k=3}^{\kappa} B_k &\le \frac{1.05x^{4/3}}{\log x}\Big(\sum_{k=3}^{26}\frac{x^{1/k-1/3}}{1+1/k} + \frac{\log x}{\log 2}\,x^{1/27-1/3}\Big)\\ &\le \frac{1.05x^{4/3}}{\log x}\Big(\sum_{k=3}^{26}\frac{x_0^{1/k-1/3}}{1+1/k} + \frac{\log x_0}{\log 2}\,x_0^{1/27-1/3}\Big) < 1.066\frac{x^{4/3}}{\log x}.\end{aligned}$$ □

The upper bound (5.10) is good for $k \ge 3$, but for $k = 2$ we need a better one. For $a \in \mathbb{C}$, let us define

$$I_a = \frac{1}{2}\int_2^{\sqrt{x}} F(t)t^a\,dt, \quad \text{with } F(t) = \frac{2t}{\log t} - \frac{t}{\log^2 t}.$$

LEMMA 5.6. *For a belonging to $\{0, \frac{1}{3}, \frac{1}{2}, 1\}$ and $x \ge x_0 = 10^{10} + 19$,*

$$I_a = \frac{2}{a+2}\,\frac{x^{(a+2)/2}}{\log x} - \frac{2a\eta x^{(a+2)/2}}{(a+2)^2\log^2 x} + \delta_a, \tag{5.11}$$

with $1 < \eta < 1.101$ and $-3.15 < \delta_a < -2.88$.

PROOF. From (2.5), we have $\int F(t)t^a\,dt = -a\,\mathrm{li}(t^{2+a}) + t^{2+a}/\log t$ and

$$I_a = -\frac{a}{2}\,\mathrm{li}(x^{(a+2)/2}) + \frac{x^{(a+2)/2}}{\log x} + \delta_a \quad \text{with } \delta_a = \frac{a}{2}\,\mathrm{li}(2^{a+2}) - \frac{2^{a+2}}{2\log 2},$$

where δ_a satisfies $-3.15 < \delta_a < -2.88$. Further, by using inequalities (2.7) and (2.10), for $x \ge x_0$, we obtain

$$\mathrm{li}(x^{(a+2)/2}) = \frac{2\,x^{(a+2)/2}}{(a+2)\log x} + \eta\frac{4\,x^{(a+2)/2}}{(a+2)^2\log^2 x},$$

with $1 < \eta < 1.101$, whence we get (5.11). □

In view of applying the explicit formula (2.37), we shall need an estimate of $S = \sum_\rho I_\rho/\rho$ where ρ is a nontrivial zero of ζ.

LEMMA 5.7. *Note that $S = \sum_\rho (I_\rho/\rho)$. Under the Riemann hypothesis, for $x \ge x_0$, we have $|S| \le 0.148x^{5/4}/\log x$.*

PROOF. Partial integration yields

$$I_\rho = \frac{1}{2}\int_2^{\sqrt{x}} F(t)t^\rho\,dt = \frac{1}{2}\int_2^{\sqrt{x}}\Big(\frac{2t}{\log t} - \frac{t}{\log^2 t}\Big)t^\rho\,dt$$
$$= \frac{x^{(\rho+2)/2}}{\rho+1}\Big(\frac{2}{\log x} - \frac{2}{\log^2 x}\Big) - \frac{2^{\rho+1}}{\rho+1}\Big(\frac{2}{\log 2} - \frac{1}{\log^2 2}\Big) - \int_2^{\sqrt{x}} \frac{t^{\rho+1}}{2(\rho+1)}F'(t)\,dt$$

and, since $F'(t)$ satisfies, for $t \geq 2$,

$$0 \leq F'(t) = \frac{2\log^2 t - 3\log t + 2}{\log^3 t} \leq \frac{2\log^2 t}{\log^3 t} = \frac{2}{\log t},$$

we have, from (2.5) and $\Re(\rho) = 1/2$,

$$|(\rho+1)I_\rho| \leq \frac{2x^{5/4}}{\log x} + \frac{2^{3/2}(2 - 1/\log 2)}{\log 2} + \int_2^{\sqrt{x}} \frac{t^{3/2}}{\log t}\,dt$$
$$= \frac{2x^{5/4}}{\log x} + \mathrm{li}(x^{5/4}) - \mathrm{li}(2^{5/2}) + \frac{2^{3/2}(2 - 1/\log 2)}{\log 2} \leq \frac{2x^{5/4}}{\log x} + \mathrm{li}(x^{5/4}). \quad (5.12)$$

Further, (5.12), (2.9) and (1.10) yield

$$|S| = \Big|\sum_\rho \frac{I_\rho}{\rho}\Big| \leq \Big(\sum_\rho \frac{1}{|\rho(\rho+1)|}\Big)\Big(\frac{2x^{5/4}}{\log x} + \mathrm{li}(x^{5/4})\Big)$$
$$\leq c\Big(2 + \frac{1.49}{5/4}\Big)\frac{x^{5/4}}{\log x} \leq 0.148\frac{x^{5/4}}{\log x}. \qquad \square$$

We now return to the proof of Proposition 5.4. From Lemma 2.1, it follows that

$$J - I_{1/2} - \frac{4}{3}I_{1/3} \leq B_2 \leq J - I_{1/2} + 2.14\, I_0 \quad \text{with } J = \frac{1}{2}\int_2^{\sqrt{x}} F(t)\psi(t)\,dt. \qquad (5.13)$$

Now, under the integral sign, we may replace $\psi(t)$ by its value in the explicit formula (2.37), and using equality (2.39) of Lemma 2.11, we obtain

$$J = I_1 - S - J_1 \quad \text{with } S = \sum_\rho \frac{1}{\rho} I_\rho$$

and

$$J_1 = \frac{1}{2}\int_2^{\sqrt{x}} F(t)\Big(\log(2\pi) + \frac{1}{2}\log\Big(1 - \frac{1}{t^2}\Big)\Big)\,dt.$$

