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The Kummer ratio of the relative class number for prime cyclotomic fields

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ABSTRACT

Kummer's conjecture predicts the asymptotic growth of the relative class number of prime cyclotomic fields. We substantially improve the known bounds of Kummer's ratio under three scenarios: no Siegel zero, presence of Siegel zero and assuming the Riemann Hypothesis for the Dirichlet L-series attached to odd characters only. The numerical work in this paper extends and improves on our earlier preprint https://arxiv.org/abs/1908.01152 and demonstrates our theoretical results.

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1. Introduction

Let K be a number field, $\mathcal{O}$ its ring of integers and s a complex variable. For $\Re(s) > 1$ the *Dedekind zeta function* is defined by

$$\zeta_K(s) = \sum_{\mathfrak{a}} \frac{1}{N\mathfrak{a}^s} = \prod_{\mathfrak{p}} \frac{1}{1 - N\mathfrak{p}^{-s}},$$

where $\mathfrak{a}$ ranges over the non-zero ideals in $\mathcal{O}$, $\mathfrak{p}$ ranges over the prime ideals in $\mathcal{O}$, and $N\mathfrak{a}$ denotes the *absolute norm* of $\mathfrak{a}$, that is the index of $\mathfrak{a}$ in $\mathcal{O}$. It is known that $\zeta_K(s)$ can be analytically continued to $\mathbb{C} \setminus \{1\}$, and that it has a simple pole at $s = 1$. Notice that $\zeta_{\mathbb{Q}}(s)$ equals $\zeta(s)$, the *Riemann zeta function*.

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Let $q \geqslant 3$ be a prime number and $K = \mathbb{Q}(\zeta_q)$ a *prime cyclotomic field*. Denote as $\mathbb{Q}(\zeta_q)^+ := \mathbb{Q}(\zeta_q + \zeta_q^{-1})$ the *maximal real cyclotomic field*. We have the factorization

$$\zeta_{\mathbb{Q}(\zeta_q)}(s) = \zeta(s) \prod_{\chi \neq \chi_0} L(s,\chi), \tag{1}$$

where χ runs over the non-principal characters modulo q. Likewise we have

$$\zeta_{\mathbb{Q}(\zeta_q)^+}(s) = \zeta(s) \prod_{\substack{\chi \neq \chi_0 \\ \chi(-1)=1}} L(s,\chi), \tag{2}$$

where the product is over all even characters modulo q.

1.1. Kummer's conjecture

Let $h_1(q)$ be the ratio of the class number $h(q)$ of $\mathbb{Q}(\zeta_q)$ and the class number of its maximal real subfield $\mathbb{Q}(\zeta_q)^+$. Kummer proved that this is an integer. It is now called either the *relative class number*, or the *first factor of the class number*, and played an important role in Kummer's research on Fermat's Last Theorem. Indeed, it is not difficult to show that if $q \nmid h(q)$, then $x^q + y^q = z^q$ has no non-trivial solution with q coprime to xyz [45, Ch. 1]. Kummer showed that q divides $h(q)$ if and only if q divides $h_1(q)$. As there is no easy way to compute $h(q)$, this is a very important result.

Some authors related $h_1(q)$ to a determinant and tried to estimate it in this way (cf. [15, §2]). Most famous is here the connection with the Maillet determinant due to Carlitz and Olsen [4] (independently obtained by Chowla and Weil, who however did not publish their result). For any integer n co-prime to q, let n' be the smallest positive integer such that $nn' \equiv 1 \pmod q$ and let $A(n,q)$ be the smallest positive residue of n modulo q. Let $M_q = (A(mn',q))_{1 \leqslant m,n \leqslant (q-1)/2}$. Then $\det(M_q)$ is called Maillet's determinant. In 1955, Carlitz and Olson proved that $\det(M_q) = \pm q^{(q-3)/2} h_1(q)$. From this Carlitz [3] deduced the appealing bounds $h_1(q) \leqslant (\frac{q-5}{4})!$ when $q \equiv 1 \pmod 4$, and $h_1(q) \leqslant (\frac{q-7}{4})!(\frac{q-3}{4})^{\frac{1}{2}}$ when $q \equiv 3 \pmod 4$. Much more recently Guo [17] proved that suitable normalizations of the determinants of $(\cot(jk\pi/q))_{j,k}$ and $(\tan(jk\pi/q))_{j,k}$ for $1 \leqslant j,k \leqslant (q-1)/2$ have $h_1(q)$ as factor.

In 1972, Metsänkylä [31] (simpler proof in [32]), established the elegant bound $h_1(q) < 2q(q/24)^{(q-1)/4}$. In 1982, Feng [11] showed using a determinantal approach that

$$h_1(q) < 2q\Big(\frac{q-1}{31.997158}\Big)^{(q-1)/4}.$$

Fung et al. [15] used determinants to exactly compute $h_1(q)$ for $q < 3000$, extending earlier computations by others. Kummer himself impressively computed by hand up to $q = 163$, only making three mistakes.

Definition 1. Let q be a prime number,

$$G(q) := 2q\Big(\frac{q}{4\pi^2}\Big)^{\frac{q-1}{4}}, \quad R(q) := \frac{h_1(q)}{G(q)} \quad \textit{and} \quad r(q) := \log R(q). \tag{3}$$

The ratio $R(q)$ is called *Kummer ratio*. In 1851, Kummer [22] conjectured that $h_1(q)$ asymptotically grows in the same way as the elementary function $G(q)$.

Conjecture 1. *As q tends to infinity, $R(q)$ tends to* 1.

For a generic prime q the Kummer ratio $R(q)$ is close to 1 (see Sections 3 and 6 for a theoretical, respectively numerical, underpinning). However, in this paper our focus is on the extremal behavior of $R(q)$. Our starting point in studying $R(q)$ will be the identity

$$R(q) = \prod_{\chi(-1)=-1} L(1, \chi), \tag{4}$$

where the product is over all the odd characters modulo q (cf. Hasse [19]). It follows from this, (1) and (2) that

$$R(q) = \lim_{s \downarrow 1} \frac{\zeta_{\mathbb{Q}(\zeta_q)}(s)}{\zeta_{\mathbb{Q}(\zeta_q)^+}(s)} = \lim_{s \downarrow 1} \prod_{\chi(-1)=-1} L(s, \chi),$$

where $s \downarrow 1$ means that $s > 1$ tends to 1. The reason why only the odd Dirichlet characters are involved into (4) follows from the fact that, using (1)-(2), in the ratio $\frac{\zeta_{\mathbb{Q}(\zeta_q)}(s)}{\zeta_{\mathbb{Q}(\zeta_q)^+}(s)}$ the Riemann zeta and the even characters contributions cancel out. We refer the interested reader to [21] to explore the bounds of the product $\prod_{\chi \neq \chi_0} L(1, \chi)$, where χ varies over all the non-principal characters modulo q.

Masley and Montgomery [29, Thm. 1] gave an *effective* bound for $R(q)$, which in combination with numerical work, allowed them to prove Kummer's conjecture that $h(q) = 1$ if and only if $q \leqslant 19$. Using their method ineffective, but rather sharper, estimates for $R(q)$ were obtained by Puchta [36][1] and more recently by Lu-Zhang [28] and Debaene [9].

Our main result, Theorem 1, improves on all of these (see also Section 5 for more details). It involves the *exponential integral function* (defined as $E_1(x) := \int_x^\infty e^{-t}\, dt/t$ for $x > 0$), and the *Siegel zero* (defined in Section 2.2).

Theorem 1. *Let $\ell(q)$ be a function that tends arbitrarily slow and monotonically to infinity as q tends to infinity. There is an effectively computable prime q_0 (possibly depending on ℓ) and an effectively computable prime q_1 such that the following statements are true:*

1) *If for some $q \geqslant q_0$ the family of Dirichlet L-series $L(s, \chi)$, with χ any odd character modulo q, has no Siegel zero, for example if $q \equiv 1 \pmod 4$, then*

$$\max\{R(q), R(q)^{-1}\} < e^{0.41} (\log q)\, \ell(q).$$

2) *If for some $q \geqslant q_0$ the family of Dirichlet L-series $L(s, \chi)$, with χ any odd character modulo q, has a Siegel zero β_0 then*

$$\max\{R(q)e^{E_1(1-\beta_0)}, R(q)^{-1}e^{-E_1(1-\beta_0)}\} < e^{0.41} (\log q)^2\, \ell(q).$$

3) *If the Riemann Hypothesis holds for every Dirichlet L-series $L(s, \chi)$, with χ an odd character modulo q for some prime $q \geqslant q_1$, then*

$$\max\{R(q), R(q)^{-1}\} < e^{0.41} \log q.$$

Notice that $\max\{R(q), R(q)^{-1}\} = e^{|r(q)|}$. Several other comments are in order. Here we state the most relevant ones, and refer to Section 5 for further ones.

[1] In Theorem 1 of [36] one should read $(p + 3)/4$ instead of $(p - 3)/4$.

Remark 1. Note that when compared with the no Siegel zero situation, assuming the Riemann Hypothesis for the Dirichlet L-series attached to odd characters only allows one to remove a factor that tends to infinity arbitrarily slowly.

Remark 2. The value 0.41 in Theorem 1 can be further sharpened to 0.39 by arguing as in Remark 5 below.

Remark 3. We have $1 \ll E_1(1-\beta_0) < \varepsilon \log q + c(\varepsilon)$, where $c(\varepsilon)$ is ineffective (see Section 5 for a proof).

The reader might wonder how close Theorem 1 is to the truth. Sharp estimates were conjectured by Granville [16, § 9], who speculated that for $\epsilon > 0$ and q large enough, we have

$$\max\{R(q), R(q)^{-1}\} < (\log_2 q)^{\frac{1}{2}+\epsilon},$$

with this result being false if $\frac{1}{2}$ is being replaced by any smaller number (where here and in the sequel $\log_2 q$ denotes $\log\log q$). The optimum is related to strong failure of prime number equidistribution, an extremely rare situation that is very far from being understood.

The paper is organized as follows: In Section 2 we recall results we need (mainly from prime number theory) and in Section 3 we present the Kummer ratio conjecture and we prove an explicit constant version of a classical result by Ankeny and Chowla (Lemma 1). In Section 4 we prove Theorem 1. Many comments and remarks about comparing Theorem 1 with similar results in the literature are collected in Section 5. Section 6 expands on our earlier preprint [26]. It provides an efficient algorithm to compute $R(q)$ and some numerical data and graphical representations regarding the distribution of $r(q)$ that might be the starting point for future works. For example, the presence of secondary "spikes" close to $\pm\frac{1}{4}$ and $\pm\frac{1}{8}$ demonstrates in a beautiful way the contributions of the primes q for which $2q \pm 1$, or $4q \pm 1$, are prime too.

