Explicit estimates: from $\Lambda(n)$ in arithmetic progressions to $\Lambda(n)/n$

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Abstract

We denote by $\tilde{\psi}(x;q,a)$ the sum of $\Lambda(n)/n$ for all $n \leq x$ and congruent to $a \bmod q$ and similarly by $\psi(x;q,a)$ the sum of $\Lambda(n)$ over the same set. We show that the error term in $\tilde{\psi}(x;q,a) - (\log x)/\varphi(q) - C(q,a)$, for a suitable constant $C(q,a)$ can be controlled by that of $\psi(y;q,a) - y/\varphi(q)$ for y of size x, up to a small error term. As a consequence, if a partial Generalized Riemann Hypothesis has been verified for the L-functions attached to characters modulo q up to height H, this error term is bounded by $\mathcal{O}(e^{-H/8})$ when $x \geq H$. Previous methods had at best $\mathcal{O}(1/H)$ instead. We further compute asymptotics for the L^2-average of a quantity closely related to $C(q,a)$.

1   Introduction

Let $q \geq 1$ be a modulus and a be an integer prime to q. We classically define

$$\psi(x;q,a) = \sum_{\substack{n \leq x, \\ n \equiv a[q]}} \Lambda(n), \quad \tilde{\psi}(x;q,a) = \sum_{\substack{n \leq x, \\ n \equiv a[q]}} \Lambda(n)/n.$$

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There has been significant progress towards finding explicit asymptotics for $\psi(x; q, a)$, see for instance [5], [10], [21], [22], [31], [33], [34], [35] and [37]. The quantity $\tilde{\psi}(x; q, a)$, however, has received less attention, though Mertens gave very early, in [23], elementary and rather sharp bounds for these quantities. Rosser & Schoenfeld's landmark paper [34, Theorem 6] gives an estimate when $q = 1$. In [26], the second author devised a method that yielded fairly good numerics for $\tilde{\psi}(x; q, a)$. This question is also addressed in [6] and [24]. More recently the second author [27] obtained a satisfactory answer when $q = 1$. The present paper extends this approach in two ways: the effect of a numerical zero-free region is much stronger on the final result, see Theorem 1.2 below, and it is also valid for primes in arithmetic progressions.

Since a lot of work has been done on $\psi(x; q, a)$, the starting idea is to derive good estimates for $\tilde{\psi}(x; q, a)$ from those for $\psi(x; q, a)$. Rosser & Schoenfeld's paper does not follow such a line. The aim of this paper is to provide a method to achieve this, see Theorem 1.1 and 1.2 below.

Let us note that the prime number Theorem in the form $\psi(x) = (1+o(1))x$ is classically equivalent to

$$\tilde{\psi}(x) = \log x - \gamma + o(1). \tag{1}$$

So in a sense, we are concerned with a quantitative version of this equivalence. A simple integration by parts is *not* enough, as it loses a log-factor. In effect, an estimate of the form $|(\psi(x) - x)/x| \leq 0.01$ for x large enough transfers in something like $|\tilde{\psi}(x) - \log x + \gamma| \leq 0.01 \log x$ which is of little interest. The Landau equivalence Theorem can however be made explicit, but does not admit a saving better than $1/\sqrt{\log x}$ in a rough form; allowing a saving of any power of $\log x$ is already theoretically not obvious, see [2] and [18]. Concerning primes in arithmetic progression, the classical theory tells us that there exists a constant $C(q, a)$ (see the paper [26, Corollaire 1] for instance) such that

$$\tilde{\psi}(x; q, a) = \frac{\log x}{\varphi(q)} + C(q, a) + o_q(1).$$

(Where $o_q(1)$ designates here a function of x that may depend on q and that goes to 0 when x goes to infinity). Our general conjecture is that there exists a constant $C > 0$ independant on $q \leq x$ such that

$$\left| \tilde{\psi}(x; q, a) - \frac{\log x}{\varphi(q)} + C(q, a) \right| \leq C \max_{x/10 < y \leq 10x} \frac{|\psi(y; q, a) - (y/\varphi(q))|}{y} + C \frac{\log x}{\sqrt{x}}. \tag{2}$$

This conjecture is now justified by Theorem 1.2 below, which shows that such an inequality holds under the Generalized Riemann Hypothesis (on selecting $\kappa = 1$ and $H = 10 \log x$). However [9] indicates that this inequality does not hold in the case of Beurling generalized integers without any further assumption; interestingly, [25] shows that an equivalent of the Mertens formula is always valid in any Beurling system. The present method relies on zeroes of L-series and is not applicable to an arbitrary Beurling system. Here is a theorem that quantifies the strength of our approach:

Theorem 1.1. *Let $x \geq 10$ and $1 \leq q \leq x$ with q not an exceptional modulus (see Lemma 10.7). Then there exists a constant $c > 0$ such that, for every a invertible modulo q, we have*

$$\left| \tilde{\psi}(x; q, a) - \frac{\log x}{\varphi(q)} - C(q, a) \right| \ll \max_{x \leq y \leq 2x} \frac{|\psi(y; q, a) - \frac{y}{\varphi(q)}|}{y} + \exp\left(-c \frac{\log x}{\log(q \log x)} \right).$$

We discuss at the end of the proof the modifications necessary to cover the case when q is exceptional. We note here that a similar question concerning derivation of bounds for $\sum_{n \leq x} \mu(n)/n$ from bounds for $\sum_{n \leq x} \mu(n)$ (and some related sums) is addressed in [4], [3, Proposition 8] and [29, (1.4)]. A conjecture similar to (2) has been proposed in several talks by the second named author. We complete this detour by mentioning the conjecture given at the bottom of the first page of [28] that proposes a very similar link between $\sum_{n \leq x} \mu(n)/n$ and $\sum_{n \leq x} \Lambda(n)$.

Though all the quantities of the end-product are elementarily defined, the proof uses zeros of L-functions, and indeed an elementary proof would be likely to ignore the effect of the possible exceptional zero and lead to some strong informations on this one.

