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THE HEXAGONAL VERSUS THE SQUARE LATTICE

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Abstract. Schmutz Schaller's conjecture regarding the lengths of the hexagonal versus the lengths of the square lattice is shown to be true. The proof makes use of results from (computational) prime number theory.

Using an identity due to Selberg, it is shown that, in principle, the conjecture can be resolved without using computational prime number theory. By our approach, however, this would require a huge amount of computation.

1. Introduction

In [17, p. 201] Schmutz Schaller, motivated by considerations from hyperbolic geometry, makes the conjecture that in dimensions 2 to 8 the best known lattice sphere packings have 'maximal lengths', that is, that their length spectrum dominates the length spectrum of every other lattice of the same dimension and covolume at every position, and goes on to write: "In dimension 2 the conjecture means in particular that the hexagonal lattice is 'better' than the square lattice. More precisely, let $0 < h_1 < h_2 < \cdots$ be the positive integers, listed in ascending order, which can be written as $h_i = x^2 + 3y^2$ for integers x and y. Let $0 < q_1 < q_2 < \cdots$ be the positive integers, listed in ascending order, which can be written as $q_i = x^2 + y^2$ for integers x and y. Then the conjecture is that $q_i \le h_i$ for $i = 1, 2, 3, \ldots$." That he uses the words 'in particular' is a bit surprising since the conjecture for dimension 2 implies that if a plane lattice having the same covolume as the hexagonal lattice Σ fails to be isometric to Σ, then its length spectrum is dominated by that of Σ at every position, which is weaker than the conjecture between the quotation marks, which asserts that the length spectrum of Σ, thought of as the Eisenstein numbers, dominates that of the square lattice in its realization as Gaussian integers (note that the Eisenstein numbers have smaller covolume than the Gaussian integers).

The reader might also be surprised to see the norm form $x^2 + 3y^2$ appearing in the quotation, rather than x^2+xy+y^2. However, both represent the same integers. Notice that $x^2 + 3y^2$ is the norm form of the sublattice $[1, 2\zeta_3]$ of index 2 of Σ. The two other sublattices of index 2 are easily seen to be $[2, \zeta_3]$ and $[-1 + \zeta_3, 1 + \zeta_3]$. As under multiplication by ζ_3 the sublattices are transformed into each other, they each have the same length spectrum. Since the union of the three sublattices is Σ, the length spectrum of every sublattice of index 2 must be the same as that of Σ itself.

For a more introductory account to Schmutz Schaller's work than [17], see [18]. For some progress regarding Schmutz Schaller's general conjecture in dimension 2 see [8] (this case of the conjecture is also mentioned in [4]).

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For $j \geq 1$ let $b_j(n) = 1$ if n is represented by the quadratic form $X^2 + jY^2$ and $b_j(n) = 0$ otherwise. The characteristic functions b_1 and b_3 are well understood. The following result was already known to Fermat.

Lemma 1. *A positive integer n is represented by the form $X^2 + Y^2$ if and only if every prime factor p of n of the form $p \equiv 3 (\mathrm{mod}\ 4)$ occurs to an even power. A positive integer n is represented by the form $X^2 + 3Y^2$ if and only if every prime factor p of n of the form $p \equiv 2 (\mathrm{mod}\ 3)$ occurs to an even power.*

(In general the natural numbers n that are represented by a quadratic form $X^2 + mY^2$ are rather more difficult to describe, cf. the beautiful book of D. Cox [5].) Lemma 1 implies that b_1 and b_3 are multiplicative functions.

Let $B_i(x) = \sum_{n \leq x} b_i(n)$ for $i = 1$ and $i = 3$. Schmutz Schaller's conjecture regarding the square versus the hexagonal lattice can be reformulated as follows in terms of B_1 and B_3.

Conjecture 1. *We have $B_1(x) \geq B_3(x)$ for every x.*

The first asymptotic result on $B_1(x)$ goes back to Landau [9], who proved in 1908 that

$$B_1(x) \sim C_{b_1} \frac{x}{\sqrt{\log x}}, \tag{1}$$

where

$$C_{b_1} = \frac{1}{\sqrt{2}} \prod_{p \equiv 3 (\mathrm{mod}\ 4)} (1 - p^{-2})^{-1/2} = \frac{\pi}{4} \prod_{p \equiv 1 (\mathrm{mod}\ 4)} (1 - p^{-2})^{1/2} \approx 0.764. \tag{2}$$

(Here and in the sequel the letter p is used to indicate primes.) Landau's proof uses contour integration. It is not difficult to use his method to show, cf. [20], that for every $k \geq 2$ there exist constants $C_{b_1}(2), \ldots, C_{b_1}(k)$ such that

$$B_1(x) = C_{b_1} \frac{x}{\sqrt{\log x}} \left(1 + \frac{C_{b_1}(2)}{\log x} + \cdots + \frac{C_{b_1}(k)}{\log^{k-1} x} + O\left(\frac{1}{\log^k x} \right) \right). \tag{3}$$

This result can also be established by methods not using complex analysis, cf. [14, p. 288]. At the beginning of 1913 a then unknown Hindu clerk by the name of Ramanujan wrote in his first letter to Hardy [2] that he could prove that

$$B_1(x) = C_{b_1} \int_2^x \frac{dt}{\sqrt{\log t}} + O(x^{1-\varepsilon}), \tag{4}$$

for some $\varepsilon > 0$. (For a reconstruction of Ramanujan's speculative argument see [1, pp. 60-66].) Note the similarity of Ramanujan's claim with the prime number theorem. From (4) we infer that $C_{b_1}(2) = 1/2$ by partial integration. Shanks [21] showed, however, that $C_{b_1}(2) \neq 1/2$, thus disproving Ramanujan's claim. (Ramanujan gave the correct formula and numerical approximation for C_{b_1}, though.) The constants C_{b_1} and $C_{b_1}(2)$ are known as the *Landau-Ramanujan constant* and the *second order Landau-Ramanujan constant*, respectively. For more on the evaluation of these constants see Section 5. For more on mathematical constants in general, see, e.g., [7].

Ramanujan [3] stated several claims similar to (4) in his 'unpublished' manuscript on the partition and tau functions, see Section 6. All of them are disproved in [11]. It can be shown, however, that in each case Ramanujan's claims give the correct asymptotic main term.

Table 1. $B_1(x)$ versus $B_3(x)$

x	$B_1(x)$	$B_3(x)$	x	$B_1(x)$	$B_3(x)$
2^1	2	1	2^{14}	4357	3645
2^2	3	3	2^{15}	8363	6993
2^3	5	4	2^{16}	16096	13456
2^4	9	8	2^{17}	31064	25978
2^5	16	14	2^{18}	60108	50248
2^6	29	25	2^{19}	116555	97446
2^7	54	45	2^{20}	226419	189291
2^8	97	82	2^{21}	440616	368338
2^9	180	151	2^{22}	858696	717804
2^{10}	337	282	2^{23}	1675603	1400699
2^{11}	633	531	2^{24}	3273643	2736534
2^{12}	1197	1003	2^{25}	6402706	5352182
2^{13}	2280	1907	2^{26}	12534812	10478044

Similarly to (3), it can be shown that for arbitrary $k \geq 2$ there exist constants $C_{b_3}(2), \ldots, C_{b_3}(k)$ such that

$$B_3(x) = C_{b_3} \frac{x}{\sqrt{\log x}} \left(1 + \frac{C_{b_3}(2)}{\log x} + \cdots + \frac{C_{b_3}(k)}{\log^{k-1} x} + O\left(\frac{1}{\log^k x}\right)\right), \tag{5}$$

where

$$C_{b_3} = \frac{1}{\sqrt{2}} \frac{1}{3^{1/4}} \prod_{p \equiv 2 (\mathrm{mod}\ 3)} (1-p^{-2})^{-1/2} = \frac{\pi 3^{1/4} \sqrt{2}}{9} \prod_{p \equiv 1 (\mathrm{mod}\ 3)} (1-p^{-2})^{1/2} \approx 0.639.$$

We thus arrive at the following conclusion.

Proposition 1. *Conjecture 1 is asymptotically true.*

Table 1 (copied from [22] and verified by the second author) suggests that Conjecture 1 is true for small x as well. The literature thus provides us with good indications that Conjecture 1 is true. The purpose of this paper is to go beyond this and prove that Conjecture 1 is indeed true.

Theorem 1. *We have $B_1(x) \geq B_3(x)$ for every x. That is, Schmutz Schaller's conjecture that the hexagonal lattice is 'better' than the square lattice is true.*

Landau's classical result (1) has been generalised in many directions; see [12] for a survey with over 50 references. Despite this rich history, nobody but the first of the present authors (in [10]) seems to have been concerned with proving effective results in this area, which is precisely what is needed to establish Theorem 1.