2. Preliminaries

2.1. Prime number distribution

In this section, we recall the material we need on the distribution of prime numbers, using the notations

$$\pi(t) = \sum_{p \leqslant t} 1, \qquad \pi(t;d,a) = \sum_{\substack{p \leqslant t \\ p \equiv a \pmod d}} 1,$$

$$\theta(t) = \sum_{p \leqslant t} \log p, \qquad \theta(t;d,a) = \sum_{\substack{p \leqslant t \\ p \equiv a \pmod d}} \log p,$$

and

$$\psi(t) = \sum_{n \leqslant t} \Lambda(n), \qquad \psi(t;d,a) = \sum_{\substack{n \leqslant t \\ n \equiv a \pmod d}} \Lambda(n),$$

where Λ denotes the von Mangoldt function. For fixed coprime integers a and d, we have asymptotic equidistribution:

$$\pi(t;d,a) \sim \frac{\pi(t)}{\varphi(d)}, \quad \theta(t;d,a) \sim \frac{\theta(t)}{\varphi(d)} \quad \text{and} \quad \psi(t;d,a) \sim \frac{\psi(t)}{\varphi(d)} \quad (t \to \infty),$$

with φ Euler's totient. While the asymptotics for the quantities above is available only for small d, say, $d \leqslant (\log t)^A$, $A > 0$, the following celebrated result concerns the accuracy of the first approximation on average when the moduli d are allowed to be large with respect to t. For every $A > 0$, we have the bound

$$\sum_{d \leqslant \mathcal{Q}} \max_{t \leqslant u} \max_{(a,d)=1} \left| \psi(t; d, a) - \frac{\psi(t)}{\varphi(d)} \right| \ll \frac{u}{(\log u)^A}, \tag{5}$$

where $\mathcal{Q} = \mathcal{Q}(u)$ is a suitable function, and the implicit constant may depend on A and $\mathcal{Q}$. The upper bound (5), with $\mathcal{Q}(u) = \sqrt{u}/(\log u)^B$, $B = B(A) > 0$, was independently proved by Bombieri and A. I. Vinogradov in 1965, see [6, § 9.2].

A similar statement for $t = u$ and $\mathcal{Q}(u) = u^{1-\varepsilon}$ with $0 < \varepsilon < 1$, is unproved yet and commonly called the *Elliott-Halberstam conjecture*, see [6,10].

Conjecture 2 *(Elliott-Halberstam). For every $\varepsilon > 0$ and $A > 0$,*

$$\sum_{q \leqslant u^{1-\varepsilon}} \max_{(a,q)=1} \left| \pi(u; q, a) - \frac{\pi(u)}{\varphi(q)} \right| \ll_{A,\varepsilon} \frac{u}{(\log u)^A}.$$

Statements equivalent to (5) and the Elliott-Halberstam conjecture with the $\psi(t; q, a), \psi(t)$-functions replaced by the $\pi(t; q, a), \pi(t)$-functions, or the $\theta(t; q, a), \theta(t)$-ones, can be easily obtained via partial summation.

An important tool we will use is the following theorem.

Classical Theorem 1 *(Brun-Titchmarsh). Let $x, y > 0$ and a, q be positive integers such that $(a, q) = 1$. Then*

$$\pi(x + y; q, a) - \pi(x; q, a) < \frac{2y}{\varphi(q) \log(y/q)}, \tag{6}$$

for all $y > q$.

For a proof, see, e.g., Montgomery-Vaughan [33, Theorem 2].

2.2. Siegel zeros

Let $K \neq \mathbb{Q}$ be an algebraic number field having d_K as its absolute discriminant over the rational numbers. Then, see Stark [42, Lemma 3], $\zeta_K(s)$ has at most one zero in the region in the complex plane determined by

$$\Re(s) \geqslant 1 - \frac{1}{4 \log d_K}, \qquad |\Im(s)| \leqslant \frac{1}{4 \log d_K}.$$

If such a zero exists, it is real, simple and often called *Siegel zero*. When $K = \mathbb{Q}(\zeta_q)$, using (1) it is easy to see that the Siegel zero is attached to the family of Dirichlet L-series $\pmod q$. In this case, the Dirichlet character χ such that $L(s, \chi)$ has the Siegel zero is called the *exceptional character* and it is a well known fact that it is quadratic.

We will also use the Riemann Hypothesis ($\mathrm{RH}_{\mathrm{odd}}(q)$) for the Dirichlet L-series attached to odd Dirichlet characters.

Conjecture 3 *($RH_{odd}(q)$). Let q be an odd prime. The non-trivial zeros of the Dirichlet L-series $L(s, \chi)$, where χ runs over the set of the odd Dirichlet characters $\pmod q$, are on the line $\Re(s) = \frac{1}{2}$.*

2.3. Admissible sets of large measure

Let $\mathcal{A} = \{a_1, \ldots, a_s\}$ be a set of s distinct natural numbers. We define the measure

$$\mu(\mathcal{A}) = \sum_{k=1}^{s} \frac{1}{a_k}.$$

Given a prime p, let $\omega(p)$ denote the number of solutions modulo p of the equation

$$X \prod_{i=1}^{s} (a_i X + 1) \equiv 0 \pmod{p}. \tag{7}$$

A set $\mathcal{A}$ is said to be *admissible* if $\omega(p) < p$ for every prime p. As $\omega(p) \leqslant s+1$, we see that $\mathcal{A}$ is admissible, if and only if $\omega(p) < p$ for every prime $p \leqslant s+1$. We observe that if we change every term $a_iX + 1$ by $a_iX - 1$ in (7), the number of solutions is also still $\omega(p)$.

The admissible sets are relevant for determining which sets of linear forms can (presumably) be infinitely often all simultaneously prime.

Conjecture 4 *(Hardy-Littlewood [18], lower bound version). Suppose $\mathcal{A} = \{a_1, \ldots, a_s\}$ is an admissible set. Choose $b \in \{-1, 1\}$. Then the number of integers $n \leqslant x$ such that the integers $n, a_1n + b, \ldots, a_sn + b$ are all prime is of cardinality $\gg_{\mathcal{A}} x/(\log x)^{s+1}$.*

Conjecture 5 *(Hardy-Littlewood [18] for Sophie Germain primes). There are $\gg x/(\log x)^2$ primes $p \leqslant x$ for which $2p + 1$ is also prime.*

The following result, conjectured by Erdős (1988), shows that there are admissible sets having arbitrarily large measure μ.

Theorem *(Granville [16]). There is a sequence of admissible sets $\mathcal{A}_1, \mathcal{A}_2, \ldots$ such that $\lim_{j\to\infty} \mu(\mathcal{A}_j) = \infty$. We have $\overline{\mathcal{M}} = [0, \infty]$, with $\overline{\mathcal{M}}$ the closure of the set $\{\mu(\mathcal{A}) : \mathcal{A}$ is an admissible set$\}$.*

3. Connecting Kummer's ratio conjecture with prime power sums

The orthogonality property of odd characters

$$\frac{2}{q-1} \sum_{\chi(-1)=-1} \chi(a)\overline{\chi}(b) = \begin{cases} \pm 1, & b \equiv \pm a \pmod{q}, \\ 0, & \text{otherwise}, \end{cases}$$

gives us

$$\sum_{\chi(-1)=-1} \log(L(s,\chi)) = \frac{q-1}{2} \lim_{x\to\infty} \Big(\sum_{\substack{m\geqslant 1;\ p^m \leqslant x \\ p^m \equiv 1 \pmod{q}}} \frac{1}{mp^{ms}} - \sum_{\substack{m\geqslant 1;\ p^m \leqslant x \\ p^m \equiv -1 \pmod{q}}} \frac{1}{mp^{ms}} \Big).$$

In the papers [9,29,36] just mentioned, the authors consider the latter function in a neighborhood of $s = 1$ (but whereas Debaene [9] and Puchta [36] take higher derivatives into account, Masley and Montgomery [29] stopped at the first derivative). Here, we will actually set $s = 1$, which in combination with (4) yields

$$r(q) = \log R(q) = \frac{q-1}{2} \lim_{x\to\infty} \Big(\sum_{\substack{m\geqslant 1;\ p^m \leqslant x \\ p^m \equiv 1 \pmod{q}}} \frac{1}{mp^{m}} - \sum_{\substack{m\geqslant 1;\ p^m \leqslant x \\ p^m \equiv -1 \pmod{q}}} \frac{1}{mp^{m}} \Big). \tag{8}$$

Definition 2. The argument in the limit we denote by $f_q(x)$ and $f_q := \lim_{x\to\infty} f_q(x)$.

Note that Kummer's conjecture is equivalent with $f_q = o(1/q)$ as q tends to infinity. The idea is now to choose x as small as possible so that the resulting error $f_q - f_q(x)$ is still reasonable. In attempting to decrease x, the Bombieri-Vinogradov theorem and the Brun-Titchmarsh inequality play a crucial role. The main contribution to $f_q(x)$ comes from the term with $m = 1$, and is denoted by $g_q(x)$:

$$g_q(x) := \sum_{\substack{p\leqslant x \\ p\equiv 1 \pmod q}} \frac{1}{p} - \sum_{\substack{p\leqslant x \\ p\equiv -1 \pmod q}} \frac{1}{p}. \tag{9}$$

In the following, we will also use the notation

$$S_q(b,x) := \sum_{\substack{p\leqslant x \\ p\equiv b \pmod q}} \frac{1}{p}, \tag{10}$$

where $b \in \{-1, 1\}$, so that $g_q(x) = S_q(1, x) - S_q(-1, x)$.

Taking all this into account Granville [16] showed that if Kummer's conjecture is true then for every $\delta > 0$ we must have

$$g_q(q^{1+\delta}) = o\Big(\frac{1}{q}\Big),$$

for all but at most $2x/(\log x)^3$ primes $q \leqslant x$. He used this to show that $c^{-1} \leqslant R(q) \leqslant c$ for a positive proportion $\rho(c)$ of primes $q \leqslant x$, where $\rho(c) \to 1$ as c tends to infinity.

Murty and Petridis [35] improved this as follows.

Theorem. *There exists a constant $c > 1$ such that for a sequence of primes with natural density 1 we have*

$$\max\{R(q), R(q)^{-1}\} \leqslant c.$$

If the Elliott-Halberstam conjecture (Conjecture 2) is true, then we can take $c = 1 + \epsilon$ for any fixed $\epsilon > 0$.

Although typically $R(q)$ is close to 1, conjecturally very different behavior also occurs (on very thin sets of primes).

Theorem *(Granville [16, Theorems 2 and 4]). If the lower bound version of the Hardy-Littlewood conjecture (Conjecture 4) is true, and also the Elliott-Halberstam conjecture (Conjecture 2), then for any admissible set $\mathcal{A}$, the numbers $e^{\mu(\mathcal{A})/2}$ and $e^{-\mu(\mathcal{A})/2}$ are both limit points of the sequence $\{R(q) : q$ is prime$\}$. Furthermore, this sequence has $[0, \infty]$ as set of limit points.*

Corollary. *Under the above conjectures, Kummer's ratio Conjecture 1 is false.*

Actually, on taking $\mathcal{A} = \{2\}$, it suffices to assume the Hardy-Littlewood conjecture for Sophie German primes (Conjecture 5) instead of the full Hardy-Littlewood conjecture (Conjecture 4), and Granville proved that $\min\{R(q), R(q)^{-1}\} > e^{0.249}$ for $\gg x/(\log x)^2$ primes $q \leqslant x$. Likewise, other cases where $\mathcal{A}$ contains only one element produce a relatively thick set of $R(q)$ outliers, something also our numerics show. The value distribution of $r(q)$ was studied in detail by Croot and Granville [7].