Let us end the general part of this introduction with a remark: in [15], the authors exhibit, under the Riemann Hypothesis, a pseudo-periodical function that (essentially) takes the value $(\tilde{\psi}(e^{-y}; q, a) + y/\varphi(q)) e^{y/2}$ when $y < 0$ and $(\psi(e^y; q, \bar{a}) - e^y/\varphi(q)) e^{-y/2}$ when $y > 0$ and $\bar{a}a \equiv 1[q]$. This gives a connection between $\tilde{\psi}(x; q, a)$ and $\psi(x; q, \bar{a})$ and *not* with $\psi(x; q, a)$.

The aim of the present method is numerical. Good bounds for $|\psi(y; q, a) - \frac{y}{\varphi(q)}|/y$ are obtained from the verification that the non-trivial zeros $\rho = \beta + i\gamma$ of bounded imaginary part (say $|\gamma| \leq H$) of any Dirichlet L-functions associated with a character modulo q have a real part equal to $1/2$. We shorten the description of this hypothesis by simply saying that $\mathrm{GRH}(q, H)$ has been satisfied.

Before we state our results on $\tilde{\psi}(x; q, a)$, we need some notation. When χ is a character modulo q, we denote by $Z(\chi)$ the set of the zeros of $L(s, \chi)$ that have a real part between 0 and 1, both extremes being excluded. We have $Z(\chi) = Z(\chi')$ whenever χ and χ' are induced by a same character, and in particular, when χ is induced by the primitive character χ_1, we have $Z(\chi) = Z(\chi_1)$. The zeros of $L(s, \chi)$ that belong to $Z(\chi)$ are called the *non-trivial zeros*. They are usually written as $\rho = \beta + i\gamma$ where β and γ are real numbers. This γ has no a priori connection with the Euler constant! There are $\varphi^*(q) = (\varphi \star \mu)(q)$ primitive characters modulo q, see [38, Theorem 8] or [30, Lemma 4.1] with the notation φ^* of [13, (3.7)]. Let further $b(\chi)$ be the constant term in the Laurent expansion of $L'/L(s, \chi)$ around $s = 0$. We have more explicitely:

$$
b(\chi) = \begin{cases} \dfrac{L'(0, \chi)}{L(0, \chi)} & \text{when } \mathfrak{a} = 0, \\[2ex] \lim_{s \to 0} \left(\dfrac{L'(s, \chi)}{L(s, \chi)} - \dfrac{1}{s} \right) & \text{when } \mathfrak{a} = 1 \text{ and } q > 1, \\[2ex] \log(2\pi) & \text{when } q = 1. \end{cases} \tag{3}
$$

See also Lemma 8.1 for a different expression for $b(\chi)$.

Theorem 1.2. *Let $\kappa > 0$ and $H \geq 100$ be two real parameters. We assume that $H/(4(1 + \kappa^{-1}))$ is an integer ≥ 10. We select a modulus $q \geq 1$ and assume $GRH(q, H)$. We have, for any $x \geq q \geq 1$ such that $x \geq H$, and any invertible residue class a modulo q:*

$$
\left| \tilde{\psi}(x; q, a) - \frac{\log x}{\varphi(q)} - C(q, a) - \frac{\psi(x; q, a) - \frac{x}{\varphi(q)}}{x} \right| \leq \int_x^{(1+\kappa)x} \left| \psi(y; q, a) - \frac{y}{\varphi(q)} \right| \frac{dy}{y^2}
$$

$$
+ \frac{U(q, H)}{\sqrt{x}} + \frac{V(q, x)}{x} + \frac{e^{-H/(4(1+\kappa^{-1}))}}{H^2} (1 + x^{-1/2}) W(q, H, \kappa)
$$

where

$$
U(q, H) = \frac{1}{\varphi(q)} \sum_{\chi \bmod q} \sum_{\substack{\rho \in Z(\chi), \\ |\gamma| \leq H}} 1/|\rho(1 - \rho)|, \tag{4}
$$

$$
V(q, x) = \frac{\sum_{d|q} \sum_{\chi \bmod^* d} |b(\chi)|}{\varphi(q)} + (1 + \log x)(1 + f(q)) + \frac{5}{4} \tag{5}
$$

$$
W(q, x, \kappa) = \sqrt{\kappa + 1} \left(\frac{1.81}{\kappa} \log \frac{qH}{2\pi e} + 4.41 \log(qH) + 10.6 \right), \tag{6}
$$

and

$$
f(q) = \sum_{p|q} \frac{1}{p - 1}. \tag{7}
$$

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We assume $H/(4(1+\kappa^{-1}))$ to be an integer to simplify the computations and avoid some integer parts. In [27] we investigated this line of approach, and obtained a first inequality, via an analog of Lemma 3.1 below. See also [41] (this is [42, chapter 4]) for some corrections and an improved error term. Since a partial Riemann Hypothesis has been satisfied to a very large height, this led to efficient estimates. Roughly speaking, up to the present paper, verifying the Riemann Hypothesis up to height H enabled to majorize the relative error term between the one of $\tilde{\psi}(x) - \log x + \gamma$ and the one of $(\psi(y) - y)/y$ by $\mathcal{O}(1/H)$. The proof we present below leads to the bound $\mathcal{O}(e^{-cH})$ (for any constant $c < 1/4$).

Numerically, the first named author has checked GRH in [7] for every primitive character to modulus $q \le 400\,000$ to height $\max\left(\frac{10^8}{q}, \frac{A \cdot 10^7}{q} + 200\right)$ with $A = 7.5$ in the case of even characters and $A = 3.75$ for odd characters. This improves on the earlier works [5] and [36]. Two main factors contribute to this improvement: the use of new algorithms that exploit the efficiency of Fast Fourier transforms to reduce the running time in its q-dependence from $\mathcal{O}(q^2)$ to $\mathcal{O}(q \log q)$, and the availability of more modern hardware. These computations were carried using interval arithmetic.

We readily see that $U(q, H) = \mathcal{O}(\log^2 q)$ while an individual explicit upper bound of the shape $|b(\chi)| = \mathcal{O}(\log^2 q)$, when χ is non exceptional, is provided by (30). The quantity that appear is however the average of these values. We state in a theorem our numerical finding.