For $t \geq 2$, we have $F(t) > 0$ and $0 < \log 2\pi + \frac{1}{2}\log\frac{3}{4} \leq \log 2\pi + \frac{1}{2}\log(1 - (1/t^2)) < \log 2\pi < 1.84$, whence

$$0 \leq J_1 \leq \log(2\pi) I_0 \leq 1.84\, I_0$$

and, with the upper bound of B_2 given by (5.13),

$$B_2 \leq I_1 + |S| - I_{1/2} + 2.14\, I_0.$$

From Lemmas 5.6 and 5.7, we obtain

$$B_2 \le \frac{2\,x^{3/2}}{3\log x} - \frac{2\,x^{3/2}}{9\log^2 x} - 2.88 + 0.148\frac{x^{5/4}}{\log x} - \frac{4x^{5/4}}{5\log x} + \frac{4.404x^{5/4}}{25\,\log^2 x} + 3.15 + 2.14\Big(\frac{x}{\log x} - 2.88\Big)$$
$$\le \frac{2x^{3/2}}{3\log x} - \frac{2x^{3/2}}{9\log^2 x} + \frac{x^{5/4}}{\log x}\Big(-\frac{4}{5} + 0.148 + \frac{17.616}{100\log x} + \frac{2.14}{x^{1/4}}\Big)$$

and, as the expression in parentheses above is decreasing for $x \ge x_0$ and its value for $x = x_0$ is negative, we get

$$B_2 \le \frac{2\,x^{3/2}}{3\log x} - \frac{2\,x^{3/2}}{9\log^2 x}.$$

We now use (5.9) to obtain

$$\sum_{k=2}^{\kappa} B_k \le \frac{2x^{3/2}}{3\log x} + \frac{x^{3/2}}{\log^2 x}\Big(-\frac{2}{9} + \frac{1.066\log x}{x^{1/6}}\Big)$$
$$\le \frac{2x^{3/2}}{3\log x} + \frac{x^{3/2}}{\log^2 x}\Big(-\frac{2}{9} + \frac{1.066\log x_0}{x_0^{1/6}}\Big) \le \frac{2x^{3/2}}{3\log x} + \frac{0.31x^{3/2}}{\log^2 x}, \tag{5.14}$$

which proves the upper bound of (5.8). Note that for $x > 8.48 \times 10^{12}$ the expression in parentheses in (5.14) is negative and that $\sum_{k=2}^{\kappa} B_k \le 2x^{3/2}/(3\log x)$.

Similarly, we have the lower bound

$$B_2 \ge J - I_{1/2} - \frac{4}{3}I_{1/3} \ge I_1 - |S| - J_1 - I_{1/2} - \frac{4}{3}I_{1/3}$$
$$\ge I_1 - |S| - 1.84\,I_0 - I_{1/2} - \frac{4}{3}I_{1/3}$$
$$\ge \Big(\frac{2x^{3/2}}{3\log x} - \frac{2.202\,x^{3/2}}{9\log^2 x} - 3.15\Big) - \Big(\frac{4x^{5/4}}{5\log x} - \frac{4}{25}\frac{x^{5/4}}{\log^2 x} - 2.88\Big) - 0.148\frac{x^{5/4}}{\log x}$$
$$-\frac{4}{3}\Big(\frac{6x^{7/6}}{7\log x} - \frac{6\,x^{7/6}}{49\log^2 x} - 2.88\Big) - 1.84\Big(\frac{x}{\log x} - 2.88\Big)$$
$$\ge \frac{2x^{3/2}}{3\log x} - \frac{2.202\,x^{3/2}}{9\log^2 x} - 0.948\frac{x^{5/4}}{\log x} - \frac{8x^{7/6}}{7\log x} - 1.84\frac{x}{\log x}$$
$$= \frac{2x^{3/2}}{3\log x} - \frac{x^{3/2}}{\log^2 x}\Big(\frac{2.202}{9} + \frac{0.948\log x}{x^{1/4}} + \frac{8\log x}{7x^{1/3}} + \frac{1.84\log x}{x^{1/2}}\Big)$$

and, as the expression in the final parentheses is decreasing on x for $x \ge x_0$ and its value for $x = x_0$ is < 0.327, we obtain

$$\sum_{k=2}^{\kappa} B_k \ge B_2 \ge \frac{2x^{3/2}}{3\log x} - 0.327\frac{x^{3/2}}{\log^2 x}$$

which completes the proof of Proposition 5.4. □

5.4. Estimate of $\mathrm{li}(\theta^2(x)) - \pi_1(x)$.

PROPOSITION 5.8. *Under the Riemann hypothesis, for $x \geq x_0 = 10^{10} + 19$,*

$$\left(\frac{2}{3} - c\right)\frac{x^{3/2}}{\log x} - 0.426\frac{x^{3/2}}{\log^2 x} \leq \pi_1(x) - \mathrm{li}(\theta^2(x)) \leq \left(\frac{2}{3} + c\right)\frac{x^{3/2}}{\log x} + 0.36\,\frac{x^{3/2}}{\log^2 x}, \quad (5.15)$$

with c defined in (1.10).

PROOF. From (5.1) and (5.3) we deduce

$$\begin{aligned}\mathrm{li}(\theta^2(x)) &= \Pi_1(x) - \frac{x\Lambda(x)}{2\log x} + \sum_\rho \frac{x^{\rho+1}}{(\rho+1)\log x} - K_2(x) + \frac{x}{\log x}(\theta(x) - x) + K_1(x) \\ &= \pi_1(x) + \sum_\rho \frac{x^{\rho+1}}{(\rho+1)\log x} + K_1(x) - K_2(x) + A(x), \qquad (5.16)\end{aligned}$$

with

$$A(x) = \Pi_1(x) - \pi_1(x) - \frac{x\Lambda(x)}{2\log x} + \frac{x}{\log x}(\theta(x) - x).$$