One can also wonder how large $R(q)$ can be as a function of q, an issue that we discussed just after Remark 8.

3.1. A useful lemma

The following lemma, inspired by a result of Ankeny-Chowla, see the estimate of C_4 in [1] and [16, Lemmas 1 and 2], will be a crucial ingredient in the proof of Theorem 1. Let

$$t_q := \sum_{\substack{m\geqslant 2\\ p^m\equiv 1 \pmod q}} \frac{1}{mp^m} - \sum_{\substack{m\geqslant 2\\ p^m\equiv -1 \pmod q}} \frac{1}{mp^m}. \tag{11}$$

By (8)-(9) and (11) we have

$$r(q) = \frac{q-1}{2}\big(t_q + \lim_{x\to\infty} g_q(x)\big).$$

Lemma 1. *There exists a constant $c > 0$ such that for every odd prime q we have*

$$|t_q| < \frac{1}{q}\Big(\frac{43}{13} - \frac{18}{13}\zeta(3)\Big) + \frac{c}{q\log q}.$$

Proof. Given any integer b we put

$$S_q(b) := \sum_{\substack{m\geqslant 2\\ p^m\equiv b \pmod q}} \frac{1}{mp^m}. \tag{12}$$

In the rest of the proof we will assume that $b \in \{-1, 1\}$. By (11) we have $t_q = S_q(1) - S_q(-1)$, and using $S_q(b) > 0$, we obtain $-S_q(-1) \leqslant t_q \leqslant S_q(1)$. Thus,

$$|t_q| \leqslant \max\{S_q(1), S_q(-1)\}. \tag{13}$$

We split $S_q(b)$ into three subsums according to whether $p^m \leqslant q(\log q)^2$, $q(\log q)^2 < p^m < q^2$ or $p^m > q^2$. The contribution to the final estimate of the sums over the first range will be less than c_1/q, with a constant $c_1 > 0$ that will be explicitly determined, while the others contribute $\ll 1/(q\log q)$.

We first consider the case $p^m > q^2$. For any prime $p > q \geqslant 3$ we have

$$\sum_{m\geqslant 2} \frac{1}{mp^m} \leqslant \frac{1}{2}\frac{1}{p(p-1)} < \frac{1}{p^2}.$$

Moreover, for $p \leqslant q$, the condition $p^m > q^2$ implies $m \geqslant 3$ and hence

$$\sum_{\substack{m\geqslant 2;\, p\leqslant q\\ p^m>q^2}} \frac{1}{mp^m} \leqslant \frac{1}{3}\sum_{\substack{m\geqslant 3;\, p\leqslant q\\ p^m>q^2}} \frac{1}{p^m} = \frac{1}{3p^3}\sum_{j\geqslant 0}\frac{1}{p^j} \leqslant \frac{1}{3q^2}\frac{p}{p-1} < \frac{1}{q^2}.$$

Combining these estimates we arrive at

$$\begin{aligned}\sum_{\substack{m\geqslant 2;\ p^m>q^2\\ p^m\equiv b \pmod q}} \frac{1}{mp^m} &\leqslant \sum_{p>q}\sum_{m\geqslant 2}\frac{1}{mp^m} + \sum_{p\leqslant q}\sum_{\substack{m\geqslant 2\\ p^m>q^2}}\frac{1}{mp^m} < \sum_{p>q}\frac{1}{p^2} + \sum_{p\leqslant q}\frac{1}{q^2}\\ &= 2\int_q^\infty \frac{\pi(t)}{t^3}dt \ll \int_q^\infty \frac{dt}{t^2\log t} \ll \frac{1}{q\log q},\end{aligned} \tag{14}$$

where we used the partial summation formula and the Chebyshev bound in the weaker form $\pi(t) \ll t/\log t$. From the proof of [16, Lemma 1] we obtain

$$\sum_{\substack{m\geqslant 2;\ q(\log q)^2<p^m<q^2 \\ p^m\equiv b \pmod q}} \frac{1}{mp^m} \leqslant \sum_{m=2}^{\lfloor 4\log q\rfloor} \frac{1}{m}\frac{2m}{q(\log q)^2} \ll \frac{1}{q\log q}. \tag{15}$$

We now proceed as in the proof of [16, Lemma 2]. We are left in (12) with the cases $p^m \equiv b \pmod q$, $m \geqslant 2$ and $p^m \leqslant q(\log q)^2$. There are at most m values of p for which $p^m \equiv b \pmod q$ and $p^m \leqslant q(\log q)^2$, so each sum can be maximized by assuming that $q+b$ and $2q+b$ are squares, $3q+b$, $4q+b$ and $5q+b$ are cubes, and so on. Setting

$$\alpha(m) := \frac{1}{2}(m^2-m), \quad \beta(m) := \frac{1}{2}(m^2+m)-1,$$

we obtain

$$\begin{aligned}\sum_{\substack{m\geqslant 2;\, p^m\leqslant q(\log q)^2 \\ p^m\equiv b \pmod q}} \frac{1}{mp^m} &\leqslant \sum_{m\geqslant 2}\frac{1}{m}\sum_{r=\alpha(m)}^{\beta(m)}\frac{1}{rq+b} \leqslant \sum_{m\geqslant 2}\frac{1}{m}\sum_{r=\alpha(m)}^{\beta(m)}\frac{1}{rq-1} \\ &= \sum_{m\geqslant 2}\frac{1}{m}\sum_{r=\alpha(m)}^{\beta(m)}\frac{1}{rq}\Big(1+\frac{1}{rq-1}\Big) \\ &\leqslant \frac{1}{q}\Big(\frac{3}{4}+\frac{1}{2q-2}+\frac{1}{8q-4}\Big)+\frac{1}{q}\Big(1+\frac{1}{3q-1}\Big)\sum_{m\geqslant 3}\frac{1}{m}\sum_{r=\alpha(m)}^{\beta(m)}\frac{1}{r},\end{aligned} \tag{16}$$

in which we have isolated the contribution of the terms corresponding to $m=2$. The innermost sum in (16) can be bounded as follows:

$$\begin{aligned}\sum_{r=\alpha(m)}^{\beta(m)}\frac{1}{r} &\leqslant \frac{2}{m^2-m}+\int_{\alpha(m)}^{\beta(m)}\frac{du}{u} = \frac{2}{m^2-m}+\log\Big(1+\frac{2}{m}\Big) \\ &\leqslant \frac{2}{m^2-m}+\frac{2}{m}\frac{3m+1}{3m+4} = \frac{2}{m}\Big(\frac{m}{m-1}-\frac{3}{3m+4}\Big) \leqslant \frac{2}{m-1}-\frac{18}{13m^2},\end{aligned}$$

in which we used the inequalities $\log(1+x) \leqslant \frac{x}{2}\cdot\frac{x+6}{2x+3}$ for every $x \geqslant 0$, see [44, eq. (22)], and $3m+4 \leqslant \frac{13}{3}m$, which holds for every $m \geqslant 3$. Hence

$$\sum_{m\geqslant 3}\frac{1}{m}\sum_{r=\alpha(m)}^{\beta(m)}\frac{1}{r} \leqslant \sum_{m\geqslant 3}\frac{2}{m(m-1)}-\frac{18}{13}\Big(\zeta(3)-\frac{9}{8}\Big) = \frac{133}{52}-\frac{18}{13}\zeta(3). \tag{17}$$

Inserting the bound for the double sum in (17) into (16) we obtain

$$\sum_{\substack{m\geqslant 2;\, p^m\leqslant q(\log q)^2 \\ p^m\equiv b \pmod q}} \frac{1}{mp^m} \leqslant \frac{1}{q}\Big(\frac{43}{13}-\frac{18}{13}\zeta(3)+\frac{c_2}{q}\Big), \tag{18}$$

where $c_2 > 0$ is a suitable constant. Inserting (14)-(15) and (18) into (12) we deduce that there exists a constant $c > 0$ such that

$$S_q(b) < \frac{1}{q}\Big(\frac{43}{13} - \frac{18}{13}\zeta(3)\Big) + \frac{c}{q\log q}. \tag{19}$$

The result immediately follows from (19) and (13). □

Remark 4. Lemma 1 allows one to improve the estimate $\Sigma_2 = \frac{q-1}{2}t_q$ in [46],[2] and hence to improve some of the results there.

Remark 5. The leading constant in Lemma 1 can be further improved by isolating more initial terms of the sum over m in equation (16); in fact, with the aid of a computer program, it is not hard to see that isolating the contribution of the first 10 values of m (corresponding with $r = 1, \dots, 54$), the value of this constant can be reduced from $\frac{43}{13} - \frac{18}{13}\zeta(3) = 1.64330\dots$ to $1.60091\dots < 1.601$. Moreover, again using a computer program, it is also possible to directly compute $\sum_{m=2}^{T}\frac{1}{m}\sum_{r=\alpha(m)}^{\beta(m)}\frac{1}{r}\big(1+\frac{1}{rq-1}\big)$ with $T = 2000$ (so $r = 1, \dots, 2\,000\,999$). This leads to a value > 1.59908, and so the upper bound 1.601 is almost optimal.

4. Proof of Theorem 1

Using (4), the Euler product for $L(1,\chi)$, $\chi \neq \chi_0$, we obtain

$$r(q) = -\sum_{\chi(-1)=-1}\sum_{p}\log\Big(1-\frac{\chi(p)}{p}\Big) = \sum_{\chi(-1)=-1}\sum_{p}\sum_{m\geqslant 1}\frac{\chi(p^m)}{mp^m} = \Sigma_1 + \Sigma_2, \tag{20}$$

say, where Σ_1 is the contribution of the primes ($m = 1$) and Σ_2 that of the prime powers ($m \geqslant 2$). We have, see the introduction of Section 3,

$$\Sigma_1 = \sum_{\chi(-1)=-1}\sum_{p}\frac{\chi(p)}{p} = \frac{q-1}{2}\lim_{x\to\infty} g_q(x),$$

and

$$\Sigma_2 = \frac{q-1}{2}\Big(\sum_{\substack{m\geqslant 2\\ p^m\equiv 1 \pmod q}}\frac{1}{mp^m} - \sum_{\substack{m\geqslant 2\\ p^m\equiv -1 \pmod q}}\frac{1}{mp^m}\Big) = \frac{q-1}{2}t_q.$$

Lemma 1 then yields

$$|\Sigma_2| < \frac{43}{26} - \frac{9}{13}\zeta(3) + \frac{c}{\log q}, \tag{21}$$

where c is a positive constant. We will use this inequality in the proofs of all the three parts of this theorem.