Theorem 1.3. *For every $q \le 10^4$, we have*

$$V_2^\sharp(q) = \frac{1}{\varphi^*(q)} \sum_{\chi \bmod^* q} \left| b(\chi) + \log \frac{q}{2\pi} - \gamma \right|^2$$

$$= \frac{1}{\varphi^*(q)} \sum_{\chi \bmod^* q} \left| \frac{L'}{L}(1, \chi) \right|^2 \le \sum_{n \ge 1} \frac{\Lambda(n)^2}{n^2}.$$

The constant $\sum_{n \ge 1} \Lambda(n)^2/n^2 = 0.805 \cdots$ has been guessed by the numerics and is shown to be relevant by the following theorem.

Theorem 1.4. *We have*

$$\frac{1}{\varphi^*(q)} \sum_{\chi \bmod^* q} \left| \frac{L'}{L}(1, \chi) \right|^2 = \sum_{n \ge 1} \frac{\Lambda(n)^2}{n^2} - \sum_{p|q} \frac{\log^2 p}{h(p, q)} + \mathcal{O}(q^{-1/10})$$

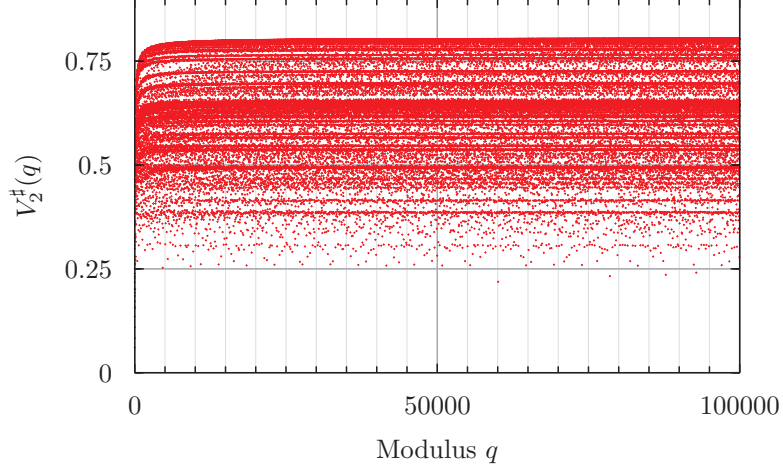*where $h(p, q) = (p - 1)^2$ when $p^2|q$ and $h(p, q) = p^2 - 1$ otherwise.*

Figure 1: $V_2^\sharp(q)$ vs. q

This is in this case a q-equivalent of the Plancherel formula for Mellin transforms. We did not try to get the best exponent in the error term, but just ensured that it was a negative power of q. Numerically however, it seems that this error term is non-positive; if this fact is a consequence of our Theorem when q has some prime factor $\leq q^{1/20}$ and is large enough, it is surprising in general and calls for some explanation that we failed to uncover. (We in fact checked this fact, but with lesser numerical accuracy for all moduli up to 10^5). This paper took quite some time to be put together, and we mention that in between, Sumaia Saad Eddin [11] proved that the values $(|L'/L|(1,\chi))_{\chi \bmod^* q}$ have a distribution when q ranges the primes.

Numerical computations give us the following for $U(q, H)$ (the average over every characters) and $U^*(q, H)$ (same quantity as for $U(q, H)$, but averaged over primitive characters, see (1.6)).

Theorem 1.5. *For $q \in [1, 10^4]$, we have*

$$U(q, 200) < 0.736 \log q.$$

In particular, for $q \leq 10^4$ we have $U(q, 200) < 6.772$.

Theorem 1.6. *For $q \in [3, 10^4]$, we have*

$$U^*(q, 200) = \frac{1}{\varphi^*(q)} \sum_{\chi \bmod^* q} \sum_{\substack{\rho \in Z(\chi), \\ |\gamma| \leq 200}} 1/|\rho(1-\rho)| < 0.737 \log q.$$

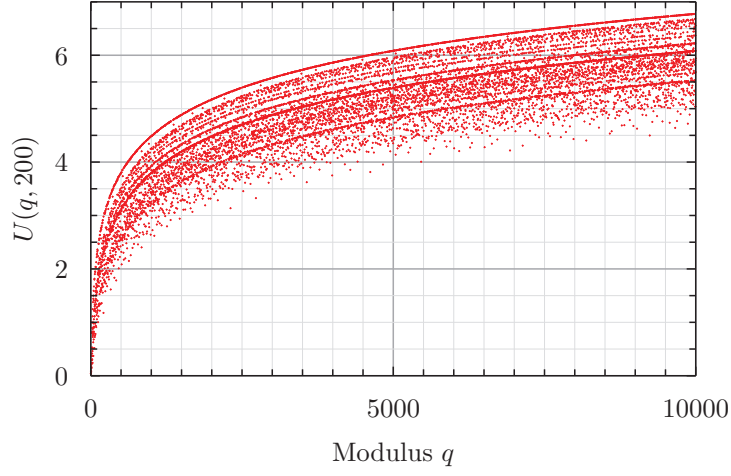*In particular, for $q \leq 10^4$ we have $U^*(q, 200) < 6.773$.*

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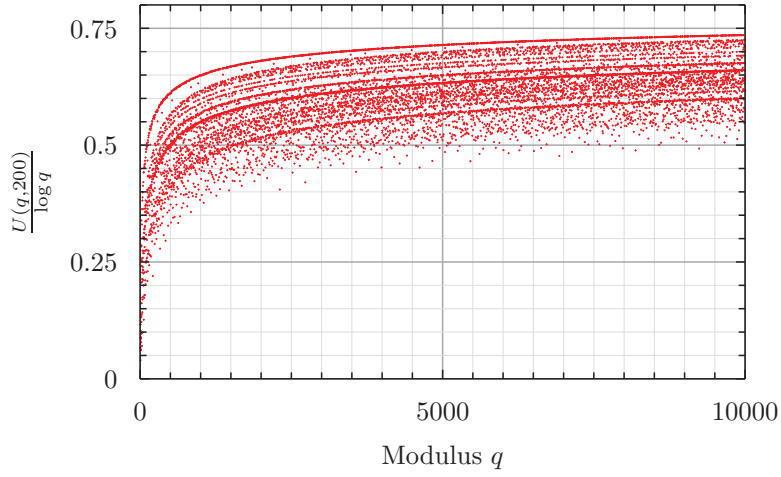
Figure 2: $U(q, 200)$ vs. q

Figure 3: $U(q, 200)/\log q$ vs. q

The computation of U and U^* were implemented in C++ using interval arithmetic. The positions of the zeros, accurate to more than 100 bits, were computed rigorously using the algorithms described in [7].