Further, from Equation (5.6) of Lemma 5.3 and from the explicit formula (2.37) of $\psi(t)$, we have

$$\begin{aligned}A(x) &= \frac{x}{\log x}(\psi(x) - x) - \frac{x\Lambda(x)}{2\log x} - \sum_{k=2}^{\kappa} B_k \\ &= \frac{x}{\log x}\left(-\sum_\rho \frac{x^\rho}{\rho} - \log(2\pi) - \frac{1}{2}\log\left(1 - \frac{1}{x^2}\right)\right) - \sum_{k=2}^{\kappa} B_k,\end{aligned}$$

and (5.16) implies $\mathrm{li}(\theta^2(x)) = \pi_1(x) - \sum_\rho (x^{\rho+1}/\rho(\rho+1)\log x) + K_3(x)$ with

$$K_3(x) = K_1(x) - K_2(x) - \frac{x}{\log x}\left(\log(2\pi) + \frac{1}{2}\log\left(1 - \frac{1}{x^2}\right)\right) - \sum_{k=2}^{\kappa} B_k.$$

For $x \geq x_0$, we have $0 < \log(2\pi) + \frac{1}{2}\log(1 - (1/x^2)) < \log(2\pi) \leq 1.84$, and from (5.1), (5.3) and (5.8), we obtain the upper bound

$$\begin{aligned}K_3(x) &\leq 0.0008x\log^3 x + \frac{0.04625\,x^{3/2}}{\log^2 x} - \frac{2x^{3/2}}{3\log x} + \frac{0.327\,x^{3/2}}{\log^2 x} \\ &= -\frac{2x^{3/2}}{3\log x} + \frac{x^{3/2}}{\log^2 x}\left(0.04625 + 0.327 + 0.0008\frac{\log^5 x}{x^{1/2}}\right) \\ &\leq -\frac{2x^{3/2}}{3\log x} + \frac{0.426\,x^{3/2}}{\log^2 x}\end{aligned}$$

for $x \ge x_0$. In the same way, we obtain the lower bound for $x \ge x_0$:

$$\begin{aligned} K_3(x) &\ge -\frac{0.04625x^{3/2}}{\log^2 x} - \frac{1.84x}{\log x} - \frac{2x^{3/2}}{3\log x} - \frac{0.31x^{3/2}}{\log^2 x} \\ &= -\frac{2x^{3/2}}{3\log x} - \frac{x^{3/2}}{\log^2 x}\Big(0.31 + 0.04625 + \frac{1.84\log x}{x^{1/2}}\Big) \\ &\ge -\frac{2x^{3/2}}{3\log x} - \Big(0.31 + 0.04625 + \frac{1.84\log x_0}{x_0^{1/2}}\Big)\frac{x^{3/2}}{\log^2 x} \\ &\ge -\frac{2x^{3/2}}{3\log x} - 0.3567\frac{x^{3/2}}{\log^2 x}, \end{aligned}$$

which completes the proof of Proposition 5.8. □

5.5. Bounds of b_n for n large. For convenience, in this and the next section we will use the following notation:

$$\begin{gathered} x = p_k \ge x_0 = 10^{10} + 19, \quad \sigma = \sigma_k = \pi_1(x), \\ L = \log\sigma \ge L_0, \quad \lambda = \log L \ge \lambda_0, \quad \nu = \lambda/L \le \nu_0. \end{gathered} \tag{5.17}$$

Proposition 5.9. *Assume the Riemann hypothesis. Let $n \ge n_0$, b_n be defined by (1.9) and c by (1.10). Then*

$$\frac{2}{3} - c - 0.22\frac{\log\log n}{\log n} < b_n < \frac{2}{3} + c + 0.77\frac{\log\log n}{\log n}. \tag{5.18}$$

Proof. First, in Sections 5.5.1 and 5.5.2, we consider the case $n = \sigma_k = \pi_1(x)$.

5.5.1. Lower bound of b_{σ_k}. By (5.15), (5.17) and the fact that $0.69(2/3 - c) > 0.426$, we can write

$$\mathrm{li}(\theta^2(x)) \le \pi_1(x) - \delta = \sigma - \delta \quad \text{with } \delta = \Big(\frac{2}{3} - c\Big)\frac{x^{3/2}}{\log x}\Big(1 - \frac{0.69}{\log x}\Big). \tag{5.19}$$

From (1.14), we have $\theta(x) = \log N_k = \log h(\sigma)$. As $\sigma = \sum_{p\le x} p < x^2$, we have $\log\sigma < 2\log x$ and $1 - 0.69/\log x > 1 - 1.38/\log\sigma \ge 1 - 1.38\lambda/(\lambda_0 L) = 1 - 1.38\nu/\lambda_0 > 1 - 0.37\nu$ so that

$$\delta \ge \Big(\frac{2}{3} - c\Big)\frac{x^{3/2}}{\log x}(1 - 0.37\,\nu). \tag{5.20}$$

Further, since the function $t \mapsto t^{3/2}/\log t$ is increasing, from (2.28), we obtain

$$\frac{x^{3/2}}{\log x} \ge \frac{(\sigma\log\sigma)^{3/4}(1 + 0.365\nu)^{3/2}}{\frac{1}{2}L + \frac{1}{2}\lambda + \log(1 + 0.365\nu)} \ge \frac{(\sigma\log\sigma)^{3/4}(1 + 0.365\nu)^{3/2}}{\frac{1}{2}L + \frac{1}{2}\lambda + 0.365\nu}$$

which, as the denominator satisfies

$$\frac{L}{2} + \frac{\lambda}{2} + 0.365\nu = \frac{L}{2}\Big(1 + \nu\Big(1 + \frac{0.73}{L}\Big)\Big) \le \frac{L}{2}\Big(1 + \nu\Big(1 + \frac{0.73}{L_0}\Big)\Big) \le \frac{L}{2}(1 + 1.018\nu),$$

yields

$$\frac{x^{3/2}}{\log x} \geq 2\Big(\frac{\sigma^3}{L}\Big)^{1/4}\frac{(1+0.365\nu)^{3/2}}{1+1.018\nu}. \tag{5.21}$$