From now on, we will assume that $b \in \{-1, 1\}$ and that q is a sufficiently large prime. We now consider Σ_1; we split the prime sum into the ranges $p \leqslant x_1$ and $p > x_1$ (where x_1 will be chosen later on), and proceed to estimate these subsums. The first ingredient is supplied by the following inequalities valid for any $x > 0$:

$$-\frac{q-1}{2}S_q(-1,x) \leqslant \sum_{\chi(-1)=-1}\sum_{p\leqslant x}\frac{\chi(p)}{p} \leqslant \frac{q-1}{2}S_q(1,x), \tag{22}$$

where $S_q(b,x)$ is defined in (10). Using $S_q(b,x) > 0$, from (22) we obtain

[2] Also [46, Lemma 2.2] makes use of [28, Lemma 10] in which a term $-\log_2 2$ is missing, see also footnote 3 on page 11.

$$\Big|\sum_{\chi(-1)=-1}\sum_{p\leqslant x}\frac{\chi(p)}{p}\Big| \leqslant \frac{q-1}{2}\max\{S_q(1,x),S_q(-1,x)\}. \tag{23}$$

We now proceed to estimate $S_q(b,x)$. Letting $x \geqslant q^2$, by partial summation and the Brun-Titchmarsh theorem, see Classical Theorem 1, we have

$$\begin{aligned}\frac{q-1}{2}\sum_{\substack{kq<p\leqslant x\\ p\equiv b \pmod q}}\frac{1}{p} &= \frac{q-1}{2}\Big(\frac{\pi(x;q,b)}{x}-\frac{\pi(kq;q,b)}{kq}+\int_{kq}^{x}\frac{\pi(u;q,b)}{u^2}du\Big)\\ &\leqslant \frac{q-1}{2}\Big(\frac{2}{(q-1)\log(x/q)}+\frac{2}{(q-1)}\int_{kq}^{x}\frac{du}{u\log(u/q)}\Big)\\ &\leqslant \log_2\Big(\frac{x}{q}\Big)-\log_2 k+\frac{1}{\log q},\end{aligned} \tag{24}$$

where $k \geqslant 3$ is an odd integer we will choose later. Since k is odd and $q \geqslant 3$, any prime $p \leqslant kq$ with $p \equiv b \pmod q$ is of the form $p = 2jq + b$, with $j \in \{1, \dots, \frac{k-1}{2}\}$. So

$$\frac{q-1}{2}\sum_{\substack{p\leqslant kq\\ p\equiv b \pmod q}}\frac{1}{p} \leqslant \frac{1}{2}\sum_{j=1}^{(k-1)/2}\frac{q-1}{2jq-1} < \frac{1}{4}\sum_{j=1}^{(k-1)/2}\frac{1}{j} = \frac{1}{4}H_{\frac{k-1}{2}}, \tag{25}$$

with $H_n := \sum_{j=1}^{n}\frac{1}{j}$ is the n-th harmonic number. Combining (24)-(25) we obtain

$$\frac{q-1}{2}S_q(b,x) < \log_2\Big(\frac{x}{q}\Big)+c_1(k)+\frac{1}{\log q}, \tag{26}$$

where $c_1(k) := \frac{1}{4}H_{\frac{k-1}{2}} - \log_2 k$. We now choose k such that $c_1(k)$ is minimal. It is not hard to see that this happens for $k = 55$ and that $C_1 := c_1(55) < -0.4152617906$.

Let $\ell(q)$ be a function that tends to infinity arbitrarily slowly and monotonically as q tends to infinity. Taking $x = x_1 := q^{\ell(q)}$ and $k = 55$ in (26), we have

$$\frac{q-1}{2}S(b,x_1) < \log_2 q+\log\ell(q)+C_1+\frac{1}{\log q}. \tag{27}$$

Inserting (27) into (23), we obtain[3]

$$\Big|\sum_{\chi(-1)=-1}\sum_{p\leqslant x_1}\frac{\chi(p)}{p}\Big| < \log_2 q+\log\ell(q)+C_1+\frac{1}{\log q}. \tag{28}$$

This inequality will be used in the proofs of the first two parts of this theorem.

If there is no odd character modulo q such that $L(s,\chi)$ has a Siegel zero, then in addition to the estimate (28) by [28, Lemmas 1, 7 and 8][4] we also have

[3] There is an oversight in the proof of [28, Lemma 10] since the (positive) term $-\log_2 2$ is missing. The reasoning that leads to (28) is an amended and improved version of the argument of Lu-Zhang.

[4] Note that [28, Lemma 7] holds for every T, x_1 such that $\lim_{q\to\infty}\log(qT)/\log x_1 = 0$. This allows us to choose $T = q^4$ and $x_1 = q^{\ell(q)}$, where $\ell(q)$ tends to infinity arbitrarily slowly and monotonically as q tends to infinity. The final error term in [28, Lemma 8] is then $\ll 1/\ell(q) = o(1)$ as q tends to infinity.

$$\Big|\sum_{\chi(-1)=-1}\sum_{p>x_1}\frac{\chi(p)}{p}\Big| \ll \frac{1}{\ell(q)}. \tag{29}$$

We remark that (29) also holds if $q \equiv 1 \pmod 4$ since this implies that there does not exist any odd quadratic Dirichlet character modulo q and hence its attached Dirichlet L-series has no Siegel zero. Using equations (28) and (29), we have

$$|\Sigma_1| < \log_2 q + \log \ell(q) + C_1 + o(1). \tag{30}$$

Combining (21) and (30), we obtain

$$|r(q)| < \log_2 q + \log \ell(q) + C_1 + \frac{43}{26} - \frac{9}{13}\zeta(3) + \frac{1}{1000} < \log_2 q + \log \ell(q) + 0.41.$$

This completes the proof of Part 1).

We now prove Part 2). The starting point is again (20), but we need a more accurate analysis of the contribution of Σ_1. To do so, the first step is to split the prime sum Σ_1 in three subsums S_1, S_2, S_3 defined according to whether $p \leqslant x_1$, $x_1 < p \leqslant x_2$ or $p \geqslant x_2$, where $x_2 = e^q$ and $x_1 = q^{\ell(q)}$, with $\ell(q)$ being any function that tends to infinity arbitrarily slowly and monotonically as q tends to infinity.

We already estimated S_1 in (28) and will proceed to estimate S_3. By [28, Lemma 1], we have

$$S_3 \ll q^2 e^{-c_1\sqrt{q}}, \tag{31}$$

where $c_1 > 0$ is an absolute constant.

For S_2 we follow the first part of the argument in [28, Lemma 8]. Recall (see, e.g., [8, Ch. 19]) that if χ is a non principal character modulo q and $2 \leqslant T \leqslant x$, then

$$\theta(x,\chi) := \sum_{p\leqslant x}\chi(p)\log p = -\delta_{\beta_0}\frac{x^{\beta_0}}{\beta_0} - {\sum_{|\gamma|\leqslant T}}' \frac{x^\rho}{\rho} + O\Big(\frac{x(\log qx)^2}{T} + \sqrt{x}\Big), \tag{32}$$

where $\delta_{\beta_0} = 1$ if the Siegel zero β_0 exists and is zero otherwise, and $\sum'$ is the sum over all non-trivial zeros $\rho = \beta + i\gamma$ of $L(s,\chi)$, with the exception of β_0 and its symmetric zero $1-\beta_0$.

Assume that there exists a Siegel zero β_0 with odd associated character. Then, by the partial summation formula and (32) with $T = q^4$, we have

$$\begin{aligned} S_2 := \sum_{\chi(-1)=-1}\sum_{x_1<p\leqslant x_2}\frac{\chi(p)}{p} &= \sum_{\chi(-1)=-1}\Big(\frac{\theta(x_2,\chi)}{x_2\log x_2} - \frac{\theta(x_1,\chi)}{x_1\log x_1} + \int_{x_1}^{x_2}\theta(u,\chi)\frac{1+\log u}{(u\log u)^2}du\Big) \\ &= -\int_{x_1}^{x_2}\frac{u^{\beta_0-2}}{\log u}du - \int_{x_1}^{x_2}\Big(\sum_{\chi(-1)=-1}{\sum_{|\gamma|\leqslant q^4}}' u^{\rho-2}\Big)\frac{du}{\log u} + \frac{q-1}{2}E_q, \end{aligned} \tag{33}$$

where

$$E_q \ll \int_{x_1}^{x_2}\Big(\frac{(\log qu)^2}{q^4 u} + \frac{1}{u^{3/2}}\Big)\frac{du}{\log u} \ll \frac{1}{q^2}.$$

By using [28, Lemmas 7 and 8],[5] we obtain that

[5] See footnote 4 on page 11.

$$\int_{x_1}^{x_2} \Big(\sum_{\chi(-1)=-1} \sideset{}{'}\sum_{|\gamma|\leqslant q^4} u^{\rho-2} \Big) \frac{du}{\log u} \ll \frac{1}{\ell(q)}. \tag{34}$$

We now proceed to evaluate the term depending on β_0 in (33). A direct computation using that $\log x_2 = q$ gives

$$\int_{x_1}^{x_2} \frac{u^{\beta_0-2}}{\log u} du = \int_{\log x_1}^{\log x_2} \frac{dt}{te^{(1-\beta_0)t}} = E_1(1-\beta_0) - \int_{1-\beta_0}^{(1-\beta_0)\log x_1} \frac{dt}{te^t} - E_1(q(1-\beta_0)),$$

where $E_1(u)$ denotes the exponential integral function. Recalling that $x_1 = q^{\ell(q)}$, where $\ell(q)$ tends to infinity arbitrarily slowly and monotonically as q tends to infinity, we have

$$\int_{1-\beta_0}^{(1-\beta_0)\log x_1} \frac{dt}{te^t} \leqslant \log_2 x_1 = \log_2 q + \log \ell(q) \quad \text{and} \quad E_1(q(1-\beta_0)) \ll \frac{1}{q}. \tag{35}$$

Inserting (34)-(35) into (33), we finally obtain

$$|S_2 + E_1(1-\beta_0)| \leqslant \log_2 q + \log \ell(q) + o(1). \tag{36}$$

Combining (28), (31) and (36), we obtain

$$|\Sigma_1 + E_1(1-\beta_0)| < 2\log_2 q + 2\log \ell(q) + C_1 + o(1). \tag{37}$$

Recalling that Σ_2 is estimated in (21), by combining (20)-(21) and (37), Part 2) follows.