2. Preliminaries

Let f be a multiplicative function from the natural numbers to $\mathbb{R}_{\geq 0}$. We define $M_f(x) = \sum_{n \leq x} f(n)$, $\mu_f(x) = \sum_{n \leq x} f(n)/n$ and $\lambda_f(x) = \sum_{n \leq x} f(n) \log n$. We denote the formal Dirichlet series $\sum_{n=1}^{\infty} f(n) n^{-s}$ associated to f by $L_f(s)$. We define $\Lambda_f(n)$ by

$$-\frac{L_f'(s)}{L_f(s)} = \sum_{n=1}^{\infty} \frac{\Lambda_f(n)}{n^s}.$$

Notice that

$$f(n)\log n=\sum_{d|n} f(d)\Lambda_f\left(\frac{n}{d}\right). \tag{6}$$

If f is the characteristic function of a multiplicative subsemigroup of the natural integers with $(1<)\ q_1<q_2<\cdots$ as generators, then it can be shown that $\Lambda_f(n)=\log q_i$ if n equals a positive power of a generator q_i, and $\Lambda_f(n)=0$ otherwise. For $f=b_1$ we thus find, using Lemma 1,

$$\Lambda_{b_1}(n)=\begin{cases}2\log p & \text{if } n=p^{2r},\ r\ge 1 \text{ and } p\equiv 3(\text{mod } 4);\\ \log p & \text{if } n=p^{r},\ r\ge 1 \text{ and } p\equiv 1(\text{mod } 4) \text{ or } p=2;\\ 0 & \text{otherwise.}\end{cases}$$

For $f=b_3$ we find

$$\Lambda_{b_3}(n)=\begin{cases}2\log p & \text{if } n=p^{2r},\ r\ge 1 \text{ and } p\equiv 2(\text{mod } 3);\\ \log p & \text{if } n=p^{r},\ r\ge 1 \text{ and } p\equiv 1(\text{mod } 3) \text{ or } p=3;\\ 0 & \text{otherwise.}\end{cases}$$

From property (6) of $\Lambda_f(n)$, we easily infer that

$$\lambda_f(x)=\sum_{n\le x} f(n)\psi_f\left(\frac{x}{n}\right), \tag{7}$$

where $\psi_f(x)=\sum_{n\le x}\Lambda_f(n)$. The functions Λ_f and ψ_f are analogues of, respectively, the von Mangoldt function and the Chebyshev ψ-function.

3. Some related conjectures

Unfortunately it seems that M_f is not a very natural mathematical object, whereas μ_f is (as is amply demonstrated by browsing through the literature). For this reason we consider two additional conjectures:

Conjecture 2. *We have $\lambda_{b_1}(x)\ge\lambda_{b_3}(x)$ for $x\ge 8$.*

Conjecture 3. *We have $\mu_{b_1}(x)\ge\mu_{b_3}(x)$ for every x.*

Note that $\exp(\lambda_{b_1}(x)/2)$ is the product of all different lengths in the square lattice not exceeding $\sqrt{x}$. Thus Conjecture 2 can be reformulated as stating that the product of the different distances not exceeding x occurring in the square lattice always exceeds the product of the different distances not exceeding x in the hexagonal lattice, provided that $x\ge 2\sqrt{2}$.

Conjecture 1 clearly implies Conjecture 3. Furthermore we have:

Proposition 2. *Conjecture* 2 *implies Conjecture* 1.

Proof. We have, for $x\ge 2$,

$$M_f(x)=\int_{2-}^{x}\frac{d\lambda_f(t)}{\log t}=\frac{\lambda_f(x)}{\log x}+\int_2^x\frac{\lambda_f(t)}{t\log^2 t}dt. \tag{8}$$

Denote the latter integral by $I_f(x)$. It is not difficult to show that $I_{b_1}(x)\ge I_{b_3}(x)$ for $x\le 8$. Conjecture 2 then implies that the latter inequality holds for every x. The truth of Conjecture 2 together with (8) then implies that $B_1(x)\ge B_3(x)$ for $x\ge 8$. By direct computation we then infer that the latter inequality holds for every x. $\square$

Thus in order to establish Theorem 1, it suffices to establish Conjecture 2. From (7) and $\psi_{b_i}(x) \sim x/2$ as x tends to infinity it follows that $\lambda_{b_i}(x) \sim \mu_{b_i}(x)/2$, as x tends to infinity. An effective form of this relationship, together with an effective estimate for μ_{b_i} (provided by Lemma 2), then allows us to prove the main result of this paper:

Theorem 2. *Conjectures* 1, 2 *and* 3 *are all true.*

Complications arise due to the fact that

$$\lim_{x\to\infty} B_1(x)/B_3(x) = 1.1961377420\cdots,$$

which is rather close to 1, and that $\psi_{b_i}(y)$ is not so close to $y/2$ for various ranges of small y (the convolutional nature of (7) forces us to take the small y range into account).

4. The toolbox

The following result from [10] will play a crucial rôle. It is in essence an effective version of Theorem A of [25].

Lemma 2. *Let f be a multiplicative function from the natural numbers to $\mathbb{R}_{\geq 0}$. Suppose that there exist constants D_-, D_+ and τ, with $\tau > 0$, such that for every $x \geq x_0$,*

$$D_-\mu_f(x) \leq \sum_{n\leq x} \frac{f(n)}{n} \left\{ \sum_{m\leq \frac{x}{n}} \frac{\Lambda_f(m)}{m} - \tau \log \frac{x}{n} \right\} \leq D_+\mu_f(x). \tag{9}$$

Then we have, for $x > \max\{x_0, \exp(D_+)\}$,

$$\frac{C_f}{\tau} \log^\tau x \frac{\left(1-\frac{D_+}{\log x}\right)^{\tau+1}}{1-\frac{D_-}{\log x}} \leq \mu_f(x) \leq \frac{C_f}{\tau} \log^\tau x \frac{\left(1-\frac{D_-}{\log x}\right)^{\tau+1}}{1-\frac{D_+}{\log x}}, \tag{10}$$

where

$$C_f := \frac{1}{\Gamma(\tau)} \lim_{s\to 1+0} (s-1)^\tau L_f(s). \tag{11}$$

In particular, if there exist constants C_- and C_+ such that

$$C_- \leq \sum_{n\leq x} \frac{\Lambda_f(n)}{n} - \tau \log x \leq C_+ \text{ for } x \geq 1, \tag{12}$$

then (10) *holds true, for $x > \exp(C_+)$, with $D_- = C_-$ and $D_+ = C_+$.*

Remark 1. From the proof of this lemma, $\int_1^x \mu_f(t)dt/t$ appears as a more easily estimated function than $\mu_f(x)$. Interestingly, Landau [9] in his proof of (1) using contour integration, estimates $\int_1^x \mu_{b_1}(t)dt/t$ rather than $B_1(x)$ itself.

Remark 2. If $\lim_{x\to\infty}(\sum_{n\leq x}(\Lambda_f(n)/n - \tau\log x))$ exists, we denote it by B_f.

Let us put

$$L(x,\tau,D_-,D_+) = \frac{(\log x - D_+)^{\tau+1}}{\log x - D_-} \text{ and } U(x,\tau,D_-,D_+) = \frac{(\log x - D_-)^{\tau+1}}{\log x - D_+}.$$

Thus we can write (10) as $C_f L(x,\tau,D_-,D_+)/\tau \leq \mu_f(x) \leq C_f U(x,\tau,D_-,D_+)/\tau$.

Let r, s and c_1 be given. At a few instances in the sequel we want to show that for every $x \geq x_2$, with x_2 some explicit constant, we have $\mu_f(x/r) \geq c_1 \mu_g(x/s)$, where g satisfies the conditions of Lemma 2 with constants τ, D'_- and D'_+. By Lemma 2 this leads us to consider inequalities of the form

$$L\left(\frac{x}{r}, \tau, D_-, D_+\right) \geq c_2 U\left(\frac{x}{s}, \tau, D'_-, D'_+\right), \tag{13}$$

where all variables and constants are real numbers with τ, r, s and c_2 positive, $D_- \leq D_+$, $D'_- \leq D'_+$ and $x \geq x_0 := \max\{\exp(D'_+)s, \exp(D_+)r\}$. We recall the following lemma from [10]:

Lemma 3. *If* $\log s + D'_- \leq D_+ + \log r$ *and* (13) *is satisfied for some* $x_1 > x_0$*, then* (13) *is satisfied for every* $x \geq x_1$*. If* $\log s + D'_- > D_+ + \log r$ *and*

$$c_2\left(1 + \frac{D'_+ - D'_-}{\log(x_1/s) - D'_+}\right) \leq 1 + \frac{D_- - D_+}{\log(x_1/r) - D_-}$$

for some $x_1 > x_0$*, then* (13) *is satisfied for every* $x \geq x_1$*.*

We also need the following result about the difference between $U(\frac{x}{r}, \frac{1}{2}, D_-, D_+)$ and $L(\frac{x}{s}, \frac{1}{2}, D_-, D_+)$.

Lemma 4. *Assume that* $D_+ > D_-$ *and* $s \geq r \geq 1$*. The difference*

$$U\left(\frac{x}{r}, \frac{1}{2}, D_-, D_+\right) - L\left(\frac{x}{s}, \frac{1}{2}, D_-, D_+\right)$$

is monotonically decreasing for $x \geq s\exp(1.01D_+ - 0.01D_-)$*.*

The difference in the latter lemma multiplied by C_{b_i} appears if we try to bound $\mu_{b_i}(x/r) - \mu_{b_i}(x/s)$ from above. Notice that the latter difference is not monotonically decreasing from any x onwards, although it can be bounded above by a function that is monotonically decreasing for all sufficiently large x.

Our proof of Lemma 4 uses the following lemma.

Lemma 5. *Let* y *and* δ *be non-negative real numbers. Then the inequality*

$$\sqrt{y+1+\delta}(y+\delta-2)(y+1)^2 \leq \sqrt{y}(y+3)(y+\delta)^2 \tag{14}$$

holds if either $\delta \leq 2$ *or* $y \geq 0.0099945$*.*

Proof. On replacing the inequality sign in (14) with the equality sign and squaring both sides, we obtain an equation of an algebraic curve. Using continuity and, e.g., Maple's function `fsolve` (for numerically determining roots of polynomial equations), the result can then be deduced. $\square$

Remark. For $y = 0.0099944$ and $\delta \approx 5.4$ inequality (14) is not satisfied. Indeed, if we square both sides of the inequality and take the difference, then, considered as a polynomial in y, the discriminant has $27\delta^5 - 198\delta^4 + 410\delta^3 - 936\delta^2 + 1299\delta - 730$ as a factor, which has $5.44694735\cdots$ as its largest real root. Considered as a polynomial in δ, we find

$$27y^8 - 72y^7 - 2380y^6 - 12792y^5 - 33822y^4 - 48888y^3 - 32076y^2 - 2376y + 27$$

as a factor of the discriminant, which has $0.00999445028\cdots$ as its next to largest real root.