For $t \geq \mathrm{li}(e^2) = 4.54\ldots$, the function $f(t) = \sqrt{\mathrm{li}^{-1}(t)}$ is increasing and concave (see Lemma 2.5) and we have

$$f'(t) = \frac{\log(\mathrm{li}^{-1}(t))}{2\sqrt{\mathrm{li}^{-1}(t)}} \quad \text{and} \quad f''(t) = \frac{\log(\mathrm{li}^{-1}(t))(2-\log(\mathrm{li}^{-1}(t))}{4(\mathrm{li}^{-1}(t))^{3/2}}.$$

Inequality (5.19) with the increasingness of f gives $f(\mathrm{li}(\theta^2(x))) \leq f(\sigma-\delta)$. Applying Taylor's formula, with the concavity of f we get

$$\log h(\sigma) = \theta(x) = f(\mathrm{li}(\theta^2(x)) \leq f(\sigma-\delta) \leq \sqrt{\mathrm{li}^{-1}(\sigma)} - \delta f'(\sigma), \tag{5.22}$$

and we need a lower bound for $f'(\sigma)$. From (2.14), we have $\mathrm{li}^{-1}(\sigma) < \sigma(L+\lambda)$. As the function $t \mapsto \log(t)/(2\sqrt{t})$ is decreasing on t, we obtain

$$\begin{aligned} f'(\sigma) &= \frac{\log(\mathrm{li}^{-1}(\sigma))}{2\sqrt{\mathrm{li}^{-1}(\sigma)}} \geq \frac{\log(\sigma(L+\lambda))}{2\sqrt{\sigma(L+\lambda)}} = \frac{L+\lambda+\log(1+\nu)}{2\sqrt{\sigma(L+\lambda)}} \\ &\geq \frac{L+\lambda}{2\sqrt{\sigma(L+\lambda)}} = \frac{\sqrt{L(1+\nu)}}{2\sqrt{\sigma}}, \end{aligned} \tag{5.23}$$

and (5.20), (5.21) and (5.23) imply

$$\delta f'(\sigma) \geq \Big(\frac{2}{3}-c\Big)(\sigma\log\sigma)^{1/4}\frac{(1+0.365\nu)^{3/2}(1+\nu)^{1/2}(1-0.37\nu)}{1+1.018\nu}. \tag{5.24}$$

We observe that

$$\begin{aligned} &(1+0.365\nu)^3(1+\nu)(1-0.37\nu)^2 - (1+1.018\nu)^2(1-0.3405)^2 \\ &\quad = 0.315\,526\,75\,\nu^2 + 0.098\,730\,42\nu^3 - 0.198\,647\,103\,641\nu^4 \\ &\qquad +0.025\,388\,488\,412\,5\nu^5 + 0.006\,657\,053\,412\,5\nu^6. \end{aligned}$$

The above polynomial is positive for $0 < \nu \leq 1$, which implies that in (5.24) the fraction is $>1-0.3405\nu$ and

$$\delta f'(\sigma) \geq (\tfrac{2}{3}-c)(\sigma\log\sigma)^{1/4}(1-0.3405\nu).$$

Therefore, from the definition (1.9) of b_n and (5.22), for $p_k \geq x_0$, we have

$$\begin{aligned} b_{\sigma_k} = b_\sigma &\geq \frac{\delta f'(\sigma)}{(\sigma\log\sigma)^{1/4}} \geq \Big(\frac{2}{3}-c\Big)\Big(1-0.3405\,\frac{\log\log\sigma_k}{\log\sigma_k}\Big) \\ &> \frac{2}{3}-c-0.2113\,\frac{\log\log\sigma_k}{\log\sigma_k}. \end{aligned} \tag{5.25}$$

5.5.2. *Upper bound of* b_{σ_k}. The proof is similar to that for the lower bound. Using (5.15), we have

$$\operatorname{li}(\theta^2(x)) \ge \sigma - \eta \quad \text{with } \eta = \left(\frac{2}{3} + c\right)\frac{x^{3/2}}{\log x}\left(1 + \frac{0.51}{\log x}\right). \tag{5.26}$$

Further, from the left-hand-side inequality of (2.28), with $x = p_k$ and with the notation of (5.17), we obtain $x \ge \sqrt{\sigma \log \sigma}$, which implies $\log x \ge (L + \lambda)/2 > L/2$,

$$1 + \frac{0.51}{\log x} \le 1 + \frac{1.02}{L} \le 1 + \frac{1.02\,\lambda}{\lambda_0 L} \le 1 + 0.28\,\nu$$

and, from the right-hand-side inequality of (2.28) with the increasingness of $(t^{3/2}/\log t)$,

$$\frac{x^{3/2}}{\log x} \le \frac{2(\sigma L)^{3/4}(1 + \nu/2)^{3/2}}{L + \lambda}.$$

The third derivative of $t \mapsto (1 + t)^{3/2}$ is negative, so that

$$\left(1 + \frac{\nu}{2}\right)^{3/2} \le 1 + \frac{3\nu}{4} + \frac{3\nu^2}{32} = 1 + \frac{3}{4}\nu\left(1 + \frac{\nu}{8}\right) \le 1 + \frac{3}{4}\nu\left(1 + \frac{\nu_0}{8}\right) \le 1 + 0.76\,\nu$$

and

$$(1 + 0.76\,\nu)(1 + 0.28\,\nu) \le 1 + \nu(1.04 + 0.2128\,\nu_0) \le 1 + 1.06\,\nu,$$

which implies

$$\eta \le \left(\frac{2}{3} + c\right)\frac{2(\sigma L)^{3/4}}{L + \lambda}(1 + 1.06\nu). \tag{5.27}$$

From (5.26) and Taylor's formula we get

$$\log h(\sigma) = \theta(x) \ge f(\sigma - \eta) = \sqrt{\operatorname{li}^{-1}(\sigma)} - \eta f'(\sigma) + \frac{\eta^2}{2} f''(\xi) \quad \text{with } \sigma - \eta \le \xi \le \sigma. \tag{5.28}$$