It remains to prove Part 3). In this case we split Σ_1 in (20) in two subsums S_1, S_2 defined according to $p \leqslant x_1$ and $p > x_1$. Let $A > 0$ be a constant to be chosen later and let $x = q^2(\log q)^A =: x_1$ in (26). We obtain

$$|S_1| < \log_2 q + C_1 + (A+1)\frac{\log_2 q}{\log q}, \tag{38}$$

where $C_1 := c_1(55) < -0.4152617906$. Arguing as in (33), by partial summation we obtain

$$S_2 = \sum_{\chi(-1)=-1} \lim_{y\to\infty} \Big(\frac{\theta(y,\chi)}{y\log y} - \frac{\theta(x_1,\chi)}{x_1\log x_1} + \int_{x_1}^{y} \theta(u,\chi) \frac{1+\log u}{(u\log u)^2} du \Big). \tag{39}$$

Assuming Conjecture 3, we have that $\psi(x,\chi) := \sum_{n\leqslant x} \chi(n)\Lambda(n) \ll \sqrt{x}(\log x)^2$ for every odd Dirichlet character $\chi \pmod q$, see, e.g., [8, p. 125, Ch. 20]. Recalling $\psi(x,\chi) - \theta(x,\chi) \ll \sqrt{x}$, we have that (39) becomes

$$S_2 \ll \frac{q\log x_1}{\sqrt{x_1}} \ll_A (\log q)^{1-A/2} = o(1), \tag{40}$$

for every $A > 2$. Choosing $A = 3$, by combining (38) and (40) we have

$$|\Sigma_1| < \log_2 q + C_1 + \frac{c}{\sqrt{\log q}}, \tag{41}$$

where c is a suitable positive constant. Equations (21) and (41) imply that

$$|r(q)| < \log_2 q + 0.41,$$

and hence Part 3) follows. □

5. Remarks on Theorem 1

In the introduction we already made some comments on Theorem 1. Here we make some further ones.

Comment to Remark 3. It is easy to derive these estimates for $E_1(1-\beta_0)$. We recall that

$$E_1(x) = -\boldsymbol{\gamma} - \log x + \int_0^x (1-e^{-t})\frac{dt}{t} = -\boldsymbol{\gamma} - \log x - \sum_{k=1}^{\infty} \frac{(-x)^k}{(k!)k} \quad (x>0), \tag{42}$$

where $\boldsymbol{\gamma}$ is the Euler-Mascheroni constant. Since $0 < 1-e^{-x} < x$, we infer from the first equality that

$$-\boldsymbol{\gamma} - \log x < E_1(x) < -\boldsymbol{\gamma} - \log x + x \quad (x>0).$$

On using that for every $\varepsilon > 0$ there exists a constant $c_1(\varepsilon)$ such that $\beta_0 < 1-c_1(\varepsilon)q^{-\varepsilon}$, the bounds for $E_1(x)$ lead to $1 \ll E_1(1-\beta_0) < \varepsilon \log q + c(\varepsilon)$, where $c(\varepsilon)$ is ineffective. Using the weaker, but with an effective constant, estimate $\beta_0 < 1 - cq^{-1/2}(\log q)^{-2}$ we obtain that $1 \ll E_1(1-\beta_0) < \frac{1}{2}\log q + 2\log_2 q + c_1$, where $c_1 > 0$ is an effective constant.

Remark 6 *(On the role of the Brun-Titchmarsh theorem in our results, I).* The power of the $\log q$-factor in the estimates for $R(q)$ in Theorem 1 directly depends on (26) that follows from using the Brun-Titchmarsh theorem (Classical Theorem 1) in (24). In particular, a key role in (24) is played by the constant 2 present in (6); any improvement of this constant to, e.g., $2-\xi$, $\xi \in (1,2)$, will lead to replace one $\log q$-factor with $(\log q)^{1-\xi/2}$ into Theorem 1. From the works of Motohashi [34], Friedlander-Iwaniec [13], Ramaré [38, Theorem 6.5] and Maynard [30, Proposition 3.5], it is well known that replacing such a constant with any value less than 2 is equivalent with assuming there does not exist a Siegel zero for $\prod_{\chi \pmod q} L(s,\chi)$. Unfortunately, none of these results is applicable in our case since $R(q)$ depends on the odd Dirichlet characters only; hence, assuming, as in Part 1) of Theorem 1, that the Dirichlet L-series associated to the odd characters do not have any Siegel zero is not enough to imply the possibility of using (6) with a leading constant less than 2.

Remark 7 *(On the role of the Brun-Titchmarsh theorem in our results, II).* Montgomery and Vaughan, see [33, Theorem 2], under the same hypotheses of Classical Theorem 1, also proved that there exists a constant $C > 0$, which they did not make explicit, such that if $y > Cq$ then

$$\pi(x+y;q,a) - \pi(x;q,a) < \frac{2y}{\varphi(q)(\log(y/q)+\frac{5}{6})}. \tag{43}$$

Usage of this estimate potentially allows us to decrease the value of C_1 in Theorem 1, leading to improvements of the constants 0.41 and 0.39 (see also Remark 2). Once C has been made explicit, (6) can be replaced by (43). Selberg [40, vol. 2, p. 233] obtained (43) with 2.8 instead of $\frac{5}{6}$, but also did not make C explicit.

Remark 8. The first two parts of Theorem 1 sharpen Lu-Zhang [28, Theorem 1] by reducing/enlarging the exponents of the $\log q$-factor from $\frac{7}{6}$ and $-\frac{4}{3}$ to, respectively, 1 and -1. Again comparing with [28, Theorem 1], in Part 3) we assumed $\mathrm{RH}_{\mathrm{odd}}(q)$ (Conjecture 3), instead of the Generalized Riemann Hypothesis.

Part 2) of Theorem 1 improves the second part of Theorem 1.1 of Debaene [9] in two aspects: the term $-\log(1-\beta_0)$ is replaced by a more accurate description involving $E_1(1-\beta_0)$, see (42), and the exponent of the $\log q$-factor is reduced from 4 to 2. This reduction is a consequence of sharpened estimates for the quantities Σ_1, Σ_2 used in the proof of Theorem 1.

Remark 9. In Part 2) of Theorem 1 we included only the contribution of the Siegel zero β_0, and not of the zero $1-\beta_0$. We did this in order to be able to easily compare with the result of Puchta [36, Theorem 1] and Debaene [9, Theorem 1.1]. It is in fact pretty easy to obtain the contribution of the zero $1-\beta_0$: arguing as in the proof of Theorem 1 we see that it equals

$$\int_{x_1}^{x_2} \frac{u^{-1-\beta_0}}{\log u} du = \int_{\log x_1}^{\log x_2} \frac{dt}{te^{\beta_0 t}} = E_1(\beta_0) - \int_{\beta_0}^{\beta_0 \log x_1} \frac{dt}{te^t} - E_1(q\beta_0),$$

in which we also used the fact that $\log x_2 = q$. Since $x_1 = q^{\ell(q)}$ we also have

$$\int_{\beta_0}^{\beta_0 \log x_1} \frac{dt}{te^t} \leqslant 2e^{-\beta_0} \leqslant 2e^{-1/2} \quad \text{and} \quad E_1(q\beta_0) \ll \frac{1}{q}.$$

Hence, the main term in the previous formula is in the series expansion of $E_1(\beta_0)$ and it is $-\log\beta_0$. Adding the leading terms of $E_1(\beta_0)$ and $E_1(1-\beta_0)$, we have that their total contribution behaves as $-\log(\beta_0(1-\beta_0))$.

6. An efficient algorithm to compute $R(q)$

Since $R(q)$ grows very quickly as q increases, it is much better to evaluate $r(q)$ instead, and obtain $R(q)$ as $\exp(r(q))$. We addressed this problem already in the preprint [26], and here present an updated version in which we obtain more accurate results. For all these quantities we can use the algorithm in [23], see also [27], in which the Fast Fourier Transform (FFT) procedure is used to obtain the needed values of $L(1,\chi)$ which are the main ingredients for getting $r(q)$. The fundamental formula is the well-known relation, see, e.g., eq. (2.1) of Shokrollahi [41]:

$$h_1(q) = 2q \prod_{\chi(-1)=-1} \Big(-\frac{B_{1,\chi}}{2}\Big), \tag{44}$$

where $B_{1,\chi}$ is the first χ-Bernoulli number defined, see Proposition 9.5.12 of Cohen [5], as

$$B_{1,\chi} := \sum_{a=1}^{q-1} \frac{a}{q}\chi(a). \tag{45}$$

Inserting (45) and (44) into (3), we obtain[6]

$$R(q) = \Big(-\frac{\pi}{\sqrt{q}}\Big)^{\frac{q-1}{2}} \prod_{\chi(-1)=-1} \sum_{a=1}^{q-1} \frac{a}{q}\chi(a).$$

We immediately have

[6] The term $1/q$ is taken on purpose outside the inner sum, as this helps in controlling the errors in the FFT procedure.

$$r(q) = \frac{q-1}{2}\Big(\log \pi - \frac{1}{2}\log q + i\pi\Big) + \sum_{\chi(-1)=-1} \log\Big(\sum_{a=1}^{q-1} \frac{a}{q}\chi(a)\Big), \tag{46}$$

where the second logarithm is the complex one. Recalling that $R(q) > 0$, it is clear that $r(q)$ is a real number. Hence the imaginary part of the sum over the odd Dirichlet characters in (46) must be equal to $-\pi(q-1)/2$. We obtain

$$r(q) = \frac{q-1}{2}\Big(\log \pi - \frac{1}{2}\log q\Big) + \sum_{\chi(-1)=-1} \log \Big|\sum_{a=1}^{q-1} \frac{a}{q}\chi(a)\Big|. \tag{47}$$

As a possible alternative approach, one can start from (4) and use the fact that $L(1,\chi) = -\frac{1}{q}\sum_{a=1}^{q-1}\chi(a)\digamma\left(\frac{a}{q}\right)$, where $\digamma(x) = (\Gamma'/\Gamma)(x)$ is the *digamma* function. Very similar computations then lead to

$$r(q) = -\frac{(q-1)}{2}\log q + \sum_{\chi(-1)=-1} \log \Big|\sum_{a=1}^{q-1} \chi(a)\digamma\Big(\frac{a}{q}\Big)\Big|. \tag{48}$$

In practice, though, it is better to use (47) since no special function computations are needed there; nevertheless, formula (48) can be useful to double-check our results.

The summation over a in (47) can be handled using the FFT procedure, paying attention to choose only the contributions of the odd Dirichlet characters, and we can also embed here a *decimation in frequency strategy*, see Section 6.2, as we already did in [23] and [27].

The FFT procedure requires $O(q)$ memory positions and the computation of $r(q)$ via (47) has a computational cost of $O(q\log q)$ arithmetic operations plus the cost of computing $(q-1)/2$ values of the logarithm function and products: so far, this is the fastest known algorithm to compute $r(q)$, see, for other less efficient algorithms, the works of Fung-Granville-Williams [15], Shokrollahi [41] and Jha [20].