A straight forward computation shows that for $q \leq 10^4$ we have the inequality $V(q, 10^4)/100 \leq 0.277$ (with the maximum at $q = 2^{13}$) so for all $q \leq 10^4 \leq x$ we have

$$U(q, H) + \frac{V(q, x)}{\sqrt{x}} \leq 7.049, \qquad \frac{e^{-H/(4(1+\kappa^{-1}))}}{H^2} W(q, H, \kappa) \leq 8 \cdot 10^{-12}$$
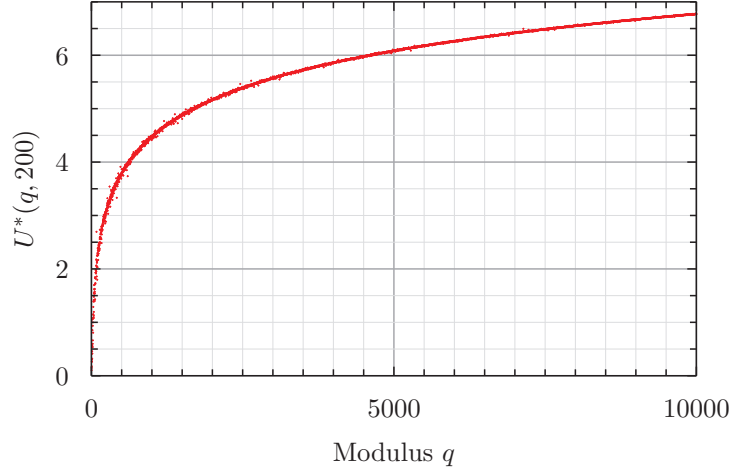
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Figure 4: $U^*(q, 200)$ vs. q

with $H = 200$ and $\kappa = 2/3$. Hence the corollary to Theorem 1.2:

Theorem 1.7. *For every* $q \leq 10^4 \leq x$, *we have*

$$\left| \tilde{\psi}(x; q, a) - \frac{\log x}{\varphi(q)} - C(q, a) - \frac{\psi(x; q, a) - \frac{x}{\varphi(q)}}{x} \right|$$

$$\leq \int_x^{5x/3} \left| \psi(y; q, a) - \frac{y}{\varphi(q)} \right| \frac{dy}{y^2} + 7.05\, x^{-1/2} + 8 \cdot 10^{-12}.$$

This result is ready for use. Here are three comments:

1. RELATIVE STRENGTH. The next step is to introduce bounds for $\psi(y; q, a) - \frac{y}{\varphi(q)}$ and derive estimates for $\tilde{R}(x; q, a) = \tilde{\psi}(x; q, a) - \frac{\log x}{\varphi(q)} - C(q, a)$. As a comparison, [26, Corollary 4] shows that $|\tilde{R}(x; q, a)| \leq 2/9$ for some moduli q and x large enough (in this result $x \geq 182$); the summand $8 \cdot 10^{-12}$ is largely negligible when we compare to such a bound.

2. INCORPORATING BOUNDS FOR $\psi(y; q, a) - \frac{y}{\varphi(q)}$. Theorem 1.7 will remain valid and be usable even if the bounds on $\psi(y; q, a) - \frac{y}{\varphi(q)}$ improve. There exists explicit bounds for primes in arithmetic progressions in the litterature, for instance in [31] or [5]. However first the number of moduli covered is much smaller than what is possible by combining [31] together with [7], and secondly, we know by private communications that several explicit bounds for $\psi(y; q, a) - \frac{y}{\varphi(q)}$ are in preparation but not quite ready.
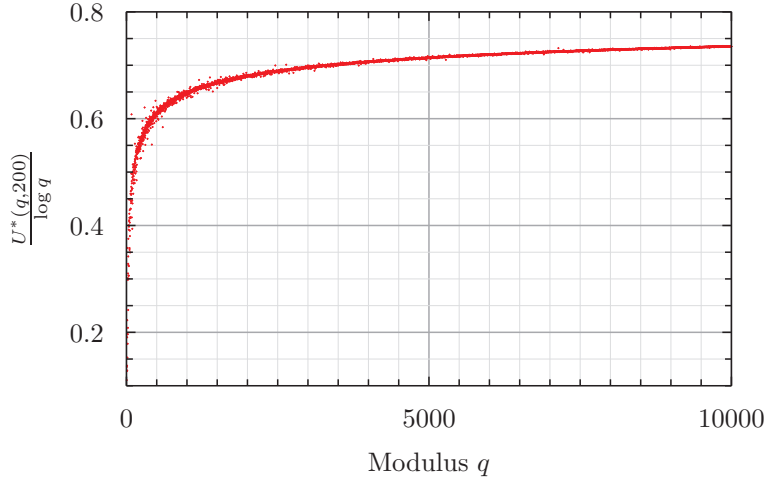
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Figure 5: $U^*(q, 200)/\log q$ vs. q

3. COMPLETING THE BOUNDS. Bounds for $\psi(x; q, a) - \frac{x}{\varphi(q)}$ will be used for x somewhat large (say greater than 10^5) to avoid some initial noise and should thus be completed for a better usability. [26, Theorem 2] gives bounds for $|\tilde{\psi}(x; q, a) - \frac{\log x}{\varphi(q)} - C(q, a)|$ when $x \leq 10^5$ and q belonging to Rumely's list. It is not straightforward to calculate the constants $C(q, a)$, and since we have the machinery ready, we complete these computations with Theorem 8.1 below.

Notation

Our set of notation is essentially standard. We use $\mathbb{1}_{q=1}$ to denote the function that takes value 1 at $q = 1$ and 0 otherwise (sometimes called the Dirac symbol at $q = 1$). We use also the natural extension of the already used definitions:

$$\tilde{\psi}(x, \chi) = \sum_{n \leq x} \Lambda(n)\chi(n)/n. \tag{8}$$

By $F(x) = \mathcal{O}^*(G(x))$ we mean $|F(x)| \leq G(x)$. Usually $s = \sigma + it$ but for a zero of an L-function we use $\rho = \beta + i\gamma$. In this case γ is not the Euler constant, though this constant is also denoted by γ. We further will use some $\gamma(\chi)$. Finally $d\|q$ means that d divides q in such a way that d and q/d are coprime.