We can now prove Lemma 4.

Proof of Lemma 4. Differentiating $U(x/r, \frac{1}{2}, D_-, D_+) - L(x/s, \frac{1}{2}, D_-, D_+)$ yields, after some tedious calculations, that the derivative is non-positive provided that (14) is satisfied with

$$y = (\log(x/s) - D_+)/(D_+ - D_-) \quad \text{and} \quad \delta = \log(s/r)/(D_+ - D_-).$$

The result then follows on invoking Lemma 5. $\square$

5. Numerical evaluation of certain constants

For our proof of Theorem 1 we need to evaluate the constants $C_{b_1}, C_{b_3}, B_{b_1}$ and B_{b_3} with enough numerical precision. The purpose of this section is to achieve this. (Recall that $B_{b_i} = \lim_{x\to\infty}(\sum_{n\le x} \Lambda_{b_i}(n)/n - (\log x)/2)$.)

We first consider the evaluation of C_{b_3} and C_{b_1} (defined by (11)). We have, for $\mathrm{Re}(s) > 1$,

$$L_{b_3}(s) = (1-3^{-s})^{-1} \prod_{p\equiv 1(\mathrm{mod}\ 3)} (1-p^{-s})^{-1} \prod_{p\equiv 2(\mathrm{mod}\ 3)} (1-p^{-2s})^{-1}$$

and

$$L_{b_3}(s)^2 = \zeta(s)L(s,\chi_{-3})(1-3^{-s})^{-1} \prod_{p\equiv 2(\mathrm{mod}\ 3)} (1-p^{-2s})^{-1}. \tag{15}$$

From this, (11), $\lim_{s\to 1+0}(s-1)\zeta(s) = 1$ and the fact that $\Gamma(\frac{1}{2}) = \sqrt{\pi}$, we obtain

$$C_{b_3}^2 = \frac{3L(1,\chi_{-3})}{2\pi} \prod_{p\equiv 2(\mathrm{mod}\ 3)} (1-p^{-2})^{-1},$$

where for any fundamental discriminant D, χ_D denotes Kronecker's extension (D/n) of the Legendre symbol [6, Chapter 5]. If χ is a real primitive character modulo k and $\chi(-1) = -1$, then

$$L(1,\chi) = -\frac{\pi}{k^{3/2}} \sum_{n=1}^{k} n\chi(n),$$

by Dirichlet's celebrated class number formula (cf. equation (17) of [6, Chapter 6]). We infer that $L(1,\chi_{-3}) = \pi/\sqrt{27}$. Using that C_{b_3} must be positive and $\zeta(2) = \pi^2/6$, we then infer that

$$C_{b_3} = \frac{1}{\sqrt{2}}\frac{1}{3^{1/4}} \prod_{p\equiv 2(\mathrm{mod}\ 3)} (1-p^{-2})^{-1/2} = \frac{\pi 3^{1/4}\sqrt{2}}{9} \prod_{p\equiv 1(\mathrm{mod}\ 3)} (1-p^{-2})^{1/2}.$$

Likewise, using that $L(1,\chi_{-4}) = \pi/4$, we find formula (2) for C_{b_1}.

Note that, for $\Re(s) > 1/2$,

$$\prod_{p\equiv 3(\mathrm{mod}\ 4)} (1-p^{-2s})^{-2} = \frac{\zeta(2s)(1-2^{-2s})}{L(2s,\chi_{-4})} \prod_{p\equiv 3(\mathrm{mod}\ 4)} (1-p^{-4s})^{-1}. \tag{16}$$

By recursion we then find from (2) and (16) the following formula:

$$C_{b_1} = \frac{1}{\sqrt{2}} \prod_{n=1}^{\infty} \left((1-2^{-2^n}) \frac{\zeta(2^n)}{L(2^n,\chi_{-4})} \right)^{1/2^{n+1}},$$

which was already known to Ramanujan [1, pp. 60-66] and Shanks [21, p. 78]. Using this expression, one computes that $C_{b_1} = 0.76422365358922066299\cdots$. Similarly one can show that

$$C_{b_3} = \frac{1}{\sqrt{2}}\frac{1}{3^{1/4}}\prod_{n=1}^{\infty}\left((1-3^{-2^n})\frac{\zeta(2^n)}{L(2^n,\chi_{-3})}\right)^{1/2^{n+1}},$$

and use it to compute $C_{b_3} = 0.63890940544534388225\cdots$, which is in agreement with the first seven (out of eight) decimals computed for C_{b_3} by Shanks and Schmid [22].

On noting that, for $\mathrm{Re}(s) \geq 1$,

$$\sum_{n=1}^{\infty}\frac{\Lambda(n)-1}{n^s} = -\frac{\zeta'(s)}{\zeta(s)} - \zeta(s),$$

and using that $\zeta(s) = 1/(s-1)+\gamma+O(s-1)$, where γ denotes Euler's constant, is the Taylor series for $\zeta(s)$ around $s=1$, one infers that

$$\sum_{n\leq x}\frac{\Lambda(n)}{n} = \sum_{n\leq x}\frac{1}{n} - 2\gamma + o(1) = \log x - \gamma + o(1). \tag{17}$$

Taking the logarithmic derivative of (15), one obtains

$$-2\frac{L'_{b_3}(s)}{L_{b_3}(s)} = -\frac{\zeta'(s)}{\zeta(s)} - \frac{L'(s,\chi_{-3})}{L(s,\chi_{-3})} + \frac{\log 3}{3^s-1} + 2\sum_{p\equiv 2(\mathrm{mod}\ 3)}\frac{\log p}{p^{2s}-1},$$

from which one easily infers that

$$2\sum_{n\leq x}\frac{\Lambda_{b_3}(n)}{n} = \sum_{n\leq x}\frac{\Lambda(n)}{n} - \frac{L'(1,\chi_{-3})}{L(1,\chi_{-3})} + \frac{\log 3}{2} + 2\sum_{p\equiv 2(\mathrm{mod}\ 3)}\frac{\log p}{p^2-1} + o(1),$$

which yields, on invoking (17),

$$2B_{b_3} = -\gamma - \frac{L'(1,\chi_{-3})}{L(1,\chi_{-3})} + \frac{\log 3}{2} + 2\sum_{p\equiv 2(\mathrm{mod}\ 3)}\frac{\log p}{p^2-1}.$$

Similarly we deduce that

$$2B_{b_1} = -\gamma - \frac{L'(1,\chi_{-4})}{L(1,\chi_{-4})} + \log 2 + 2\sum_{p\equiv 3(\mathrm{mod}\ 4)}\frac{\log p}{p^2-1}.$$

Note that the argument above yielded

$$B_{b_i} = -\lim_{s\to 1+0}\left(\frac{L'_{b_i}(s)}{L_{b_i}(s)} + \frac{1}{2(s-1)}\right).$$

This can be alternatively deduced from Serre's [20] proof of (3), cf. [11].

As to the numerical evaluation of, for example, the latter prime sum, we note that

$$2\sum_{p\equiv 3(\mathrm{mod}\ 4)}\frac{\log p}{p^2-1} = -\frac{d}{ds}\log\prod_{p\equiv 3(\mathrm{mod}\ 4)}\left(\frac{1}{1-p^{-2s}}\right)\Big|_{s=1}.$$

Then, applying (16) m times, we obtain

$$\sum_{p\equiv 3(\mathrm{mod}\ 4)} \frac{\log p}{p^2-1} = \sum_{p\equiv 3(\mathrm{mod}\ 4)} \frac{\log p}{p^{2^{m+1}}-1} + \frac{1}{2}\sum_{n=1}^{m}\left\{\frac{L'(2^m,\chi_{-4})}{L(2^m,\chi_{-4})} - \frac{\zeta'(2^m)}{\zeta(2^m)} - \frac{\log 2}{2^{2^m}-1}\right\}.$$

Similarly we have

$$\sum_{p\equiv 2(\mathrm{mod}\ 3)} \frac{\log p}{p^2-1} = \sum_{p\equiv 2(\mathrm{mod}\ 3)} \frac{\log p}{p^{2^{m+1}}-1} + \frac{1}{2}\sum_{n=1}^{m}\left\{\frac{L'(2^m,\chi_{-3})}{L(2^m,\chi_{-4})} - \frac{\zeta'(2^m)}{\zeta(2^m)} - \frac{\log 3}{3^{2^m}-1}\right\}.$$

Using these expressions, one computes $B_{b_1} = 0.1638973186345815958 56\cdots$, and similarly $B_{b_3} = 0.1535522449949958272447\cdots$.

Now we can invoke [10, Theorem 4] to compute the constants $C_{b_1}(2)$ and $C_{b_3}(2)$. They are given by $C_f(2) = (1+B_f)/2$ for $f \in \{b_1, b_3\}$. We thus find that

$$C_{b_1}(2) = 0.5819486593172907979 28\cdots,\ C_{b_3}(2) = 0.5767761224974979136 22\cdots.$$

In [22] the authors write (in our notation) "$B_3(x)$ remains so closely proportional to $B_1(x)$ that it is not clear from this data whether $C_{b_3}(2) > C_{b_1}(2)$ or $C_{b_1}(2) < C_{b_3}(2)$. It would be unlikely that they are exactly equal." We thus have resolved this matter.

The numerical data from Table 1 in conjunction with the values of C_{b_1}, $C_{b_1}(2)$ and (3) suggest that $C_{b_1}(3) > 0$ and $C_{b_1}(4) < 0$. Similarly it seems plausible that $C_{b_3}(3) > 0$ and $C_{b_3}(4) < 0$.

6. Intermezzo: On a claim of Ramanujan

In the previous section we have seen that $B_{b_3} < \log\sqrt{3}$. This knowledge suffices to disprove a claim that was made in a celebrated, hitherto unpublished, manuscript of Ramanujan [3] on the partition and tau-functions.