Using this algorithm we were able to obtain more digits of the maximal and minimal champions for $R(q)$ with $q < 10^{10}$, namely

$$R(9697282541) = 1.7247411203\ldots \quad \text{and} \quad R(116827429) = 0.5756742526\ldots,$$

see also Tables 2-3. Further records for $q > 10^{10}$, claimed to be correct up to 6 decimals, were obtained in 2021 by Broadhurst [2]. He directly evaluated the prime sums in formula (8) using x between 10^{15} and 10^{21}; then he gave a statistical estimate for the errors in such computations.

Our approach to evaluate the computational error is more classical and it is presented in Section 6.3. We did not replicate Broadhurst's computations for $q > 10^{10}$, because we did not have enough computational resources at our disposal. The problem is the huge memory resources the FFT procedure would require in these cases. For example, the largest case we were able to handle, $q = 9854964401$, already needed about 3TB of memory using FFTW [14], a software library designed to implement the FFT procedure, with the quadruple precision (128 bits) of the C programming language.

6.1. Computations with trivial summing over a (slower, more digits available)

Unfortunately in PARI/GP [43] and in `libpari` the FFT-functions work only if $q = 2^t + 1$, for some $t \in \mathbb{N}$. So we had to trivially perform these summations and hence, in practice, this part is the most time consuming one as its computational cost is quadratic in q. Nevertheless, this approach works nicely for small values of q and is able to provide the values of $R(q)$ which many decimals.

Table 1
Values of $R(q)$ (truncated) for every odd prime up to 1000.

q	$R(q)$
3	0.6045997880780726168646927525473
5	0.7895683520871486895067592799900
7	0.9566751857508418754795073381317
11	1.1091619128700057589698217531662
13	1.0771490562098575674859781589187
17	0.8553903456876526811590587393660
19	0.7070400490038472907067462197858
23	1.2730306993968550223440516296068
29	1.1950722585472314170213869230139
31	0.8898896210785440789198518157132
37	0.8961735424518262426393010568398
41	1.0109514928155133737670365161798
43	1.0003280708398792157908433519393
47	0.9951041947584376332046179459764
53	1.0023154955608046980883540349743
59	1.0311199595775858834174986891680
61	0.9154168975763615203860784058478
67	1.0323019630420196815155397633286
71	0.9465247471036236809290054627120
73	1.2821779323076053838224676118514
79	0.8457945961200297550455294076382
83	1.2232692654844146161950762139016
89	1.2863214746192234623445369458997
97	0.9046761428702376506678185793342
101	1.1104995875358644805192388808229
103	1.0556519883371874318616371348168
107	0.9926076779267250130951961237566
109	0.9155428388523018685066750024637
113	1.1618557363506180805776111458998
127	1.0626983549971763540798019088845
131	1.2789769938976286727059298824683
137	1.0018885365042079285157114283333
139	0.8716611518739232788670854213024
149	1.0488652764269119456479100644937
151	1.0961352605053081203560323292152
157	0.7430450532910889660052300286210
163	0.9516739236944299288308183830698
167	0.8540489171409883518683860745104
173	1.2575031110060486325647665223234
179	1.3189895521869900854067212054754
181	1.0164672530790178324085643879748
191	1.2985095534724676367615527171504
193	1.1738495661428052368362517610841
197	0.8714268580587022585427508674145
199	0.7977576598180326170333641097002
211	0.7096581038457700773915382688127
223	0.9001673677400910738942007486095
227	0.7629883976313712260376287117080
229	0.7241457414201049462008640419682
233	1.4310221673105806346958377026375
239	1.1852025922101838102852657887109
241	1.1190819269965132548112076907794
251	1.1804169442539285917038758350886
257	0.9055962573549657664091346453876
263	0.9371707816685296065406493231972
269	1.0105242994134286604110488301351
271	0.8412088090144110303458717890667
277	1.2228716770080365999632534704580
281	1.0907231267144641150745775682060
283	0.9873004592498935117673519297087
293	1.2884302359523728319105679845501
307	0.9135872522019948222051491689937
311	1.1458937454264730221344414268718
313	0.9389331767581916618067398442288
317	0.8067182318898481284945719857774
331	0.8135627495605184590233164933650
337	0.8611151152192259126883225579098
347	1.0851794175810526744648331305833
349	0.9839573134487701044559123913262
353	0.8860350566174460450308781577592
359	1.1600264444670825456691643273527
367	0.9086410187793691206326531982541
373	1.0750761442013325764626703553466
379	0.7214461864713844469442699568877
383	0.8324380926742871396047076038085
389	0.8499778289685450397162756349668
397	0.9975778112015857909425324661679
401	1.1399832831644707063138427893128
409	1.1991980974390954074874424479768
419	1.1897445888237693592676697100177
421	0.8645796653071174117734286953546
431	1.1375426110359346246171708562349
433	1.0717613518204177138545059520477
439	0.6848413406172976205500589562641
443	1.4108998843039798698090656834498
449	0.9053964365861442489589154746074
457	0.8373463419058562177863679134357
461	1.0311955737739740364528472490666
463	0.9613462511195984177868663523170
467	0.8974045485919283687065708373771
479	1.1050671578064206970591097893948
487	1.1304102278265606313945369715559
491	1.2722146569130496835275435498496
499	0.8297902495946506366988138268051
503	1.0995617471957832909336221046588
509	1.3969208271961266132041741065091
521	0.7448857918191827286091015924803
523	0.9951484787399289420380269322079
541	0.9447265578295298152134577952949
547	0.7386850547619545899616661320191
557	1.0180061813097044024347867514026
563	0.9232212509133752364416200184615
569	0.8664438451435738527270516828484
571	0.9966248063685197276230915134980
577	0.9137029380401851023927738920458
587	0.8125245985067212166037417395454
593	1.0773461748966493078075918844172
599	0.9640877383472306977957126847174
601	0.9282733975182409725085430055023
607	0.8363731270525144324766779910174
613	0.8770365930347214891035502029408
617	0.8424608454194671614144537884806
619	0.8046391863654823181809704923832
631	1.1396469807244276647958444773064
641	1.3429915643232847544526367324545
643	1.0183620561136068530441755349378
647	0.9023366731711887559549077220931
653	1.2708772780577246646879609833837
659	1.3910631789822655014399826852608
661	0.8354443097523214656936838597289
673	1.0366020698239863718118735321088
677	0.9242401331249736440179204466235
683	1.1352828140240947699825469113423
691	0.7692142795745405069640641103691
701	0.9208988286796986104162625438273
709	1.0564893491780186160617480034127
719	1.2030632585533392768111724372893
727	0.9985692142278032863134063960758
733	0.9801491017726198673607802262180
739	1.1026354682405308663067124546439
743	1.0349549409620577590409117683058
751	1.0185620058358507387809584897536
757	0.9670687611870859854554145544772
761	1.4695828581314155249132265698413
769	0.8989223036739211131497271647474
773	1.0681094719703144713033330503520
787	0.9717823284398633668645155647478
797	1.0307513038736094294364198652655
809	1.3197044140601871225194956764480
811	0.8028381726481542070785681890576
821	1.0652843703654964331935281465584
823	0.9676931847618204865646570591849
827	0.8655599367575844205769196995319
829	0.8225003354161554974840091964490
839	0.9187109054076576161004431766675
853	1.0822358288025334754800428361362
857	1.0507531149069469457639638202726
859	0.8808009418056817847639767572161
863	1.0569423120644476418024040128851
877	0.7228939852270574121828463785409
881	1.0973899419907535018443533637062
883	1.1331822763939321498203901268480
887	0.9691797419679082310841771993673
907	0.9026255886631148047805162360749
911	1.0779855753630487309935104370070
919	1.0400334655419995090131730345736
929	1.0441490445298916774481320172549
937	0.9001793485775001978413226252376
941	1.0940086717975223552339721484683
947	1.2258744827051074302609149043348
953	1.1608317303128388568222684560130
967	0.7286000440466886148143682504791
971	1.0793911591644004625871038160386
977	0.8389088588037128235412547247521
983	0.7886767720297385404724656676372
991	0.9094393615350512976006963975090
997	0.8557575449135065446654521786495

Being aware of such limitations, we performed the computation of $r(q)$ and $R(q)$ for every prime q in the range $3 \leqslant q \leqslant 1000$, using a precision of 100 decimals, see Table 1. We also computed their values for $q = 1451, 2741, 3331, 4349, 4391, 5231, 6101, 6379, 7219, 8209, 9049, 9689$, see the left part of Table 2. These numbers were chosen to extend the available decimals for the known data (see Fung-Granville-Williams [15] and Shokrollahi [41]). Likewise we also obtained them for $q = 37189, 42611, 149119, 198221, 305741, 401179$; see the right part of Table 2. For these values of q it became clear that the bulk of the computation time was spent on summing over a, providing experimental evidence that replacing the trivial way of summing over a with the FFT procedure is fundamental to be able to evaluate $r(q)$ and $R(q)$ for larger values of q.

Table 2
On the left: few other values of $R(q)$. On the right: maximal champions for $R(q)$. The values for $q \leqslant 305741$ were obtained using PARI/GP with a trivial summation over a and an accuracy of 100 decimals; the others using the FFTW software library (128 bits accuracy).

q	$R(q)$
1451	1.4893160720809344256113213467 52...
2741	1.498121015176665823721124535220...
3331	0.642429297634719506688741152270...
4349	1.518570512426339397454202981116...
4391	1.507776410131052825600361832032...
5231	1.556562247546690554629305894110...
6101	1.511405291132409881116244836469...
6379	0.673523026278795404982148735902...
7219	0.658084090096317378291742795450...
8209	0.672045039003857595919734222943...
9049	0.667614244171116232015569216575...
9689	1.524371504087494924535704793958...

q	$R(q)$
4391	1.507776410131052825600361832032...
5231	1.556562247546690554629305894110...
42611	1.619906571157532399867361172777...
198221	1.623477270751197661500864242418...
305741	1.661436485908786948688528096415...
6766811	1.7093790418...
1326662801	1.7097585606...
1979990861	1.7207910074...
4735703723	1.7216545866...
9697282541	1.7247411203...

Table 3
Minimal champions for $R(q)$. The values for $q \leqslant 401179$ were obtained using PARI/GP with a trivial summation over a and an accuracy of 100 decimals; the others using the FFTW software library (128 bits accuracy).

q	$R(q)$
37189	0.625231255787654795233417601859...
149119	0.624149715978401425409347395847...
401179	0.621507092276527124572758370995...
2083117	0.6142798512...
5589169	0.5869729849...
102598099	0.5861372431...
116827429	0.5756742526...

6.2. FFT-decimation in frequency

We give here a shortened version of the more general argument presented in [25, Section 8]. The way to translate eq. (47) into a problem that can be handled using the FFT procedure is based on the following remark. Recalling that q is prime, it is enough to determine a primitive root[7] g of q, to represent the Dirichlet character χ_1 mod q being uniquely determined by $\chi_1(g) = \mathbf{e}(1/(q-1))$, where $\mathbf{e}(x) := \exp(2\pi i x)$. Using χ_1 we can represent the set of non-trivial characters mod q as $\{\chi_1^j \colon j = 1, 2, \dots, q-2\}$. Hence, if for every $k \in \{0, \dots, q-2\}$, we write $g^k \equiv a_k \in \{1, \dots, q-1\}$, the innermost summation in (47) is of the type $\sum_{k=0}^{q-2} \mathbf{e}(jk/(q-1)) f(a_k/q)$, $j \in \{1, \dots, q-2\}$ is odd and f is a suitable function. As a consequence, such quantities are the Discrete Fourier Transform (DFT) of the sequence $\{f(a_k/q) \colon k = 0, \dots, q-2\}$. This observation is due to Rader [37] and it was used in [12,23,24,27] to speed up the computation of similar quantities.