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2 An explicit formula for an integrated form of $\psi(x, \chi)$

We first need to adapt [32, Lemma 4] to the case of Dirichlet character. Let χ be a primitive character modulo q. Let $\mathfrak{a} = (1 + \chi(-1))/2$. The same parameter appears in [8, Chapter 19, (4)] and equals $1 - d$, where d is the parameter of [14]. The notation $b(\chi)$ specified in (3) is the same as the one used in [21, Section 3], while it is $-B(\chi)$ in [14]. We shall bundle the contribution of the trivial zeros with the help of a simple function:

$$
\Omega(t, \chi) = \begin{cases} \frac{1}{2} \log \frac{t-1}{t+1} & \text{when } \mathfrak{a} = 0, \\ \log t + \frac{1}{2} \log(1 - t^{-2}) & \text{when } \mathfrak{a} = 1 \text{ and } q > 1, \\ \frac{1}{2} \log(1 - t^{-2}) & \text{when } q = 1. \end{cases}
\tag{9}
$$

(See [14, (2.6) and (4.5)])

Lemma 2.1. *Let g be a continuously differentiable function on $[a, b]$ with $2 \le a \le b < +\infty$. Let χ be a primitive character modulo q. Let $\mathfrak{a} = (1+\chi(-1))/2$ and $b(\chi)$ and $\Omega(t, \chi)$ be defined as above. We have*

$$
\int_a^b \psi(t, \chi)g(t)dt = \mathbb{1}_{q=1} \int_a^b tg(t)dt - \sum_\rho \int_a^b \frac{t^\rho}{\rho} g(t)dt
$$

$$
- \int_a^b \big(b(\chi) + \Omega(t, \chi)\big)g(t)dt.
$$

where ρ ranges the zeros of $L(s, \chi)$ in the critical strip (i.e. with $\Re\rho \in (0, 1)$)

Proof. The proof follows strictly the one of [32, Lemma 4]. It is enough to prove this lemma when no integer lies between a and b, a hypothesis we shall henceforth make. We recall that for $a < y < b$ and $T > 2$,

$$
\psi(y, \chi) = \mathbb{1}_{q=1}y - \sum_{|\gamma| \le T} \frac{y^\rho}{\rho} - b(\chi) - \Omega(y, \chi)
\tag{10}
$$

$$
+ \mathcal{O}\left(\frac{y \log^2 yT}{T} + \frac{y \log y}{<y>T}\right),
$$

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where $< y >= \min(y - a, b - y)$ (see [8, Chapter 17, (9)–(10)] when $q = 1$ and [8, Chapter 19, (2)–(3)] when $q > 1$). Note that the formula [32, (5)] has a wrong sign in front of $\log 2\pi$. Formula (10) is valid as such because y is not an integer in this range and the reader should consult [8] to extend the result in this case. The remainder of the proof is then straighforward, and is for instance detailled in [32, Proof of Lemma 4]. □

Lemma 2.2. *When $t \geq 1.84$ we have $|\Omega(t, \chi)| \leq \log t$.*

Proof. When $\mathfrak{a} = 0$, we have to check that

$$\tfrac{1}{2} \log \frac{t - 1}{t + 1} \overset{?}{\geq} - \log t$$

i.e. $t^2(t - 1) \geq t + 1$ whose largest (and only) real root is ≤ 1.84. When $\mathfrak{a} = 1$, we see that the only inequality that is not obvious is

$$-\tfrac{1}{2} \log(1 - t^{-2}) \overset{?}{\leq} 2 \log t.$$

It is satisfied when $t^4 - t^2 \geq 1$, i.e. when $t \geq \sqrt{(1 + \sqrt{5})/2}$. □

3 A first formula linking $\tilde{\psi}(x, \chi)$ and $\psi(x, \chi)$

Our first step is the following lemma:

Lemma 3.1. *Let χ be a primitive character modulo q. We have, for $x \geq 1$:*

$$\tilde{\psi}(x, \chi) = \mathbb{1}_{q=1} \log x - \gamma(\chi) + \frac{\psi(x, \chi) - \mathbb{1}_{q=1}x}{x} + \sum_\rho \frac{x^{\rho-1}}{\rho(\rho - 1)} + \frac{B(x, \chi)}{x}.$$

where the sum is over the zeros ρ of $L(s, \chi)$ that lie in the critical strip $0 < \Re s < 1$ (the so-called non trivial zeros), $\gamma(\chi)$ is the constant defined by

$$\gamma(\chi) = \mathbb{1}_{q=1} - \int_1^\infty (\psi(t, \chi) - \mathbb{1}_{q=1}t) \frac{dt}{t^2}$$

and $B(x, \chi)$ is the bounded function given by

$$B(x, \chi) = x \int_x^\infty (b(\chi) + \Omega(t, \chi)) \frac{dt}{t^2}.$$

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The main feature of the lemma is that the sum over the zeros is uniformly convergent, a feature not shared by the explicit formulaes for $\psi(x,\chi)$ or for $\tilde{\psi}(x,\chi)$ (see (10) for instance). In fact, the main difficulty in carried by the term $(\psi(x,\chi)-x)/x$. Note that $\gamma(1)=\gamma$, while, when $q>1$, we have

$$\gamma(\chi)=L'(1,\chi)/L(1,\chi).$$

Proof. We simply proceed by integration by parts:

$$
\begin{aligned}
\tilde{\psi}(x,\chi) &= \int_1^x \psi(t,\chi)\frac{dt}{t^2} + \frac{\psi(x,\chi)}{x} \\
&= \mathbb{1}_{q=1}\log x - \gamma(\chi) + \int_x^\infty (\psi(t,\chi)-\mathbb{1}_{q=1}t)\frac{dt}{t^2} + \frac{\psi(x,\chi)-\mathbb{1}_{q=1}x}{x}.
\end{aligned}
$$