Let τ denote Ramanujan's tau-function. Put $T_n = 0$ if $3|\tau(n)$ and $T_n = 1$ otherwise. In Ramanujan's manuscript we read [3, p. 64]: "We can show by transcendental methods that

$$\sum_{k=1}^{n} T_k = \frac{C}{3}\int_1^n \frac{dx}{\sqrt{\log x}} + O\left(\frac{n}{(\log n)^r}\right), \tag{18}$$

where r is any positive number and

$$C = \frac{2^{1/2}}{3^{1/4}}.\frac{1-7^{-2}}{1-7^{-3}}.\frac{1-13^{-2}}{1-13^{-3}}.\frac{1-19^{-2}}{1-19^{-3}}\cdots\frac{1}{\{(1-2^{-2})(1-5^{-2})(1-11^{-2})\cdots\}^{1/2}},$$

$2, 5, 11, \ldots$ being primes of the form $3k-1$ and $7, 13, 19, \ldots$ being primes of the form $3k+1$." This implies that for almost all n, $\tau(n)$ is divisible by 3.

Using that $\tau(n) \equiv n\sigma_1(n) (\mathrm{mod}\ 3)$, where $\sigma_1(n)$ denotes the sum of the positive divisors of n, it is easy to see that T_n is multiplicative and that

$$\sum_{n=1}^{\infty}\frac{T_n}{n^s} = \prod_{p\equiv 2(\mathrm{mod}\ 3)}\frac{1}{1-p^{-2s}}\prod_{p\equiv 1(\mathrm{mod}\ 3)}\frac{1+p^{-s}}{1-p^{-3s}}. \tag{19}$$

From (19) it is not difficult to verify Ramanujan's claim regarding the value of C. By logarithmic differentiation we obtain from (19) that

$$\sum_{n=1}^{\infty}\frac{\Lambda_T(n)}{n^s}=\sum_{p\equiv 2(\mathrm{mod}\ 3)}\frac{2\log p}{p^{2s}-1}+\sum_{p\equiv 1(\mathrm{mod}\ 3)}\left[\frac{\log p}{p^s+1}+\frac{3\log p}{p^{3s}-1}\right].$$

On comparing this series with that for $\sum_{n=1}^{\infty}\Lambda_{b_3}(n)n^{-s}$, it is easily seen, on using the inequality $B_{b_3}<\log\sqrt{3}$, that

$$B_T=B_{b_3}-\sum_{p\equiv 1(\mathrm{mod}\ 3)}\frac{(2p+1)\log p}{(p^2+p+1)(p+1)}-\log\sqrt{3}<B_{b_3}-\log\sqrt{3}<0;$$

indeed, we have $B_T=-0.53\cdots$. This shows that

$$\sum_{k=1}^{n}T_k=\frac{C}{3}\frac{n}{\sqrt{\log n}}\left(1+\frac{0.23\cdots}{\log n}+O\left(\frac{1}{(\log n)^{1+\epsilon}}\right)\right),$$

where $0.23\cdots=(1+B_T)/2\neq 0.5$ (here we invoked Theorem 4 of [10]) and $\epsilon>0$. Thus the above claim of Ramanujan is false for every $r>3/2$ and true for $r\leq 3/2$.

Note that if it were true that $B_T=0$, an amazing identity for Euler's constant would result. The manuscript [3] contains several further assertions of the type (18) (with 3 replaced by various other primes), all of which are disproved for $r>3/2$ in [11].

7. On the behaviour of $\sum_{n\leq x}\frac{\Lambda_{b_i}(n)}{n}-\frac{\log x}{2}$

Put $H_i(x)=\sum_{n\leq x}\Lambda_{b_i}(n)/n-\log\sqrt{x}$, for $i=1$ and $i=3$. A good understanding of the behaviour of H_i is needed in order to apply our key lemma, Lemma 2. Let us define, for $i=1$ and $i=3$, $C_+(b_i)=\sup_{x\geq 1}H_i(x)$ and $C_-(b_i)=\inf_{x\geq 1}H_i(x)$. As in [15] we define $V(x;d,a)=\sum_{\substack{n\leq x\\ n\equiv a(\mathrm{mod}\ d)}}\Lambda(n)/n$. It can be shown that as x

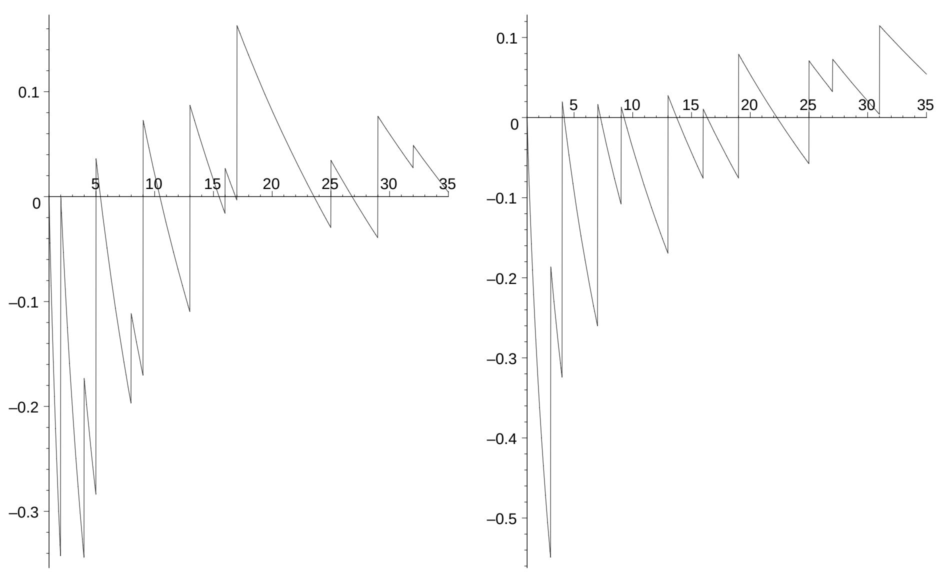

Figure 1. Plot of $H_1(x)$ (left) and $H_3(x)$ (right) for $1\leq x\leq 35$

tends to infinity $V(x;d,a) - \log x/\varphi(d)$ tends to a limit $C(d,a)$. Ramaré [15] has established the following result.

Theorem 3. [15]. *For $x \ge 68$ we have $|V(x;3,1) - \frac{1}{2}\log x - C(3,1)| \le 0.1205$ and $|V(x;4,1) - \frac{1}{2}\log x - C(4,1)| \le 0.0961$.*

We recall from [10] that

$$\sum_{\substack{p^r > \sqrt{x} \\ p \equiv a (\mathrm{mod}\ d)}} \frac{\log p}{p^{2r}} \le \frac{1.3}{\sqrt{x}} \text{ for } x \ge 289, \tag{20}$$

and that, for every fixed $v > 1$ and every $x > 0$,

$$\frac{\log v}{v-1}(1 - \frac{v}{x}) \le \sum_{r=1}^{[\log x/\log v]} \frac{\log v}{v^r} \le \frac{\log v}{v-1}. \tag{21}$$

Theorem 4. *We have:*
a) $C_-(b_1) = -\log\sqrt{2}$ *and* $C_+(b_1) < 0.2663$*;*
b) $C_-(b_3) = -\log\sqrt{3}$ *and* $C_+(b_3) < 0.276$*.*

Proof. After some computation for the interval $[1,68]$ we infer, from Theorem 3, that $C_+(b_1) \le B_{b_1} + 0.0961$ and similarly $C_+(b_3) \le B_{b_3} + 0.1205$. For the determination of $C_-(b_i)$ we use (20) and (21) in addition to Ramaré's inequalities; this yields, for $x \ge 289$, that $H_1(x) \ge \frac{1}{2}\log x + B_{b_1} - 1.3/\sqrt{x} - (\log 4)/x$ and $H_3(x) \ge \frac{1}{2}\log x + B_{b_3} - 1.3/\sqrt{x} - (\log 27)/(2x)$. □

Let RH(d) be the hypothesis that for every character χ mod d every non-trivial zero of $L(s,\chi)$ is on the critical line.

Theorem 5. *We have:*
a) $C_+(b_1) = H_1(461) = 0.1701069880305239\cdots$*, under RH*(4)*.*
b) $C_+(b_3) = H_3(3739) = 0.1554480047272349\cdots$*, under RH*(3)*.*

Proof (cf. [10, Theorem 6]*).* We recall from [10] that for $d \le 432$ and $(a,d) = 1$, there exists a constant $c_{d,a}$ such that for $x \ge 224$ we have, under RH(d), that

$$\left| \sum_{\substack{n \le x \\ n \equiv a (\mathrm{mod}\ d)}} \frac{\Lambda(n)}{n} - \frac{\log x}{\varphi(d)} - c_{d,a} \right| \le \frac{11}{32\pi\sqrt{x}}\{3\log^2 x + 8\log x + 16\}.$$

Under RH(4) it follows from this that $C_+(b_1) = \max_{v_i \le 6.15\times 10^8} H_1(v_i)$, where $2 = v_1 < v_2 < \cdots$ are the consecutive prime powers that can be written as a sum of two squares. Similarly under RH(3) we deduce that $C_+(b_3) = \max_{w_i \le 1.083\times 10^{10}} H_3(w_i)$, where $3 = w_1 < w_2 < \cdots$ are the consecutive prime powers that can be represented by the form $X^2 + 3Y^2$. On computing these maxima (for details see Section 9), the proof is then completed. □

The reason that, even under GRH, it requires a lot of computation to determine $C_+(b_1)$ and $C_+(b_3)$ is that these values are so close to B_{b_1}, respectively B_{b_3}. A similar phenomenon occurs in [10] for some of the functions considered there (cf. Theorem 6).

Using Theorem 4 and Lemma 2 together with sufficiently accurate approximations for C_{b_1} and C_{b_3}, one infers that $\mu_{b_1}(x) \ge \mu_{b_3}(x)$ for $x \ge 27500$. After some computation we then deduce that Conjecture 3 holds true.