In our case we can also use the *decimation in frequency* strategy: following the line of reasoning in [25, Section 8], letting $\overline{q} = (q-1)/2$ for every $j = 0, \dots, q-2$, $j = 2t + \ell$, $\ell \in \{0, 1\}$ and $t \in \mathbb{Z}$, we have that

[7] We recall that finding primitive roots is a computationally hard problem; but we just need to do this once for each q we will work with.

$$\sum_{k=0}^{q-2} \mathbf{e}\Big(\frac{jk}{q-1}\Big) f\Big(\frac{a_k}{q}\Big) = \sum_{k=0}^{\overline{q}-1} \mathbf{e}\Big(\frac{tk}{\overline{q}}\Big)\, \mathbf{e}\Big(\frac{\ell k}{q-1}\Big) \Big(f\Big(\frac{a_k}{q}\Big) + (-1)^{\ell} f\Big(\frac{a_{k+\overline{q}}}{q}\Big)\Big)$$
$$= \begin{cases} \sum_{k=0}^{\overline{q}-1} \mathbf{e}\big(\frac{tk}{\overline{q}}\big) b_k & \text{if } \ell = 0; \\ \sum_{k=0}^{\overline{q}-1} \mathbf{e}\big(\frac{tk}{\overline{q}}\big) c_k & \text{if } \ell = 1, \end{cases} \tag{49}$$

where $t = 0, \dots, \overline{q} - 1$,

$$b_k := f\Big(\frac{a_k}{q}\Big) + f\Big(\frac{a_{k+\overline{q}}}{q}\Big) \quad \text{and} \quad c_k := \mathbf{e}\Big(\frac{k}{q-1}\Big)\Big(f\Big(\frac{a_k}{q}\Big) - f\Big(\frac{a_{k+\overline{q}}}{q}\Big)\Big).$$

Since we just need the sum over the odd Dirichlet characters for $f(x) = x$, instead of computing an FFT of length $q - 1$ we can evaluate an FFT of half a length, applied on the sequence c_k defined in (49). Clearly this leads to a gain in speed and in a reduction in memory usage. In our case, using again $\langle g \rangle = (\mathbb{Z}/q\mathbb{Z})^*$, $a_k \equiv g^k \bmod q$ and $g^{\overline{q}} \equiv q - 1 \bmod q$, we can write that $a_{k+\overline{q}} \equiv q - a_k \bmod q$; hence

$$a_k - a_{k+\overline{q}} = a_k - (q - a_k) = 2a_k - q,$$

so that we obtain $c_k = \mathbf{e}(k/(q-1))(2a_k/q - 1)$ for every $k = 0, \dots, \overline{q} - 1$, $\overline{q} = (q-1)/2$.

6.3. FFT accuracy estimate

In order to estimate the accuracy in performing the FFT procedure, we have to recall first the definition of the Discrete Fourier Transform (DFT).

Definition 3 *(The Discrete Fourier Transform D).* Let $u_k \in \mathbb{C}$, $k = 0, \dots, N-1$, be a sequence. We define the *Discrete Fourier Transform D* of u_k as the following sequence

$$\big(D(u_k)\big)_j := \sum_{k=0}^{N-1} u_k\, \mathbf{e}\Big(-\frac{jk}{N}\Big)$$

where $j = 0, \dots, N-1$ and $\mathbf{e}(x) = \exp(2\pi i x)$. The corresponding *inverse Discrete Fourier Transform* D^{-1} is defined as the sequence

$$\big(D^{-1}(u_k)\big)_j = \Big(\frac{1}{N}\overline{D(\overline{u_k})}\Big)_j = \Big(\frac{1}{N}\sum_{k=0}^{N-1} u_k\, \mathbf{e}\Big(\frac{jk}{N}\Big)\Big)_j,$$

where $j = 0, \dots, N-1$.

It is not hard to prove that D, D^{-1} are linear, $D(D^{-1}(u_k)) = u_k$, $D^{-1}(D(u_k)) = u_k$, and $D/\sqrt{N}$, $\sqrt{N}D^{-1}$ are L^2-isometries.

We also recall that the Fast Fourier Transform F is an algorithm that evaluates the Discrete Fourier Transform D. We define analogously the Inverse Fast Fourier Transform F^{-1}.

According to Schatzman [39, § 3.4, p. 1159-1160], the root mean square relative error $\mathcal{E}$ in the FFT satisfies

$$\mathcal{E} = \frac{\|F(u_k) - D(u_k)\|_2}{\|D(u_k)\|_2} < \Delta, \text{ with } \Delta := 0.6\varepsilon\Big(\frac{\log N}{\log 2}\Big)^{1/2}, \tag{50}$$

where ε is the machine epsilon and N is the length of the transform. Moreover, the estimate in (50) holds for both F^{-1}, D^{-1} too.

According to the IEEE 754-2008 specification, we can set $\varepsilon = 2^{-64}$ for the *long double precision* (80 bits) of the C programming language. So for the largest case we are considering, $q = 9854964401$, $N = (q-1)/2$, we get that $\Delta < 1.85 \cdot 10^{-19}$. To evaluate the euclidean norm of the error we have then to multiply Δ and the euclidean norm of $x_k := 2a_k/q - 1$, where $a_k = g^k \bmod q$, $\langle q \rangle = (\mathbb{Z}/q\mathbb{Z})^*$. A straightforward computation gives

$$\|x_k\|_2 = \Big(\frac{(q-1)(q-2)}{6q}\Big)^{1/2} = 40527.69505\dots$$

Exploiting (50) and that $D/\sqrt{N}$ is an L^2-isometry, we also obtain

$$\|F(x_k) - D(x_k)\|_2 < \Delta \|D(x_k)\|_2 = \Delta\sqrt{N}\|x_k\|_2. \tag{51}$$

Recalling that $\|\cdot\|_\infty \leqslant \|\cdot\|_2$ and using (51), we can estimate that the maximal error in its FFT-computation for this sequence is bounded by $7.48 \cdot 10^{-15}$ (long double precision case).

We also estimated *in practice* the accuracy in the actual computations using the FFTW software library by evaluating at run-time the quantity $E_j(x_k) := \|F^{-1}(F(x_k)) - x_k\|_j$, $j \in \{2, \infty\}$. Note that this quantity becomes zero if we replace (F, F^{-1}) by (D, D^{-1}). Moreover, we also remark that from (51) we obtain

$$\|F(x_k)\|_2 \leqslant \|F(x_k) - D(x_k)\|_2 + \|D(x_k)\|_2 < (1+\Delta)\|D(x_k)\|_2 = (1+\Delta)\sqrt{N}\|x_k\|_2. \tag{52}$$

We also have that

$$\begin{aligned} E_2(x_k) &= \|F^{-1}(F(x_k)) - D^{-1}(D(x_k))\|_2 \\ &\leqslant \|F^{-1}(F(x_k)) - D^{-1}(F(x_k))\|_2 + \|D^{-1}[F(x_k) - D(x_k)]\|_2 \\ &< \Delta\|D^{-1}(F(x_k))\|_2 + \frac{1}{\sqrt{N}}\|F(x_k) - D(x_k)\|_2 \\ &< \frac{\Delta}{\sqrt{N}}\|F(x_k)\|_2 + \Delta\|x_k\|_2 < \Delta(2+\Delta)\|x_k\|_2, \end{aligned} \tag{53}$$

in which we used that D^{-1} is linear and $\sqrt{N}D^{-1}$ is an L^2-isometry, (50) for F^{-1}, and (51)-(52). Recalling that $\|\cdot\|_\infty \leqslant \|\cdot\|_2 \leqslant \sqrt{N}\|\cdot\|_\infty$, we also have $E_\infty(x_k) < \Delta(2+\Delta)\sqrt{N}\|x_k\|_\infty$. For $q = 9854964401$, $N = (q-1)/2$ and $\varepsilon = 2^{-64}$ in (50), we get that $\Delta(2+\Delta) < 3.70 \cdot 10^{-19}$ and, using again the previous norm-computation, we also obtain that $E_\infty(x_k) < 1.50 \cdot 10^{-14}$. Moreover, the actual computations using FFTW gave the following results:

$$\frac{E_2(x_k)}{\|x_k\|_2} < 6.27 \cdot 10^{-19}, \quad E_\infty(x_k) < 1.72 \cdot 10^{-18},$$

in agreement with (53).

Summarizing, we can conclude that at least ten decimals of our final results are correct. If necessary, more accurate results can be obtained using the *quadruple precision* (128 bits), which enables us to choose $\varepsilon = 2^{-113}$ in (50) and in the following argument, at the cost of a much slower practical execution.

A similar, but shorter, analysis of the accuracy of the FFT procedure is performed in [27, Section 5.7].