To estimate $(\eta^2/2)f''(\xi)$, we need a crude upper bound for η. From (5.27), we have

$$\eta \le \left(\frac{2}{3} + c\right)\frac{2(\sigma L)^{3/4}}{L}(1 + 1.06\nu_0) \le 1.56\frac{\sigma^{3/4}}{L^{1/4}} < \frac{\sigma}{2}. \tag{5.29}$$

As $\xi > \sigma - \sigma/2 = \sigma/2$ and $|f''(t)|$ is decreasing on t, we have

$$|f''(\xi)| \le |f''(\sigma/2)| \le \frac{\log^2(\operatorname{li}^{-1}(\sigma/2))}{4(\operatorname{li}^{-1}(\sigma/2))^{3/2}}.$$

But, from (2.15),

$$\operatorname{li}^{-1}\left(\frac{\sigma}{2}\right) > \frac{\sigma}{2}\log\left(\frac{\sigma}{2}\right) = \frac{\sigma L}{2}\left(1 - \frac{\log 2}{L}\right) \ge \frac{\sigma L}{2}\left(1 - \frac{\log 2}{L_0}\right) > 0.49\,\sigma L$$

and

$$|f''(\xi)| \le \frac{\log^2(0.49\,\sigma L)}{4(0.49\,\sigma L)^{3/2}} < \frac{(L + \lambda)^2}{4(0.49)^2(\sigma L)^{3/2}} < 1.05\,\frac{(L + \lambda)^2}{(\sigma L)^{3/2}}.$$

Therefore, from (5.29),

$$\frac{\eta^2}{2}|f''(\xi)| \le \frac{(1.56)^2 \times 1.05}{2}(1+\nu)^2 \le 1.28(1+\nu)^2 \le 1.28(1+\nu_0)^2 < 1.52. \tag{5.30}$$

Inequality (2.15), with the decreasingness of $\log t/\sqrt{t}$, implies

$$f'(\sigma) = \frac{\log(\mathrm{li}^{-1}(\sigma))}{2\sqrt{\mathrm{li}^{-1}(\sigma)}} \le \frac{\log(\sigma\log\sigma)}{2\sqrt{\sigma\log\sigma}} = \frac{L+\lambda}{2\sqrt{\sigma L}}, \tag{5.31}$$

and from (5.27),

$$\eta f'(\sigma) \le (\tfrac{2}{3}+c)(\sigma\log\sigma)^{1/4}(1+1.06\nu). \tag{5.32}$$

From (5.28), (5.30) and (5.32), we obtain

$$\log h(\sigma) \ge \sqrt{\mathrm{li}^{-1}(\sigma)} - \Big(\frac{2}{3}+c\Big)(\sigma\log\sigma)^{1/4}\Big(1+\nu\Big(1.06+\frac{1.52}{(2/3+c)\nu(\sigma L)^{1/4}}\Big)\Big).$$

But the above fraction is maximal for $\sigma = n_0$ and, therefore, is less than 0.0003, so that

$$\log h(\sigma_k) = \log(h(\sigma)) \ge \sqrt{\mathrm{li}^{-1}(\sigma_k)} - \Big(\frac{2}{3}+c\Big)(\sigma_k\log\sigma_k)^{1/4}\Big(1+1.061\,\frac{\log\log\sigma_k}{\log\sigma_k}\Big)$$

and, from (1.9) and (1.10),

$$b_{\sigma_k} \le \Big(\frac{2}{3}+c\Big)\Big(1+1.061\frac{\log\log\sigma_k}{\log\sigma_k}\Big) < \frac{2}{3}+c+0.757\frac{\log\log\sigma_k}{\log\sigma_k}. \tag{5.33}$$

5.5.3. Bounds of b_n for $n \ge n_0$. Let us recall that σ_k is defined by $\sigma_k \le n < \sigma_{k+1}$. From (5.33), it follows that $b_{\sigma_k} < 2/3 + c + 0.757\,\nu_0 < 0.78 < 1$ and we may apply Lemma 4.1 so that, from (5.25),

$$\begin{aligned} b_n &\ge \min\Big(\frac{2}{3}-c-0.2113\frac{\log\log\sigma_k}{\log\sigma_k}, \frac{2}{3}-c-0.2113\frac{\log\log\sigma_{k+1}}{\log\sigma_{k+1}}\Big) \\ &= \frac{2}{3}-c-0.2113\frac{\log\log\sigma_k}{\log\sigma_k} \ge \frac{2}{3}-c-0.2113\frac{\log\log n}{\log\sigma_k}. \end{aligned}$$

Now, from Lemma 4.4, $1/\log\sigma_k < (1+3\times 10^{-10})/\log n$ holds, which proves the lower bound of (5.18).

Note that $c + 0.22\log\log n/\log n \le c + 0.22\nu_0 < 2/3$, which implies that the lower bound in (5.18) is positive so that, for $n \ge n_0$, $b_n > 0$ and $\sqrt{\mathrm{li}^{-1}(n)} - \log h(n) > 0$ hold. Therefore, from the definition (1.9) of b_n, we have

$$\begin{aligned} b_n &= \frac{\sqrt{\mathrm{li}^{-1}(n)} - \log h(n)}{(n\log n)^{1/4}} \le \frac{\sqrt{\mathrm{li}^{-1}(n)} - \log h(n)}{(\sigma_k\log\sigma_k)^{1/4}} \\ &\le \frac{\sqrt{\mathrm{li}^{-1}(\sigma_{k+1})} - \log h(\sigma_k)}{(\sigma_k\log\sigma_k)^{1/4}} = \tau_k + b_{\sigma_k} \end{aligned} \tag{5.34}$$

with, from (4.8),

$$\tau_k = \frac{\sqrt{\mathrm{li}^{-1}(\sigma_{k+1})} - \sqrt{\mathrm{li}^{-1}(\sigma_k)}}{(\sigma_k \log \sigma_k)^{1/4}} < 1.14 \frac{(\log \sigma_k)^{3/4}}{\sigma_k^{1/4}}. \tag{5.35}$$