Unfortunately, establishing Conjecture 2 requires quite a bit more work. In particular we need values for D_- and D_+ in Lemma 2 that are closer together than those coming from Theorem 4. Without improvement of Theorem 3, the upper bounds in Theorem 4 cannot be improved. The lower bounds, however, are amenable to improvement.

Let $\Delta_f(x)$ denote the quantity sandwiched between $D_-\mu_f(x)$ and $D_+\mu_f(x)$ in (9). Using the lower bound for $H_3(x)$ appearing in the proof of Theorem 4, we deduce that $H_3(x) \geq 0$ for $x \geq 25$. We infer that

$$\Delta_{b_3}(x) \geq -\log\sqrt{3}\{\mu_{b_3}(x) - \mu_{b_3}(\frac{x}{25})\}.$$

On applying Lemma 3 with $D_- = -\log\sqrt{3}$ and $D_+ = 0.276$, we deduce that $\Delta_{b_3}(x)/\mu_{b_3}(x) \geq -0.09586\cdots$ for $x \geq 10^9$. Taking $D_- = -0.09586\cdots$ as new value and repeating the procedure, we obtain $D_- = -0.06890\cdots$. Iterating twice more, we see that for $x \geq 10^9$ we can take $D_- = -0.0672$ in Lemma 2.

For any x satisfying the conditions of Lemma 2, we can proceed as above. If the first iteration yields an improved value of our initial D_- (which we take to be $-\log\sqrt{3}$), then it is not difficult to see that every further iteration yields a value of D_- not less than the previous one (this is so since, for given $r \geq 1$, $L(x/r, \frac{1}{2}, D_-, D_+)/U(x, \frac{1}{2}, D_-, D_+)$ is increasing, considered as a function in D_-). On the other hand, the value cannot be improved beyond zero, and hence the iteration process must converge. If the first iteration does not yield an improved value for D_- (which is initially taken as $-\log\sqrt{3}$), we put $\tilde{w}_i(x) = -\log\sqrt{3}$ for every $i \geq 0$; otherwise we put $\tilde{w}_0(x) = -\log\sqrt{3}$ and define

$$\tilde{w}_{i+1}(x) = \left(\frac{L(\frac{x}{25}, \frac{1}{2}, \tilde{w}_i(x), 0.276)}{U(x, \frac{1}{2}, \tilde{w}_i(x), 0.276)} - 1\right)\frac{\log 3}{2}.$$

Empirically it seems that after n iterations we can expect to have approached the limit value $\lim_{i\to\infty}\tilde{w}_i(x)$ with $O(n)$ decimal precision.

For b_1 we proceed similarly. After some computation using the lower bound for $H_1(x)$ given in Theorem 4, we find that $H_1(x) \geq 0.065$ for $x \geq 97$. Hence

$$H_1(x) \geq \left(-\log\sqrt{2} - 0.065\right)\{\mu_{b_1}(x) - \mu_{b_1}(\frac{x}{97})\} + 0.065\mu_{b_1}(x).$$

If the first iteration does not yield an improved value for D_- (which is initially taken as $-\log\sqrt{2}$), we put $\tilde{v}_i(x) = -\log\sqrt{2}$ for every $i \geq 0$; otherwise we put $\tilde{v}_0(x) = -\log\sqrt{2}$ and define

$$\tilde{v}_{i+1}(x) = \left(\frac{L(\frac{x}{97}, \frac{1}{2}, \tilde{v}_i(x), 0.2663)}{U(x, \frac{1}{2}, \tilde{v}_i(x), 0.2663)} - 1\right)(\log\sqrt{2} + 0.065) + 0.065.$$

To sum up, we have established:

Lemma 6. *Suppose that $x \geq x_0 \geq 2$ and $i \geq 0$. Then* (9) *holds true with $f = b_1$, $D_- = \tilde{v}_i(x_0)$, $D_+ = 0.276$. It also holds true with $f = b_3$, $D_- = \tilde{w}_i(x_0)$ and $D_+ = 0.2663$.*

This lemma, although amenable to further improvement, is sufficiently sharp for our purposes.

8. The proof of Theorem 2

Before proving Theorem 2, we will need two more lemmas (which are illustrated in Figure 2). From prime number theory we recall that

$$\psi(x;d,a) = \sum_{n\le x,\ n\equiv a (\mathrm{mod}\ d)} \Lambda(n).$$

Lemma 7. *We have:*
a) $\psi_{b_1}(x) \ge 0.4924x$ *for* $x \ge 37$.
b) $\psi_{b_3}(x) \le 0.5176x$ *for* $x \ge 3793$.

Proof. Let $d \le 13$ and $(a,d) = 1$. Then $|\psi(x;d,a) - x/\varphi(d)| \le \sqrt{x}$ for $224 \le x \le 10^{10}$ by [16, Theorem 1] and $|\psi(x;d,a) - x/\varphi(d)| < 0.004560x/\varphi(d)$ for $x \ge 10^{10}$ by [16, Theorem 5.2.1]. From these inequalities the lemma follows after some computation. □

For $y \ge 3$ we define $S_{b_3}(y)$ by $0.5176y$, except for the intervals $[3,49), [49,181), [181,487), [487,1369), [1699,1933), [2287.2437)$, and $[3733,3793)$, where we define $S_{b_3}(y)$ to be (respectively) $0.653954y, 0.605778y, 0.557372y, 0.534528y$, $0.526579y$, $0.521825y$ and $0.51996y$.

Lemma 8. *For* $y \ge 2$ *we have* $\psi_{b_3}(y) \le S_{b_3}(y)$.

Proof. The points where ψ_{b_3} and S_{b_3} change value occur only at prime powers representable by $X^2 + 3Y^2$, which we denoted by $3 = w_1 < w_2 < \cdots$. We now check that $\psi_{b_3}(w_i) \le S_{b_3}(w_i)$ for every $w_i \le 3793$. For $w_i \ge 3793$ the result follows by Lemma 7. □

At last we are in position to prove Theorem 2.

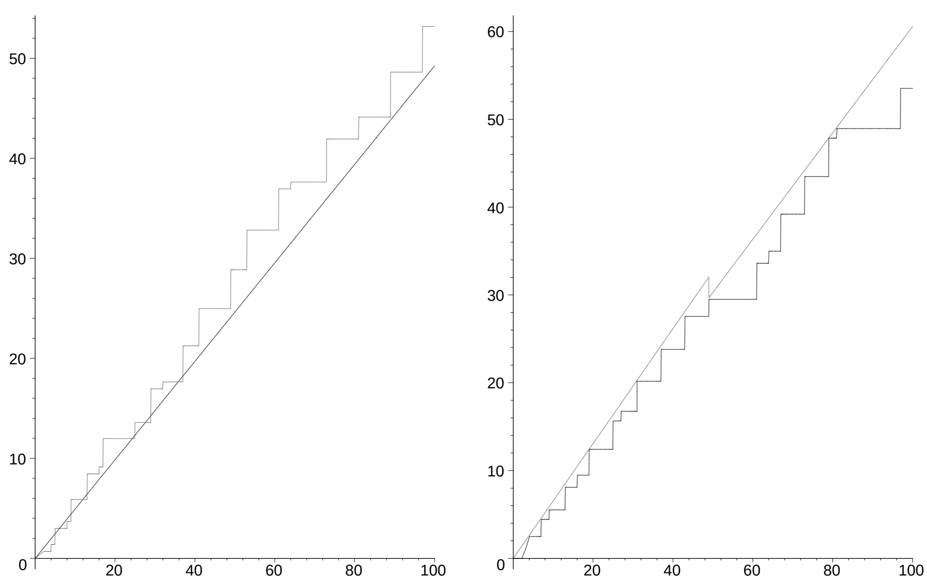

Figure 2. Plot of $\psi_{b_1}(x)$ versus $0.4924x$ (left) and plot of $\psi_{b_3}(x)$ versus $S_{b_3}(x)$ (right), for $0 \le x \le 100$

Proof of Theorem 2. As we have shown in Section 2, it suffices to establish Conjecture 2. To this end we have to prove that, for $x \geq 8$,

$$\lambda_{b_1}(x) = \sum_{n \leq \frac{x}{2}} b_1(n)\psi_{b_1}(\frac{x}{n}) \geq \sum_{n \leq \frac{x}{3}} b_3(n)\psi_{b_3}(\frac{x}{n}) = \lambda_{b_3}(x).$$

Let us denote the 6 intervals in the definition of $S_{b_3}(y)$ by $[r_i, s_i)$ for $i = 1, \ldots, 6$, and put $\alpha_i = S_{b_3}(r_i)/r_i - 0.5176$ (note that $\alpha_i > 0$). From Lemma 8 we infer that

$$\lambda_{b_3}(x) \leq \sum_{n \leq \frac{x}{3}} b_3(n)S_{b_3}(\frac{x}{n}) = 0.5176\mu_{b_3}(\frac{x}{3}) + \sum_{i=1}^{6} \alpha_i\{\mu_{b_3}(\frac{x}{r_i}) - \mu_{b_3}(\frac{x}{s_i})\}.$$

Put $x_0 = 1.5 \times 10^{11}$. Using a computer (see Section 9), Conjecture 2 can be established for $x < x_0$. Hence, assume now that $x \geq x_0$. For notational convenience we shorten $U(x/r, \frac{1}{2}, \tilde{w}_8(x_0/r), 0.276)$ to $U_3(x/r)$, $L(x/r, \frac{1}{2}, \tilde{w}_8(x_0/r), 0.276)$ to $L_3(x/r)$ and $L(x/r, \frac{1}{2}, \tilde{v}_8(x_0/r), 0.2663)$ to $L_1(x/r)$, where r is some fixed number. On applying Lemma 6, we deduce that

$$\frac{\lambda_{b_3}(x)}{2C_{b_3}} \leq 0.5176U_3(\frac{x}{3}) + \sum_{i=1}^{6} \alpha_i\{U_3(\frac{x}{r_i}) - L_3(\frac{x}{s_i})\}.$$