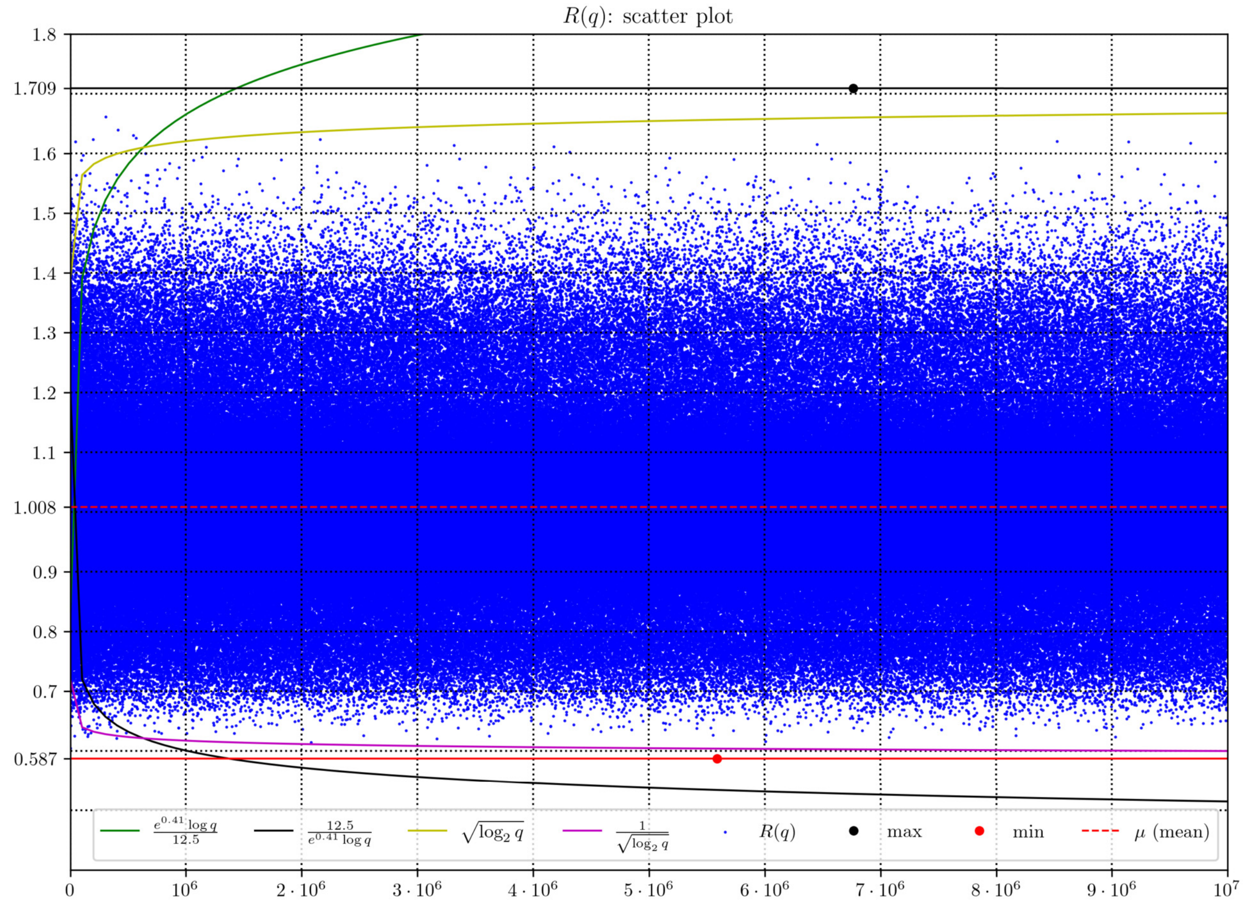

Fig. 1. The values of $R(q)$, q prime, $3 \leqslant q \leqslant 10^7$. The red dashed line represents the mean value. (For interpretation of the colors in the figure(s), the reader is referred to the web version of this article.)

6.4. Comments on the plots and on the histograms

The actual values of $r(q)$, $R(q)$ and of all the other relevant quantities presented in the herewith included plots and histograms were obtained for every odd prime q up to 10^7 using the FFTW [14] software library set to work with the *long double precision* (80 bits). Such results were then collected in some *comma-separated values* (csv) files and then all the plots and the histograms were obtained running on such stored data some suitable designed scripts written using Python (v. 3.11.6) and making use of the packages Pandas (v. 2.1.3) and Matplotlib (v. 3.8.2). The normal function used in the histograms is defined as

$$\mathcal{N}(x, \mu, \sigma) := \frac{1}{\sigma\sqrt{2\pi}} \exp\Big(-\frac{(x-\mu)^2}{2\sigma^2}\Big),$$

where μ and σ denote the mean, respectively the standard deviation, of the plotted data.

Fig. 1 shows some values for $R(q)$. The first important remark is that Fig. 2 shows that $r(q)$ has a symmetrical distribution having average equal to 0; this symmetry is not shown by the known theoretical results. The frequent values of $r(q)$ are rational numbers r for which the smallest set $\mathcal{A}$ with $\mu(\mathcal{A}) = 2r$ has very few elements. This explains the "concentration" of the computed data around the values $\pm 1/4$ (with $\mu(\{2\}) = \frac{1}{2}$ and primes q such that $2q \pm 1$ contributing, see Fig. 3). Moreover, the peak around the values $\pm 1/8$ depends on the contribution of the primes q such that $4q \pm 1$ are primes. In both cases, considering

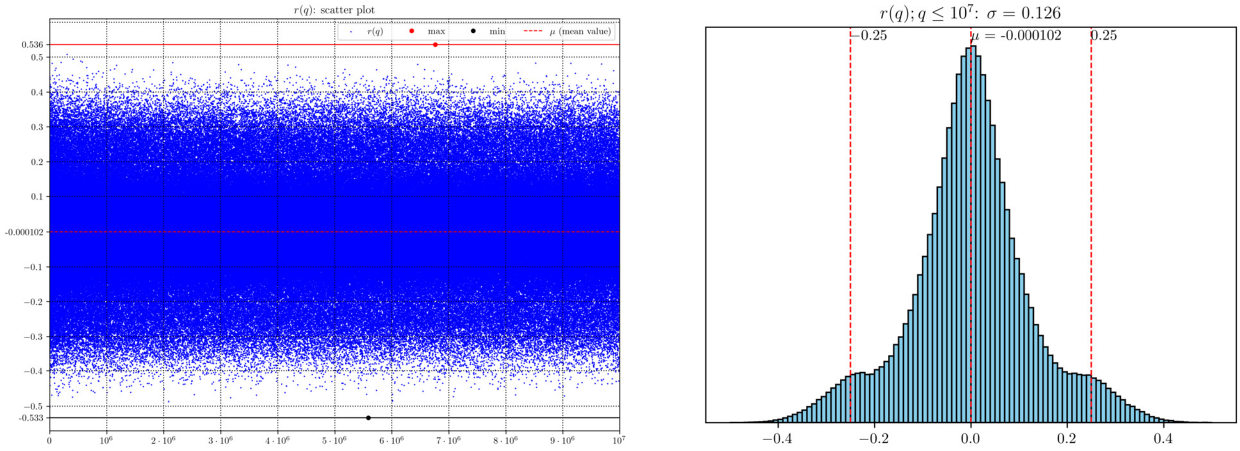

Fig. 2. On the left: the values of $r(q)$.

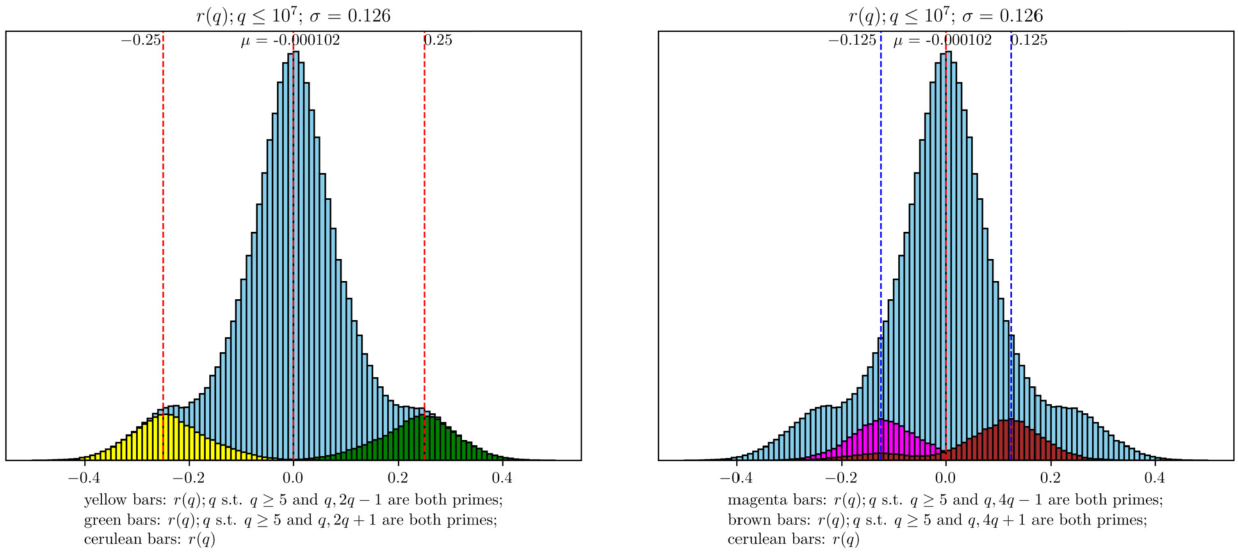

Fig. 3. On the left: the same histograms of Fig. 2 but the contributions of the primes q such that $2q+1$ is prime or $2q-1$ is prime (the "spikes") are superimposed. On the right: the contributions of the primes q such that $4q+1$ is prime or $4q-1$ is prime (the "spikes") are superimposed.

only the contribution of the primes q such that $2q \pm 1$ and $4q \pm 1$ are composite produces distributions very similar to the normal one, see Fig. 4.

The numerical results mentioned, the plots and the histograms, and the programs used to obtain $R(q)$ and $r(q)$, are available at https://www.math.unipd.it/~languasc/rq-comput-reprise.html

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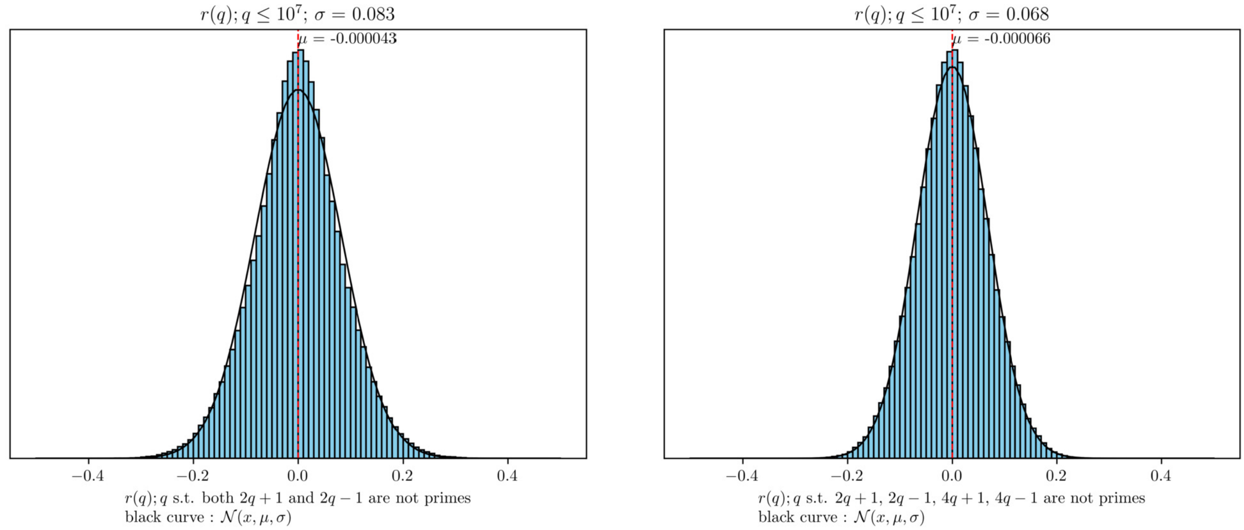

Fig. 4. On the left: the histogram for $r(q)$, q prime, $5 \leqslant q \leqslant 10^7$, such that $2q \pm 1$ are composite; on the right: the same with both $2q \pm 1$ and $4q \pm 1$ that are composite numbers. The red dashed lines represent the mean values.

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