Therefore, from (5.33) and (4.7), we obtain

$$\begin{aligned} b_n &\le \frac{2}{3} + c + \frac{\log\log \sigma_k}{\log \sigma_k}\Big(0.757 + 1.14 \frac{(\log \sigma_k)^{7/4}}{\sigma_k^{1/4} \log\log \sigma_k}\Big) \\ &< \frac{2}{3} + c + \frac{\log\log \sigma_k}{\log \sigma_k}\Big(0.757 + 1.14 \frac{(\log n_0)^{7/4}}{n_0^{1/4} \log\log n_0}\Big) \\ &< \frac{2}{3} + c + 0.763 \frac{\log\log \sigma_k}{\log \sigma_k} \\ &\le \frac{2}{3} + c + 0.763 \frac{\log\log n}{\log \sigma_k} < \frac{2}{3} + c + 0.763(1 + 3 \times 10^{-10}) \frac{\log\log n}{\log n} \end{aligned}$$

which completes the proof of (5.18) and of Proposition 5.9. □

5.6. Asymptotic bounds of b_n.

Proposition 5.10. *Under the Riemann hypothesis, for k and σ_k tending to infinity, we have*

$$b_{\sigma_k} \ge \Big(\frac{2}{3} - c\Big)\Big(1 + \frac{\log\log \sigma_k + O(1)}{4 \log \sigma_k}\Big) \tag{5.36}$$

and

$$b_{\sigma_k} \le \Big(\frac{2}{3} + c\Big)\Big(1 + \frac{\log\log \sigma_k + O(1)}{4 \log \sigma_k}\Big). \tag{5.37}$$

Proof. The proof follows the lines of the proof of Proposition 5.9, from which we retain the notation.

Lower bound. First, from (2.29), with the notation of (5.17),

$$\begin{aligned} x^{3/2} &= (\sigma L)^{3/4}\Big(1 + \frac{3(\log L + O(1))}{4L}\Big), \\ \log x &= \frac{1}{2}(L + \log L + O(1)) = \frac{L}{2}\Big(1 + \frac{\log L + O(1)}{L}\Big), \\ \frac{x^{3/2}}{\log x} &= 2\frac{(\sigma L)^{3/4}}{L}\Big(1 - \frac{\log L + O(1)}{4L}\Big), \\ \frac{x^{3/2}}{\log^2 x} &= O\Big(\frac{(\sigma L)^{3/4}}{L^2}\Big), \end{aligned}$$

whence, from (5.19),

$$\delta = \Big(\frac{2}{3} - c\Big)\frac{2\sigma^{3/4}}{L^{1/4}}\Big(1 - \frac{\lambda + O(1)}{4\,L}\Big). \tag{5.38}$$

Further, from (5.22) and (5.23), we obtain

$$b_{\sigma_k} \geq \frac{\delta f'(\sigma)}{(\sigma L)^{1/4}} \geq \frac{\delta\sqrt{L(1+\nu)}}{2\sqrt{\sigma}(\sigma L)^{1/4}} = \frac{\delta L^{1/4}}{2\sigma^{3/4}}\Big(1+\frac{\lambda+O(1)}{2L}\Big)$$

which, with (5.38), yields (5.37).

Upper bound. As for the lower bound, but using (5.26) instead of (5.19), we obtain

$$\eta = \Big(\frac{2}{3}+c\Big)\frac{x^{3/2}}{\log x} = \Big(\frac{2}{3}+c\Big)\frac{2\sigma^{3/4}}{L^{1/4}}\Big(1-\frac{\lambda+O(1)}{4L}\Big). \tag{5.39}$$

Further, (5.28) and (5.30) yield

$$\log h(\sigma) = \sqrt{\mathrm{li}^{-1}(\sigma)} - \eta f'(\sigma) + O(1),$$

which implies

$$b_{\sigma_k} = \frac{\sqrt{\mathrm{li}^{-1}(\sigma)} - \log h(\sigma)}{(\sigma L)^{1/4}} = \frac{\eta f'(\sigma)+O(1)}{(\sigma L)^{1/4}}. \tag{5.40}$$

Here, for $f'(\sigma)$, we need a sharper upper bound than that of (5.31). From (2.14) and (2.16), for σ tending to infinity, we have $\mathrm{li}^{-1}(\sigma) = \sigma(L+\lambda+O(1))$, $\log(\mathrm{li}^{-1}(\sigma)) = L+\lambda+\log(1+(\lambda+O(1))/L) = L+\lambda+O(1)$, $\sqrt{\mathrm{li}^{-1}(\sigma)} = \sqrt{\sigma L}(1+(\lambda+O(1))/(2L))$ and

$$f'(\sigma) = \frac{\log(\mathrm{li}^{-1}(\sigma))}{2\sqrt{\mathrm{li}^{-1}(\sigma)}} = \frac{L+\lambda+O(1)}{2\sqrt{\sigma L}(1+(\lambda+O(1))/(2L))} = \frac{\sqrt{L}}{2\sqrt{\sigma}}\Big(1+\frac{\lambda+O(1)}{2L}\Big). \tag{5.41}$$

Now, from (5.39) and (5.41), we obtain

$$\eta f'(\sigma) = \Big(\frac{2}{3}+c\Big)(\sigma L)^{1/4}\Big(1+\frac{\lambda+O(1)}{4L}\Big).$$

As $(\sigma L)^{1/4}/L \to \infty$, with (5.40), this yields (5.37). □

5.7. Bounds of b_n for n small.

PROPOSITION 5.11. *Recall that* $n_0 = \pi_1(10^{10}+19)$ *and that* b_n *is defined by (1.9).*

(1) *For* n, $2 \leq n < n_0$,

$$b_{17} = 0.497\,95\cdots \leq b_n \leq b_{1137} = 1.044\,14\ldots. \tag{5.42}$$

(2) *For* $78 \leq n < n_0$,

$$b_n \geq b_{100} = b_{\sigma_9} = 0.623\,28\cdots > 2/3 - c. \tag{5.43}$$

(3) *For* $157\,933\,210 \leq n \leq n_0$,

$$b_n < \frac{2}{3} + c + 0.77\frac{\log\log n}{\log n}. \tag{5.44}$$

PROOF. First, we calculate b_{σ_k} for $2 \le \sigma_k < n_0$ (see Section 3.2). For $k \ge 9$, we have

$$b_{100} = b_{\sigma_9} = 0.623\,28\cdots \le b_{\sigma_k} \le b_{31\,117} = b_{\sigma_{112}} = 0.884\,47\cdots < 1.$$

Therefore, we may apply Lemma 4.1 which implies, for $100 \le n < n_0$,

$$b_n \ge b_{100} = 0.623\,28\cdots > 2/3 - c.$$

The computation of b_n for $2 \le n < 100$ completes the proof of (5.43) and of the lower bound of (5.42).