By Lemma 4 each of the six terms in the above sum is non-increasing for $x \geq x_0$, and thus the sum is bounded above by its value in x_0, which in its turn is less than $0.0224U_3(x_0/3)$. One easily checks that $U_3(x/3) \geq U_3(x_0/3)$ for $x \geq x_0$ (on noting that $U(y, \tau, D_-, D_+)$, considered as a function of τ, is increasing for $y > \exp(D_+ + (D_+ - D_-)/\tau)$). We thus obtain that $\lambda_{b_3}(x) \leq 1.08C_{b_3}U_3(x/3)$. Using Lemma 6 and the lower bound for ψ_{b_1} given in Lemma 7, we infer that $\lambda_{b_1}(x) \geq \sum_{n \leq x/37} b_1(n)\psi_{b_1}(x/n) \geq 0.4924\mu_{b_1}(x/37) \geq 0.9848C_{b_1}L_1(x/37)$. A computation shows that $0.9848C_{b_1}L_1(x_0/37) > 1.08C_{b_3}U_3(x_0/3)$. By Lemma 3 we then have $0.9848C_{b_1}L_{b_1}(x/37) > 1.08C_{b_3}U_3(x/3)$ for every $x \geq x_0$. We thus obtain that for every $x \geq x_0$,

$$\lambda_{b_1}(x) \geq 0.9848C_{b_1}L_1(\frac{x}{37}) \geq 1.08C_{b_3}U_3(\frac{x}{3}) \geq \lambda_{b_3}(x),$$

completing the proof. □

9. Computations of results used in Theorems 2 and 5

In the proof of Theorem 2 we have used the fact that Conjecture 2 is true for $x \leq x_0$ with $x_0 = 1.5 \times 10^{11}$. We established that result as follows.

Checking Conjecture 2 requires the computation and comparison of the sums

$$\lambda_{b_i}(x) = \sum_{n \leq x} b_i(n) \log n, \ i = 1, 3,$$

and, consequently, the computation of the characteristic functions $b_1(n)$ and $b_3(n)$ for all positive integers $n \leq x_0$. Because of the size of x_0, the range of x-values for which Conjecture 2 had to be checked was split up into subintervals of length 10^6, large enough for efficiency, and small enough to avoid so-called cache misses during the computations.

We first describe the case $\lambda_{b_1}(n)$. For a given interval, say, $[A, B]$, an integer array $b(j), j = 1, 2, \ldots, B - A + 1$ of length $B - A + 1$ is initialized to 0. Here, $b(j)$ corresponds to $b_1(j + A - 1)$. Next, all the possible sums of squares $x^2 + y^2$ of integers $0 \le x \le y$, with $A \le x^2 + y^2 \le B$, hence $x \in \left[0, \sqrt{B/2}\right]$, $y \in \left[\sqrt{A/2}, \sqrt{B}\right]$, are computed as follows. First, the sequence of all the squares $y^2 \in [A/2, B]$ is precomputed and stored. Next, for each $x = 0, 1, \ldots, \left\lfloor \sqrt{B/2} \right\rfloor$, the sums $x^2 + y^2$ are computed

$$\text{for all } y^2 \in \left[\max(A - x^2, A/2), B - x^2\right] \subset [A/2, B].$$

For all the sums $x^2 + y^2 =: n$ obtained in this way, $b(n - A + 1)$ is set equal to 1.

The case $\lambda_{b_3}(n)$ is treated similarly: the same initialization of array b is carried out. Next, all the possible sums $x^2 + 3y^2$ of integers x, y, with $A \le x^2 + 3y^2 \le B$, hence $x \in \left[0, \sqrt{B}\right]$, $y \in \left[0, \sqrt{B/3}\right]$, are computed as follows. First, the sequence of all the triples of squares $3y^2 \in [0, B]$ is precomputed and stored. Next, for each $x = 0, 1, \ldots, \left\lfloor \sqrt{B} \right\rfloor$, the sums $x^2 + 3y^2$ are computed

$$\text{for all } 3y^2 \in \left[\max(0, A - x^2), B - x^2\right] \subset [0, B]$$

and for all the sums $x^2 + 3y^2 =: n$ obtained in this way, $b(n - A + 1)$ is set equal to 1. This corresponds to $b_3(n)$.

We have implemented these algorithms for $b_1(n)$ and $b_3(n)$ in Fortran and used them to compute $\lambda_{b_i}(x)$ for $i = 1, 3$, and to verify Conjecture 2 for $x = 8, 9, \ldots, 1.5 \times 10^{11}$ on one 250 MHZ processor of CWI's SGI Origin 2000 computing system. Computing time was 7.6 CPU hours. We also used our program to check the values of $B_1(x) = \sum_{n \le x} b_1(n)$, given for $x = 10^i, i = 1, \ldots, 12$, by Shiu in Table 1 of [23] (where $B_1(x)$ is called $W(x)$). Computing time to extend our results from 1.5×10^{11} to 10^{12} was 77 CPU hours. We found agreement with Shiu for $i = 1, \ldots, 10$, but differences for $i = 11$ and $i = 12$: $B_1(10^{11}) = 15\ 570\ 512\ 744$ and $B_1(10^{12}) = 148\ 736\ 628\ 858$, whereas Shiu gave $W(10^{11}) = 15\ 570\ 523\ 346$ and $W(10^{12}) = 148\ 736\ 629\ 005$. Shiu used a different, more efficient method than ours, but he has confirmed our value of $B_1(10^{11})$ after checking and correcting his program [24].

We have spot-checked our program for computing $b_1(n)$ and $b_3(n)$ on various intervals of length 10^6 with the help of Lemma 1. This requires the decomposition into primes of each n for which we wish to compute $b_1(n)$, which is extremely expensive, compared with composing all integers in a given long interval $[A, B]$ as a sum of integer squares. However, we found agreement for all the checks we did, in particular for those in the neighbourhood of $x = 10^{12}$. In Table 2, we list, for $i = 1, 3$, the values we found of $\lambda_{b_i}(x)$ and $B_i(x)$ for $x = j \times 10^{11}$, $j = 1, 1.5, 2, \ldots, 10$.

In the proof of Theorems 5a and 5b, we have used the fact that

$$\max_{v_i \le 6.15 \times 10^8} H_1(v_i) = H_1(461) = 0.170106 \cdots, \text{ respectively,} \tag{22}$$

$$\max_{w_i \le 1.083 \times 10^{10}} H_3(w_i) = H_3(3739) = 0.155448 \cdots, \tag{23}$$

We established these results as follows.

TABLE 2. $\lambda_{b_1}(x), B_1(x)$ versus $\lambda_{b_3}(x), B_3(x)$

$x/10^{11}$	$\lambda_{b_1}(x)$	$\lambda_{b_3}(x)$	$B_1(x)$	$B_3(x)$
1	378458908590.818	316358774044.179	15570512744	13015595425
1.5	572353849423.260	478438468735.511	23160971166	19360573686
2	767521856517.400	641582406621.494	30700929088	25663340448
3	1160486988190.213	970068358550.987	45678037444	38182949191
4	1555965223692.576	1300655152892.098	60558145064	50621477125
5	1953301629004.525	1632795521743.015	75367348255	63000746043
6	2352112868630.901	1966168966371.294	90120785046	75333407591
7	2752146230205.959	2300563843364.554	104828319151	87627692348
8	3153223047545.408	2635831188875.970	119496904413	99889427349
9	3555209733889.339	2971859287714.156	134131682979	112122909167
10	3958003171956.632	3308561817015.470	148736628858	124331455166

Let $x = 6.15 \times 10^8$. We first generated the primes $\le \sqrt{x}$ with the sieve of Eratosthenes, and stored the following pairs $(n, \Lambda_{b_1}(n))$:

$$(2^k, \log 2), k = 1, 2, \ldots, \lfloor \log_2 x \rfloor,$$

$$(p^{2k}, 2\log p), k = 1, 2, \ldots, \left\lfloor \frac{1}{2} \log_p x \right\rfloor, \text{ for the primes } p \equiv 3 \bmod 4 \le \sqrt{x},$$

$$(p^k, \log p), k = 1, 2, \ldots, \lfloor \log_p x \rfloor, \text{ for the primes } p \equiv 1 \bmod 4 \le \sqrt{x},$$

into an array, sorted increasingly according to the first element of the pairs. The set of numbers n in these pairs in fact contains as a subset all the prime powers $v_1, v_2, \cdots \le \sqrt{x}$ which can be written as a sum of two squares. For these $(n, \Lambda_{b_1}(n))$-pairs, we computed $H_1(n)$ and verified that

$$\max_{v_i \le \lfloor \sqrt{6.15 \times 10^8} \rfloor} H_1(v_i) = H_1(461) = 0.170106 \cdots .$$

The remaining interval $\left[\lfloor \sqrt{6.15 \times 10^8} \rfloor + 1, x\right]$ was split up in pieces of length 10^7, and for each of these intervals, $[A, B]$, say, the primes $p \equiv 1 \bmod 4$ were generated with the sieve of Eratosthenes, together with $\log p$. These pairs $(p, \log p)$ were mixed with the $(n, \Lambda_{b_1}(n))$-pairs generated above for which $n \in [A, B]$, and then it was verified that $\max_{v_i \in [A,B]} H_1(v_i) < H_1(461)$. This proved (22). Computing time was 81 CPU seconds. Relation (23) was proved in a similar way at the cost of 1340 CPU seconds.

10. An alternative approach

In the previous sections we have made essential use of asymptotic information regarding the distribution of primes. Some of the results we used depend eventually on RH(3) and RH(4) to be true up to some finite height. It might come as a surprise then that it is possible to show that $B_1(x) \ge B_3(x)$ for $x \ge 10^{9111}$, without invoking any result from computational prime number theory (one only needs the ability to compute some successive primes...).