Note that the existence of the integral requires a strong enough form of the approximation of $\psi(t,\chi)$ by $\mathbb{1}_{q=1}t$. Next we apply the explicit formula given in Lemma 2.1 and get

$$
\begin{aligned}
\int_x^Y (\psi(t,\chi)-\mathbb{1}_{q=1}t)\frac{dt}{t^2} &= -\sum_\rho \int_x^Y \frac{t^{\rho-2}dt}{\rho} + \int_x^Y (b(\chi)+\Omega(t,\chi))\frac{dt}{t^2} \\
&= -\sum_\rho \frac{Y^{\rho-1}-x^{\rho-1}}{\rho(\rho-1)} + \int_x^Y (b(\chi)+\Omega(t,\chi))\frac{dt}{t^2}.
\end{aligned}
$$

Since (1) is known to hold, and $\sum_\rho 1/|\rho(\rho-1)|$ is convergent, we can send Y to infinity and get

$$\int_x^\infty (\psi(t)-\mathbb{1}_{q=1}t)\frac{dt}{t^2} = \sum_\rho \frac{x^{\rho-1}}{\rho(\rho-1)} + \int_x^\infty (b(\chi)+\Omega(t,\chi))\frac{dt}{t^2}.$$

$\square$

4 Integration of $\psi(x,\chi)$ against a well-chosen kernel

We will need in next section to choose a proper kernel. We rely on [32] where a similar question has been addressed. We define, for any integer $m\geq 1$, the function

$$f_m(t)=\max\big(0,(4t(1-t))^m\big). \tag{11}$$

The function f_m satisfies

$$f_m^{(k)}(0)=f_m^{(k)}(1)=0 \quad (0\leq k\leq m-1). \tag{12}$$

We recall part of [32, Lemma 6]

Lemma 4.1.
$$\|f_m\|_1 = \frac{2^{2m}m!^2}{(2m+1)!} \quad , \quad \|f_m^{(m)}\|_2 = 2^{2m}\frac{m!}{\sqrt{2m+1}}, \tag{13}$$

$$\|f_m^{(m)}\|_2/\|f_m\|_1 = \frac{(2m+1)!}{m!\sqrt{2m+1}} \leq \sqrt{4m+2}\,e^{\frac{1}{24m}}(4m/e)^m. \tag{14}$$

From f_m and another real parameter $\kappa > 0$, we define

$$g_m(t,\kappa) = \begin{cases} 1 & \text{when } 0 < t \leq 1, \\ 1 - \|f_m\|_1^{-1} \int_0^{(t-1)/\kappa} f_m(u)du & \text{when } 1 \leq t \leq 1+\kappa, \\ 0 & \text{when } t \geq 1+\kappa. \end{cases} \tag{15}$$

Note that the function g_m satisfies $0 \leq g_m(t,\kappa) \leq 1$.

Lemma 4.2. *We have*

$$\int_x^\infty \frac{\psi(t,\chi) - \mathbb{1}_{q=1}t}{t^2} g_m(t/x,\kappa)dt = \sum_\rho \frac{x^{\rho-1}}{\rho(\rho-1)} - \sum_\rho \frac{x^{\rho-1}c_m(\kappa,\rho)}{\rho(\rho-1)}$$
$$+ \int_x^\infty \big(b(\chi) + \Omega(t,\chi)\big)\frac{g_m(t/x,\kappa)}{t^2}dt.$$

for some coefficients $c_m(\kappa,\rho)$ that satisfy

$$|c_m(\kappa,\rho)| \leq 1, \quad |c_m(\kappa,\rho)| \leq \frac{\|f_m^{(m)}\|_2/\|f_m\|_1}{|\rho(\rho+1)\cdots(\rho+m-1)|\kappa^m}\sqrt{\frac{(\kappa+1)^{2m+1}-1}{2m+1}}.$$

We also have

$$|c_m(\kappa,\rho)| \leq e^{\frac{1}{24m}}\sqrt{2\kappa+2}\Big(\frac{4(1+\kappa^{-1})m}{e\,|\rho|}\Big)^m. \tag{16}$$

Furthermore, the proof shows that

$$c_m(\kappa,\rho) = \frac{1}{\|f_m\|_1}\int_0^1 (1+\kappa u)^{\rho-1}f_m(u)du. \tag{17}$$

Proof. Lemma 2.1 is ready to be used in this context. We readily compute:
$$\int_x^\infty t^{\rho-2}g_m(t/x,\kappa)dt = x^{\rho-1}\int_1^\infty t^{\rho-2}g_m(t,\kappa)dt$$
$$= \frac{x^{\rho-1}}{\rho-1} - \frac{1}{\|f_m\|_1\kappa(\rho-1)}\int_1^{1+\kappa} t^{\rho-1}f_m((t-1)/\kappa)dt.$$

Repeated integration by parts on the last summand shows this one to be equal to

$$\frac{1}{\|f_m\|_1\kappa^{k+1}(\rho-1)\cdots(\rho+k-1)}\int_1^{1+\kappa} t^{\rho+k-1}f_m^{(k)}((t-1)/\kappa)dt$$

for any integer $k \leq m$ (check by recursion on k). □

5 A second formula linking $\tilde{\psi}(x, \chi)$ and $\psi(x, \chi)$; proof of Theorem 1.1

On joining Lemma 3.1 together with Lemma 4.2, we reach our fundamental formula, namely

$$
\begin{aligned}
\tilde{\psi}(x, \chi) = \ & \mathbb{1}_{q=1} \log x - \gamma(\chi) \\
& + \frac{\psi(x, \chi) - \mathbb{1}_{q=1} x}{x} + \int_x^\infty \frac{\psi(t, \chi) - \mathbb{1}_{q=1} t}{t^2} g_m(t/x, \kappa) dt \\
& + \sum_\rho \frac{x^{\rho-1} c_m(\kappa, \rho)}{\rho(\rho-1)} + \int_x^\infty \left(b(\chi) + \Omega(t, \chi) \right) \frac{(1 - g_m(t/x, \kappa))}{t^2} dt.
\end{aligned}
\tag{18}
$$

Let us explain this formula: the first line contains what we want. The second line is a part of the error term that is controlled directly by $|\psi(t, \chi) - \mathbb{1}_{q=1} t|$ for $t \in [x, (1 + \kappa)x]$ since g_m is bounded by 1. If the formula ended here, we would have proven our conjecture. The third line however appears, in which the second summand is readily seen to be $\ll (\log x)/x$. The last summand is the most important; the success of this formula relies on the fact that this sum is extremely well-behaved. Indeed, when $|\rho| \geq T$ and typically $\kappa = 1$, and on using (16), it is $\ll \frac{\log(qT)}{mT} (8m/(eT))^m$. If we take $m = \log x + \mathcal{O}(1)$ and $T = 8m$, this contribution is thus $\mathcal{O}(x^{-0.6})$. This means that only the very first zeros contribute, and indeed the ones of height $\leq 8 \log x + \mathcal{O}(1)$. For these zeros, we use $|c_m(\kappa, \rho)| \leq 1$. Asymptotically, the zero-free region ensures us that the contribution is thus bounded upto a multiplicative constant by $\exp(-c(\log x)/\log(q \log x))$ for some positive constant c. This is not as good as the $(\log x)/\sqrt{x}$ of our conjecture, but it is still much better than the error term one can get for $\tilde{\psi}(x, \chi)$ with such a zero-free region. This means that the second line really controls the error term.