To prove the upper bound of (5.42), for $\sigma_{253} = 186\,914 \le \sigma_k < n_0$, we compute $b_{\sigma_k} + \tau_k$ (with τ_k defined by (5.35)) and observe that $b_{\sigma_k} + \tau_k < 1.044$ holds, which implies (see (5.34)) that b_n is smaller than 1.044 for $186\,914 \le n < n_0$. It remains to calculate b_n for $2 \le n \le 186\,913$ to complete the proof of (5.42).

The proof of (5.44) is more complicated. If the inequality

$$b_{\sigma_k} + \tau_k < \frac{2}{3} + c + \frac{0.77\ \log\log\sigma_{k+1}}{\log\sigma_{k+1}} \tag{5.45}$$

holds, then, from (5.34),

$$b_n < \frac{2}{3} + c + \frac{0.77\log\log\sigma_{k+1}}{\log\sigma_{k+1}} < \frac{2}{3} + c + \frac{0.77\log\log n}{\log n} \tag{5.46}$$

for $\sigma_k \le n < \sigma_{k+1}$. At the same time we compute all the b_{σ_k} for $2 \le \sigma_k \le n_0$ (see the beginning of this proof), and we check that inequality (5.45) holds for $305\,926\,023 \le \sigma_k < n_0$, so that we have (5.46) for $305\,926\,023 \le n < n_0$.

It remains to compute the largest $n \le n_1 = 305\,926\,023$ such that inequality (5.44) does not hold. This could be expensive because the computation of b_n is not very fast. Let us recall that for an n which is not of the form $n = \sigma_k$, to compute $h(n)$ we have to compute $G(p_k, n - \sigma_k)$, and this costs about 0.004 seconds. If we used the trivial method, computing $h(n)$ for $n = n_1 - 1, n_2 - 1, \ldots$ until we find n not satisfying (5.44), we should have to compute about 1.5×10^8 values of $h(n)$, requiring about a week of computation.

Lemma 4.3 gives us a test, proving in $O(1)$ time that all the ns in $[n_1, n_2]$ satisfy (5.44). Moreover, there are a lot of intervals $[n_1, n_2]$ passing this test. The boolean function `good_interval(n1, n2)` returns true if and only if $[n_1, n_2]$ is such an interval, that is, if (n_1, n_2) satisfy inequality (4.5) with $\mu = 0.77$.

Now, using Python programming language, we define below, by a dichotomous recursion, a boolean function `ok_rec(n1, n2)` which returns true if and only if every n in $[n_1, n_2]$ satisfies (5.44). Furthermore, when it returns false, it prints the largest n in $[n_1, n_2]$ which does not satisfy this inequality.

```
def ok(n):
   if bn(n) >= 2/3 + c + 0.77 * log log n / log n :
      print n, ' does not satisfy inequality (iv) of Theorem 1.1 '
      return False
   return True

def ok_rec(n1, n2):
   if n2 - n1 >= 2:
       if good_interval(n1,n2):
          return True
       nmed = (n1 + n2)//2
       if not ok_rec(nmed,n2):
           return False
       return ok_rec(n1,nmed)

   if n1==n2:
      return ok(n1)

   if n2 == n1 + 1:
      if ok(n2):
         return ok(n1)
      return False
```

The correctness of `ok_rec(n1, n2)` is proved by recursion about the size of $n_2 - n_1$. The largest n which does not satisfy (5.44), $n = 157\,933\,209$, is given by the call `ok_rec(2,305926023)`. It computed four values of `ok(n)` and 11 395 values of `good_interval(n1,n2)`, and took 35.27 seconds. □

5.8. Completing the proof of Theorem 1.1. Proposition 5.9 implies that, for $n \geq n_0 = \pi_1(10^{10} + 19)$,

$$0.6010\ldots = \frac{2}{3} - c - 0.22\,\frac{\log\log n_0}{\log n_0} < b_n < \frac{2}{3} + c + 0.77\,\frac{\log\log n_0}{\log n_0} = 0.781\ldots,$$

which, together with inequality (5.42), proves statement (ii) of Theorem 1.1.

- Point (i) is equivalent to $b_n > 0$ which follows from (ii).
- From inequalities (5.18) and (5.43), one deduces $b_n > \frac{2}{3} - c - 0.22\,(\log\log n/\log n)$ for $n \geq 78$, and the computation of b_n for $2 \leq n < 78$ proves (iii).
- Similarly, inequalities (5.18) and (5.44) imply $b_n < \frac{2}{3} + c + 0.77\,(\log\log n/\log n)$ for $n \geq 157\,933\,210$.
- Statement (v) follows from (iii) and (iv).
- To prove (vi), we assume $n \to \infty$ and $\sigma = \sigma_k \leq n \leq \sigma_{k+1}$ so that $n = \sigma + O(p_k)$ holds. From Lemma 2.10, $\sigma = \sigma_k = \pi_1(p_k)$ yields

$$n = \sigma + O(\sqrt{\sigma\log\sigma}) = \sigma(1 + O(\sqrt{(\log\sigma)/\sigma}) \sim \sigma.$$

This implies

$$\begin{aligned}
\log n &= \log\sigma + O(\sqrt{(\log\sigma)/\sigma}) = (\log\sigma)(1 + O(1/\sqrt{\sigma\log\sigma}))\\
\log\log n &= \log\log\sigma + O(1)\\
\frac{\log\log\sigma + O(1)}{\log\sigma} &= \frac{\log\log n + O(1)}{(\log n)\Big(1 + \dfrac{O(1)}{\log\log n}\Big)}\\
&= \frac{\log\log n + O(1)}{\log n} = \frac{\log\log\sigma_{k+1} + O(1)}{\log\sigma_{k+1}}.
\end{aligned}$$

From Lemma 4.1 and (5.36), we get

$$b_n \ge \min(b_{\sigma_k}, b_{\sigma_{k+1}}) \ge \Big(\frac{2}{3} - c\Big)\Big(1 + \frac{\log\log n + O(1)}{4\log n}\Big),$$

which proves the lower bound of (vi).