Our method of establishing this is inspired by Selberg's [19, pp. 183-185] method of obtaining an asymptotic evaluation for $N(x; 4, 1)$, where $N(x; d, a)$ denotes the number of integers $n \le x$ that have no prime factor p with $p \not\equiv a (\text{mod } d)$. Unfortunately Selberg's method does not seem to generalise well; for example we have no idea how to generalise it so as to show that $N(x; 4, 3) \ge N(x; 4, 1)$ for $x \ge x_0$, with

x_0 some effectively computable constant. See [13] for generalisations of Selberg's method.

Lemma 9. *a) For $x \geq 2$ we have*

$$|B_1(x) - C_{b_1}\frac{x}{\sqrt{\log x}}| \leq 9.62\frac{x}{\log x}.$$

b) For $x \geq 2$ we have

$$|B_3(x) - C_{b_3}\frac{x}{\sqrt{\log x}}| \leq 8.53\frac{x}{\log x}.$$

Corollary 1. *For $x \geq 10^{9111}$ we have $B_1(x) \geq B_3(x)$.*

In the proof of Lemma 9 we will make use of the following result. For a plot of the function g, see Figure 3.

Lemma 10. *Let $c_2 = 2e^\gamma$ and $c_3 = \sqrt{3}e^\gamma$. For $z \geq 1$ we put*

$$f(z) = z\sum_{n\leq z,\ 2\nmid n}\frac{1}{n} - \frac{z}{2}\log(c_2 z) \text{ and } g(z) = z\sum_{n\leq z,\ 3\nmid n}\frac{1}{n} - \frac{2}{3}z\log(c_3 z).$$

Then

$$\sup_{z\geq 1}|f(z)| = -f(3^-) = \frac{3}{2}\{\log 6 + \gamma\} - 3 = 0.55346270119438\cdots$$

and

$$\sup_{z\geq 1}|g(z)| = -g(4^-) = \frac{8}{3}\log(4\sqrt{3}e^\gamma) - 6 = 0.70084312094794\cdots.$$

Proof. We only prove the statement concerning $f(z)$; the statement regarding $g(z)$ can be proved in a similar way.

Since $z\log(c_2 z)$ is monotonically increasing, we obtain, cf. [10, Lemma 4], that $\sup_{z\geq 1}|f(z)| = \sup\{|f(1)|, |f(3^-)|, |f(3)|, |f(5^-)|, |f(5)|, \ldots\}$. Using the Euler-MacLaurin summation formula, cf. [26, p. 6], one finds that for integers $n \geq 1$,

$$\sum_{m\leq n}\frac{1}{m} = \log n + \gamma + \frac{1}{2n} - \frac{1}{12n^2} + \frac{\theta_1(n)}{60n^4}, \tag{24}$$

where $\theta_1(n) \in [0, 1]$. Clearly

$$\sum_{m\leq n,\ 2\nmid m}\frac{1}{m} = \sum_{m\leq n}\frac{1}{m} - \frac{1}{2}\sum_{m\leq n/2}\frac{1}{m}. \tag{25}$$

Let $n \geq 3$ be an odd integer. Notice that $f(n^-) = f(n) - 1$. Using (24) and (25), it is not difficult to deduce that

$$-\frac{1}{2} \leq f(n) \leq \frac{n}{2}\log(\frac{n}{n-1}) + \frac{n}{6(n-1)^2} + \frac{1}{60n^3}$$

and

$$-\frac{1}{2} \leq -f(n^-) \leq \frac{1}{2} + \frac{1}{2(n-1)} + \frac{1}{12n^2} + \frac{2}{15(n-1)^4}.$$

Using that the latter two right-hand sides are monotonically decreasing in n and noting that $\sup_{z\geq 1}|f(z)| \geq |f(3^-)|$, we see that $\sup_{z\geq 1}|f(z)| = \sup_{1\leq z\leq 11}|f(z)| = |f(3^-)|$. □

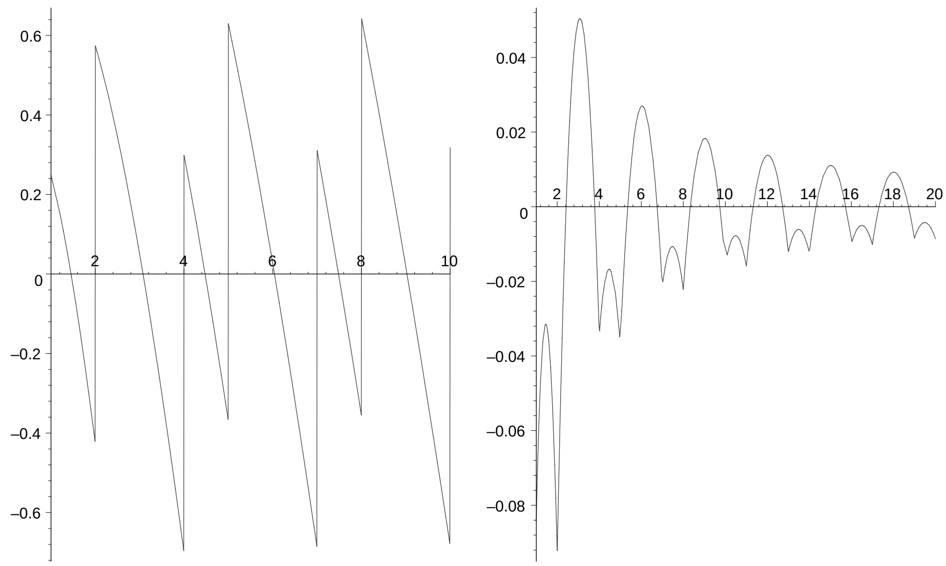

FIGURE 3. Plot of $g(x)$ for $1 \le x \le 10$ (left) and of $g(x)$ minus its limit function for $1 \le x \le 20$ (right)

Let $\{z\} = z - [z]$ denote the fractional part of z. Using (24) it can be shown that the functions f and g are almost periodic in the sense that they converge uniformly to the periodic functions $\frac{1}{2} - \{\frac{z-1}{2}\}$, respectively $1 - \{\frac{z-1}{3}\} - \{\frac{z+1}{3}\}$ (cf. Figure 3).

11. Proof of Lemma 9

Let P_2, P_3 denote the set of primes p that satisfy $p \equiv 2(\text{mod } 3)$, respectively $p \equiv 3(\text{mod } 4)$. Let $(P_2), (P_3)$ denote the set of natural numbers that have no prime divisor p with $p \not\equiv 2(\text{mod } 3)$, respectively $p \not\equiv 3(\text{mod } 4)$. Let $\psi_3(x), \psi_4(x)$ denote the number of integers $1 \le n \le x$ that have no prime divisor p with $p \not\equiv 2(\text{mod } 3)$, respectively $p \not\equiv 3(\text{mod } 4)$.

Proof of part a. Put $c_2 = 2e^\gamma$. We consider the expression

$$\begin{aligned} &\sum_{j=0}^{\infty} \sum_{m \in (P_3)} \sum_{\substack{1 \le n \le x/(2^j m^2) \\ n \equiv 1 (\text{mod } 4)}} \sum_{\substack{d \mid n \\ d \in (P_3)}} \mu(d) \log \frac{c_2 x}{2^j m^2 d} \\ &= \sum_{j=0}^{\infty} \sum_{m \in (P_3)} \sum_{\substack{d \in (P_3) \\ d \le x/(2^j m^2)}} \mu(d) \log \frac{c_2 x}{2^j m^2 d} \sum_{\substack{d \mid n,\ 1 \le n \le x/(2^j m^2) \\ n \equiv 1 (\text{mod } 4)}} 1. \end{aligned} \tag{26}$$

By approximating both sides of this equation in terms of the function B_1, we will arrive at an approximate functional equation, (34), for B_1 which on solving will yield an explicit lower bound for B_1.

On recalling that $\sum_{d|n} \mu(d) \log d = -\Lambda(n)$, one sees that, when $n \equiv 1 (\mathrm{mod}\ 4)$ and $d \le x/(2^j m^2)$, we have

$$\sum_{\substack{d|n \\ d\in(P_3)}} \mu(d) \log \frac{c_2 x}{2^j m^2 d} = \begin{cases} \log \frac{c_2 x}{2^j m^2} & \text{if } n \text{ has no divisor } p \text{ from } P_3; \\ \log p & \text{if } n \text{ is divisible by exactly one } p \text{ from } P_3; \\ 0 & \text{if } n \text{ has } \ge 2 \text{ distinct prime factors from } P_3. \end{cases}$$

On noting that

$$B_1(x) = \sum_{j=0}^{\infty} \sum_{m\in(P_3)} \psi_4(\frac{x}{2^j m^2}),$$

we see that the left-hand side of (26) equals

$$B_1(x) \log c_2 x + \sum_{\substack{p\in P_3 \\ r\ge 1}} \log p \ B_1(\frac{x}{p^{2r}}) - \sum_{j=0}^{\infty} \sum_{m\in(P_3)} \log(2^j m^2) \psi_4(\frac{x}{2^j m^2}), \tag{27}$$

which we write as

$$B_1(x) \log c_2 x + I_1(x) - I_2(x). \tag{28}$$

We write $z = x/2^j$ and consider the expression formed by the three inner sums in (26), that is,

$$\sum_{m\in(P_3)} \sum_{\substack{d\in(P_3) \\ d\le z/m^2}} \mu(d) \log \frac{c_2 z}{m^2 d} \sum_{\substack{d|n,\ 1\le n\le z/m^2 \\ n\equiv 1(\mathrm{mod}\ 4)}} 1. \tag{29}$$