6 From $\tilde{\psi}(x; q, a)$ to $\tilde{\psi}(x, \chi)$ for primitive χ

We rely on [31, Section 4.3]. When χ is a character modulo q, we denote by χ_1 its associated primitive character. We define

$$
w_q(n, a) = \frac{1}{\varphi(q)} \sum_{\chi \bmod q} \chi_1(n) \overline{\chi(a)}.
\tag{19}
$$

It is proved in [31, Section 4.3] (the proof is easy) that, if K is the largest divisor of q coprime to n, we have

$$w_q(n, a) = \begin{cases} \varphi(K)/\varphi(q) & \text{when } n \equiv a \bmod K \\ 0 & \text{otherwise.} \end{cases} \tag{20}$$

We consider

$$\tilde{\psi}^*(x; q, a) = \sum_{n \leq x} w_q(n, a)\Lambda(n)/n, \quad \psi^*(x; q, a) = \sum_{n \leq x} w_q(n, a)\Lambda(n). \tag{21}$$

The paper [31] contains also, next to equation (4.3.1) the inequality (recall (7))

$$\psi^*(x; q, a) = \psi(x; q, a) + \mathcal{O}^*(f(q)\log x).$$

In the next lemma, we need only to register the existence of the constant $C(q, a)$, but we take the opportunity to explicitate it here. We define $\nu_p(q)$ to be the p-adic valuation of q, so that $p^{\nu_p(q)}|q$ and p is coprime to $q/p^{\nu_p(q)}$. We define $\varpi(p, a, q)$ to be the smallest positive integer ℓ such that $p^\ell \equiv a[q/p^{\nu_p(q)}]$ and ∞ if no such ℓ exists. We define finally

$$C_0(q, a) = \sum_{p|q} \frac{p^{1+\varpi(p,1,q)} \log p}{(p-1)(p^{\varpi(p,1,q)} - 1)p^{\nu_p(q)+\varpi(p,a,q)}}. \tag{22}$$

Lemma 6.1. *We have, when $x \geq 1$,*

$$\tilde{\psi}(x; q, a) = \tilde{\psi}^*(x; q, a) - C_0(q, a) + \mathcal{O}^*(\tfrac{5}{4}/x).$$

Proof. Indeed, we find that

$$\begin{aligned}
\tilde{\psi}^*(x; q, a) &= \tilde{\psi}(x; q, a) + \sum_{p|q} \frac{1}{(p-1)p^{\nu_p(q)-1}} \sum_{\substack{\ell \geq 1, p^\ell \leq x, \\ p^\ell \equiv a[q/p^{\nu_p(q)}]}} \frac{\log p}{p^\ell} \\
&= \tilde{\psi}(x; q, a) + \sum_{p|q} \frac{1}{(p-1)p^{\nu_p(q)-1}} \sum_{\substack{\ell \geq 1, \\ p^\ell \equiv a[q/p^{\nu_p(q)}]}} \frac{\log p}{p^\ell} \\
&\quad + \mathcal{O}^*\left(\sum_{p|q} \frac{\log p}{(p-1)^2 p^{\nu_p(q)-1}}/x\right).
\end{aligned}$$

After some easy work, the reader will recover (22). Concerning the remainder term, we note that

$$\sum_{p \geq 2} \frac{\log p}{(p-1)^2} \leq 1.23 \leq 5/4.$$

$\square$

On using (19), we readily derive from (18) the following formula

$$
\begin{aligned}
\tilde{\psi}^*(x; q, a) = \ & \frac{\log x}{\varphi(q)} + C^*(q, a) \\
& + \frac{\psi^*(x; q, a) - \frac{x}{\varphi(q)}}{x} + \int_x^\infty \frac{\psi^*(t; q, a) - \frac{t}{\varphi(q)}}{t^2} g_m(t/x, \kappa) dt \\
& + \frac{1}{\varphi(q)} \sum_{d|q} \sum_{\chi \bmod^* d} \overline{\chi(a)} \sum_{\rho \in Z(\chi)} \frac{x^{\rho-1} c_m(\kappa, \rho)}{\rho(\rho - 1)} \\
& + \frac{1}{\varphi(q)} \sum_{d|q} \sum_{\chi \bmod^* d} \overline{\chi(a)} \int_x^\infty \big(b(\chi) + \Omega(t, \chi)\big) \frac{(1 - g_m(t/x, \kappa))}{t^2} dt.
\end{aligned}
\tag{23}
$$

where

$$
C^*(q, a) = \frac{-\gamma}{\varphi(q)} - \frac{1}{\varphi(q)} \sum_{\substack{d|q, \ \chi \bmod^* d \\ d > 1}} \overline{\chi}(a) \frac{L'}{L}(1, \chi)
\tag{24}
$$

The reader will easily check that $f(q)$ is at most of order $\log\log\log(100q)$. We replace $\tilde{\psi}^*$ by $\tilde{\psi}$ at the cost of a modification of the constant and a $\mathcal{O}^*(\frac{5}{4}/x)$. We replace $\psi^*(x; q, a)$ by $\psi(x; q, a)$ at a cost of $\mathcal{O}^*(f(q)(\log x)/x)$ and $\psi^*(t; q, a)$ by $\psi(t; q, a)$ at a cost of $\mathcal{O}^*(f(q)(1 + \log x)/x)$. We appeal to Lemma 2.2 and get that the last summand is, in absolute value,

$$
\leq \frac{1}{\varphi(q)x} \sum_{d|q} \sum_{\chi \bmod^* d} |b(\chi)| + \frac{1 + \log x}{x}.
$$