- From (5.34), (5.35) and (5.37), we obtain

$$\begin{aligned}
b_n \le b_{\sigma_k} + \tau_k &= \Big(\frac{2}{3} + c\Big)\Big(1 + \frac{\log\log\sigma_k + O(1)}{4\log\sigma_k}\Big) + O\Big(\frac{\log^{3/4}\sigma}{\sigma^{1/4}}\Big)\\
&= \Big(\frac{2}{3} + c\Big)\Big(1 + \frac{\log\log n + O(1)}{4\log n}\Big),
\end{aligned}$$

which proves the upper bound of (vi) and concludes the proof of Theorem 1.1.

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References

[1] M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions* (Dover Publications, New York).

[2] C. Axler, ‘New bounds for the sum of the first n prime numbers’, *J. Théor. Nombres Bordeaux* (to appear) (2016), arXiv:1606.06874.

[3] C. Axler, ‘New estimates for some functions defined over primes’, *Intergers* (to appear) (2017), arXiv:1703.08032.

[4] B. C. Berndt, *Ramanujan’s Notebooks, Part IV* (Springer, New York, 1994), 126–131.

[5] H. Cohen, *Number Theory*, Analytic and Modern Tools, Volume II (Springer, New York, 2007).

[6] M. Deléglise and J.-L. Nicolas, ‘Le plus grand facteur premier de la fonction de Landau’, *Ramanujan J.* **27** (2012), 109–145.

[7] M. Deléglise and J.-L. Nicolas, ‘Maximal product of primes whose sum is bounded’, *Proc. Steklov Inst. Math.* **282** (2013), 73–102; (Issue 1, Supplement).

[8] M. Deléglise and J.-L. Nicolas, ‘On the largest product of primes with bounded sums’, *J. Integer Sequences* **18** (2015), Article 15.2.8.

[9] M. Deléglise, J.-L. Nicolas and P. Zimmermann, ‘Landau’s function for one million billions’, *J. Théor. Nombres Bordeaux* **20** (2008), 625–671.

[10] M. Deléglise and J. Rivat, 'Computing $\pi(x)$: The Meissel, Lehmer, Lagarias, Miller, Odlyzko method', *Math. Comp.* **65** (1996), 235–245.
[11] M. Deléglise and J. Rivat, 'Computing $\psi(x)$', *Math. Comp.* **67** (1998), 1691–1696.
[12] P. Dusart, 'Explicit estimates of some functions over primes', *Ramanujan J.* **45** (2018), 227–251.
[13] H. M. Edwards, *Riemann's Zeta Function* (Academic Press, New York, 1974).
[14] W. J. Ellison and F. Ellison, *Prime Numbers* (Wiley, New York, 1985).
[15] W. J. Ellison and M. Mendès France, *Les nombres premiers* (Hermann, Paris, 1975).
[16] E. Landau, *Handbuch der Lehre von der Verteilung der Primzahlen, I*, 2nd edn (Chelsea, New York, 1953).
[17] J.-P. Massias and G. Robin, 'Bornes effectives pour certaines fonctions concernant les nombres premiers', *J. Théor. Nombres Bordeaux* **8** (1996), 215–242.
[18] J.-P. Massias, J.-L. Nicolas and G. Robin, 'Évaluation asymptotique de l'ordre maximum d'un élément du groupe symétrique', *Acta Arith.* **50** (1988), 221–242.
[19] J.-P. Massias, J.-L. Nicolas and G. Robin, 'Effective bounds for the maximal order of an element in the symmetric group', *Math. Comp.* **53**(188) (1989), 665–678.
[20] J.-L. Nicolas, 'Small values of the Euler function and the Riemann hypothesis', *Acta Arith.* **155** (2012), 311–321.
[21] D. J. Platt and T. Trudgian, 'On the first sign change of $\theta(x) - x$', *Math. Comp.* **85**(299) (2016), 1539–1547.
[22] G. Robin, 'Grandes valeurs de la fonction somme des diviseurs et hypothèse de Riemann', *J. Math. Pures Appl.* **63** (1984), 187–213.
[23] B. Salvy, 'Fast computation of some asymptotic functional inverses', *J. Symbolic Comput.* **17** (1994), 227–236.
[24] L. Schoenfeld, 'Sharper bounds for the Chebyshev functions $\theta(x)$ and $\psi(x)$ II', *Math. Comp.* **30** (1976), 337–360.
[25] https://github.com/mhdeleglise/PsiTheta.
[26] http://math.univ-lyon1.fr/homes-www/deleglis/calculs.html.
[27] http://math.univ-lyon1.fr/homes-www/nicolas/calculhdenHR.html.
[28] http://www.dtc.umn.edu/ odlyzko/zeta_tables/zeros2.

MARC DELÉGLISE, Univ Lyon, Université Claude Bernard,
Lyon 1, CNRS UMR 5208,
Institut Camille Jordan, Mathématiques,
Bât. Doyen Jean Braconnier,
43 Bd du 11 Novembre 1918,
F-69622 Villeurbanne cedex,
France
e-mail: m.h.deleglise@gmail.com

JEAN-LOUIS NICOLAS, Univ Lyon, Université Claude Bernard,
Lyon 1, CNRS UMR 5208,
Institut Camille Jordan, Mathématiques,
Bât. Doyen Jean Braconnier,
43 Bd du 11 Novembre 1918,
F-69622 Villeurbanne cedex,
France
e-mail: nicolas@math.univ-lyon1.fr