Given an integer k, let $\xi(k)$ denote the product of the distinct primes that occur to an odd power in the prime factorisation of k. We put $\xi(k) = 1$ if there is no prime that occurs to an odd power in k. Note that

$$\sum_{m^2 d = k} \mu(d) = \mu(\xi(k)), \tag{30}$$

where the sum is over all integers m and d such that $m^2 d = k$. On writing $m^2 d = k$ in (29), and invoking (30), we deduce that the triple sum in (29) equals

$$\sum_{\substack{k\in(P_3) \\ k\le z}} \mu(\xi(k)) \log \frac{c_2 z}{k} \sum_{\substack{k_1\le z/k \\ k_1\equiv k(\mathrm{mod}\ 4)}} 1.$$

The right-hand side of (26) is thus seen to equal

$$\sum_{j=0}^{\infty} \sum_{\substack{k\in(P_3) \\ k\le x/2^j}} \mu(\xi(k)) \log \frac{c_2 x}{2^j k} \sum_{\substack{k_1\le x/(2^j k) \\ k_1\equiv k(\mathrm{mod}\ 4)}} 1,$$

which simplifies to

$$\sum_{\substack{d\in(P_3') \\ d\le x}} \mu(\xi(d')) \log \frac{c_2 x}{d} \sum_{\substack{k_1\le x/d \\ k_1\equiv d'(\mathrm{mod}\ 4)}} 1,$$

where d' denotes the largest odd divisor of d and $P_3' = P_3 \cup \{2\}$ and (P_3') is defined as (P_3), but where now no prime divisor p with $p \equiv 1 (\mathrm{mod}\ 4)$ is allowed. The right-hand side of (26) is thus seen to equal

(31)
$$\sum_{\substack{d\in(P_3')\\ d\le x}}\left[\frac{x}{4d}+\frac{2+(-1)^{\frac{d'-1}{2}}}{4}\right]\mu(\xi(d'))\log\frac{c_2x}{d}=\frac{x}{4}\sum_{\substack{d\in(P_3')\\ d\le x}}\frac{\mu(\xi(d'))}{d}\log\frac{c_2x}{d}+I_3(x),$$

where

$$|I_3(x)|\le\frac{3}{4}\sum_{\substack{d\in(P_3')\\ d\le x}}\log\frac{c_2x}{d}. \tag{32}$$

For $1\le d\le x$ we have, recalling the definition of f (made in Lemma 10),

$$\frac{1}{2}\log\frac{c_2x}{d}=\sum_{n\le x/d,\ 2\nmid n}\frac{1}{n}-f(\frac{x}{d})\frac{d}{x}.$$

Combining the latter equation with the sum in the right-hand side of (31) yields

$$\frac{x}{4}\sum_{\substack{d\in(P_3')\\ d\le x}}\frac{\mu(\xi(d'))}{d}\log\frac{c_2x}{d}=\frac{x}{2}\sum_{\substack{dn\le x,\ d\in(P_3')\\ 2\nmid n}}\frac{\mu(\xi(d'))}{dn}+I_4(x),$$

where

$$|I_4(x)|\le\frac{1}{2}\sum_{\substack{d\in(P_3')\\ d\le x}}|f(\frac{x}{d})|. \tag{33}$$

Note that

$$\frac{x}{2}\sum_{\substack{dn\le x,\ d\in(P_3')\\ 2\nmid n}}\frac{\mu(\xi(d'))}{dn}=\frac{x}{2}\sum_{k\le x}\frac{1}{k}\sum_{\substack{dn=k,\ d\in(P_3')\\ 2\nmid n}}\mu(\xi(d')).$$

Denote the latter inner sum by $h(k)$. We claim that $h(k)=b_1(k)$. First let us consider the case where k is odd. Then

$$h(k)=\sum_{dn=k,\ d\in(P_3)}\mu(\xi(d))=\sum_{dn=k}\mu(\xi(d))2^{-\omega(d)}\prod_{p|d}(1-(-1)^{\frac{p-1}{2}}),$$

where $\omega(d)$ denotes the number of distinct primes dividing d. We see that for odd k, h is the Dirichlet convolution of two multiplicative functions and is thus itself a multiplicative function. For arbitrary k we note that $h(k)=h(k')$, where k' is the largest odd divisor of k. Thus h is a multiplicative function. An easy computation shows that for every prime power q we have $h(q)=b_1(q)$. Since both h and b are multiplicative, this completes the proof of the claim. We thus infer that

$$\begin{aligned}\frac{x}{2}\sum_{\substack{dn\le x,\ d\in(P_3')\\ 2\nmid n}}\frac{\mu(\xi(d'))}{dn}&=\frac{x}{2}\sum_{m\le x}\frac{b_1(m)}{m}\\ &=\frac{x}{2}\int_1^x\frac{dB_1(t)}{t}=\frac{B_1(x)}{2}+\frac{x}{2}\int_1^x\frac{B_1(t)}{t^2}dt.\end{aligned}$$

Thus the right-hand side of (26) equals

$$\frac{B_1(x)}{2}+\frac{x}{2}\int_1^x\frac{B_1(t)}{t^2}dt+I_3(x)+I_4(x).$$

Equating it with the expression (28) for the left-hand side of (26), we get

$$B_1(x)\log c_2x - \frac{x}{2}\int_1^x \frac{B_1(t)}{t^2}dt = -I_1(x) + I_2(x) + I_3(x) + I_4(x) + \frac{B_1(x)}{2}. \tag{34}$$

Next we will consider effective estimates for $I_j(x)$ for $1 \le j \le 4$. Using the trivial estimate $B_1(x) \le x$, we obtain that

$$0 \le I_1(x) \le x \sum_{p\in P_3} \frac{\log p}{p^2-1} < .23x.$$

On noting that

$$\sum_{j=0}^{\infty} \sum_{m\in(P_3)} \frac{\log(2^j m^2)}{2^j m^2} = 2\sum_{m\in(P_3)} \frac{\log(2m^2)}{m^2} < 2.7$$

and $\psi_4(x) \le x$, we deduce that $0 \le I_2(x) < 2.7x$. Using (32), we deduce that

$$|I_3(x)| \le \frac{3}{4}\sum_{d\in(P_3'),\ d\le x} \log\frac{cx}{d} \le \frac{3}{4}\sum_{1\le d\le x}\int_d^{cx}\frac{dt}{t} \le \frac{3}{4}cx < 2.68x.$$

For $I_4(x)$ we have, by (33) and Lemma 10, $|I_4(x)| \le 0.277x$.

Put $A(x) = \int_1^x B_1(t)dt/t^2$. An easy calculation (divide by $x^2\log^{3/2}x$ and integrate) now shows that if

$$-\alpha_- x \le x^2 \log x A'(x) - \frac{x}{2}A(x) \le \alpha_+ x, \text{ for } x \ge x_0, \tag{35}$$

then there exists a constant c_0 such that

$$c_0\sqrt{\log x} - 2\alpha_+ \le A(x) \le c_0\sqrt{\log x} + 2\alpha_-, \text{ for } x \ge x_0.$$

On inserting the latter estimate in (35) and invoking (1), it then follows that

$$\Big|B_1(x) - C_{b_1}\frac{x}{\sqrt{\log x}}\Big| \le (\alpha_- + \alpha_+)\frac{x}{\log x}, \text{ for } x \ge x_0. \tag{36}$$

From our estimates for $I_j(x)$ with $j = 1, \ldots, 4$, we see that we can take $\alpha_- = 3.96$, $\alpha_+ = 5.66$ and $x_0 = 2$. □

Proof of part b. Making the obvious modifications in the proof of part a, we deduce that

$$B_3(x)\log c_3x - \frac{x}{2}\int_1^x \frac{B_3(t)}{t^2}dt = -J_1(x) + J_2(x) + J_3(x) + J_4(x) + \frac{B_3(x)}{2}, \tag{37}$$

where

$$J_1(x) = \sum_{p\in P_2,\ r\ge 1} \log p\ B_3(\frac{x}{p^{2r}}),$$

$$J_2(x) = \sum_{j=0}^{\infty}\sum_{m\in(P_2)} \log(3^j m^2)\psi_3(\frac{x}{3^j m^2}),$$

$$|J_3(x)| \le \frac{2}{3}\sum_{d\in(P_2'),\ d\le x} \log\frac{c_3x}{d},$$

and

$$|J_4(x)| \le \frac{1}{2}\sum_{d\in(P_2'),\ d\le x} |g(\frac{x}{d})|,$$

with $P_2' = P_2 \cup \{3\}$ and (P_2') defined as (P_2), but where now no prime divisor p with $p \equiv 1 (\mathrm{mod}\ 3)$ is allowed. Reasoning as before, we find that

$$0 \le J_1(x) < x \sum_{p \in P_2} \frac{\log p}{p^2 - 1} < 0.36x$$

and

$$0 \le J_2(x) < \frac{3}{4} x \sum_{m \in (P_2)} \frac{\log(3m^4)}{m^2} < 2.7x.$$

Furthermore we find that $|J_3(x)| \le 2xc_3/3 < 2.06x$ and $|J_4(x)| \le 0.36x$. From these estimates and (37) we infer that we can take $\alpha_+ = 5.12$, $\alpha_- = 3.41$ and $x_0 = 2$ in the analogue of (36). $\square$

Remark. In the proof of part a we have used the trivial estimates $\psi_4(x) \le x$ and $B_1(x) \le x$. Using that the integers n counted by $\psi_4(x)$ satisfy $n \equiv 1 (\mathrm{mod}\ 4)$ and $3 \nmid n$, we obtain the sharper estimate

$$\psi_4(x) \le [\frac{x+11}{12}] + [\frac{x+7}{12}] \le \frac{x}{6} + \frac{7}{6}. \tag{38}$$

Similarly, some computation yields that $B_1(x) \le x/2 + 2$. In this way the value 9.62 appearing in Lemma 9 a can still be further decreased, but we have not carried this out. Similarly the estimates in the proof of part b can be improved.

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