After some straightforward manipulations, we reach

$$
\begin{aligned}
\tilde{\psi}(x; q, a) = \ & \frac{\log x}{\varphi(q)} + C(q, a) \\
& + \frac{\psi(x; q, a) - \frac{x}{\varphi(q)}}{x} + \int_x^\infty \frac{\psi(t; q, a) - \frac{t}{\varphi(q)}}{t^2} g_m(t/x, \kappa) dt \\
& + \frac{1}{\varphi(q)} \sum_{d|q} \sum_{\chi \bmod^* d} \overline{\chi(a)} \sum_{\rho \in Z(\chi)} \frac{x^{\rho-1} c_m(\kappa, \rho)}{\rho(\rho - 1)} \\
& + \mathcal{O}^* \left(\frac{\sum_{d|q} \sum_{\chi \bmod^* d} |b(\chi)|}{\varphi(q)x} + \frac{1 + 2\log x}{x}(1 + f(q)) + \frac{5/4}{x} \right).
\end{aligned}
\tag{25}
$$

where (see (22) and (24))

$$
C(q, a) = -C_0(q, a) + C^*(q, a).
\tag{26}
$$

7 On the constants $b(\chi)$

On reading the proof of [21, Lemma 3.5] and more precisely the equality before (3.16), we see that we have, *when χ is primitive* (i.e. equals χ_1 in the notation of [21])

$$|b(\chi)| \leq \left|\frac{\zeta'}{\zeta}(2)\right| + \mathfrak{a} + \sum_{\rho \in Z(\chi)} \frac{2}{\rho(2-\rho)}. \tag{27}$$

We read [21, Top of page 275] and find, that, when χ is not exceptional (for otherwise there may be a zero close to 1 and by symmetry – since this would correspond to a real character – a zero close to 0), we have

$$|b(\chi)| \leq 0.57 + 1 + 11(\pi^{-1} + C_1)\log^2 q + 11(C_2 - \pi^{-1}\log(2\pi e))\log q$$
$$+ (4\pi^{-1} + 2C_1)\log q - 4\pi^{-1}\log(2\pi) + C_1 + 2C_2 \tag{28}$$

where we can take $C_1 = 0.9185$ and $C_2 = 5.512$ as in [31, Lemma 4.1.1] (be careful to the change of notation between both papers!). As a consequence, we find that

$$|b(\chi)| \leq 6 + 54\log q + 14\log^2 q \quad (\chi \text{ not exceptional.}) \tag{29}$$

This bound can be improved in several ways, for instance on invoking the improved zero-free region for L-function proved in [16] (see also [17]). This result is heavily influenced by the small zeros for which a better result may be known. Furthermore, and since we only need to bound the average $\sum_\chi |b(\chi)|$, several other tools could be used. We keep these improvements for a later paper. On using [31, Lemma 4.1.4] together with (27), we infer that, when $L(s, \chi)$ has no zeros on the critical strip of height ≤ 1 (in absolute value) that are off the critical line (i.e. $\Re s = 1/2$), we have

$$|b(\chi)| \leq 14.3 + 3.94\log q \quad (\text{when } L(s, \chi) \text{ satisfies GRH(q,1)})$$

By [7], this condition is known to hold for every character to any modulus $\leq 4 \cdot 10^5$; we combine both estimates to get

$$|b(\chi)| \leq 14 + 19\log^2 q \quad (\chi \text{ not exceptional.}) \tag{30}$$

Note again that [7] demonstrates that there are no exceptional characters when $q \leq 4 \cdot 10^5$.

8   On the constants $b(\chi)$ and $C(q,a)$, II

Our first task here is to express $b(\chi)$ in terms of values at $s = 1$, when $q \neq 1$. This is achieved in the next lemma.

Lemma 8.1. *For a primitive non-principal Dirichlet character χ, we have*

$$b(\chi) = -\log \frac{q}{2\pi} + \gamma - \frac{L'}{L}(1, \overline{\chi}).$$

Proof. We consider the completed L-series defined by

$$\Phi(s, \chi) = (q/\pi)^{(s+\mathfrak{a})/2} \Gamma\left(\frac{s + \mathfrak{a}}{2}\right) L(s, \chi) \tag{31}$$

where $\mathfrak{a} = (1 - \chi(-1))/2$. Its logarithmic derivative is given by

$$\frac{\Phi'(s, \chi)}{\Phi(s, \chi)} = \tfrac{1}{2}\log\frac{q}{\pi} + \frac{\Gamma'}{2\Gamma}\left(\frac{s + \mathfrak{a}}{2}\right) + \frac{L'}{L}(s, \chi). \tag{32}$$

When $\mathfrak{a} = 1$, the functional equation at $s = 0$ gives us

$$\tfrac{1}{2}\log\frac{q}{\pi} + \frac{\Gamma'}{2\Gamma}(1/2) + \frac{L'}{L}(0, \chi) + b(\chi) = -\tfrac{1}{2}\log\frac{q}{\pi} - \frac{\Gamma'}{2\Gamma}(1) - \frac{L'}{L}(1, \overline{\chi}) \tag{33}$$

Thus, on recalling the special values of the digamma function $F = \Gamma'/\Gamma$ (see [1, (6.3.1)]):

$$F(1) = -\gamma, \quad F(1/2) = -\gamma - 2\log 2, \tag{34}$$

we find that

$$b(\chi) = -\log\frac{q}{2\pi} + \gamma - \frac{L'}{L}(1, \overline{\chi}) \qquad (\mathfrak{a} = 1). \tag{35}$$

When $\mathfrak{a} = 0$, the functional equation at $s = 0$ gives us

$$\tfrac{1}{2}\log\frac{q}{\pi} + \lim_{s \to 0}\left(\frac{\Gamma'}{2\Gamma}(s/2) + \frac{1}{s}\right) + b(\chi) = -\tfrac{1}{2}\log\frac{q}{\pi} - \frac{\Gamma'}{2\Gamma}(1/2) - \frac{L'}{L}(1, \chi).$$

Note that, by $\Gamma(z + 1) = z\Gamma(z)$, we find that

$$F(s/2) + \frac{2}{s} = F(1 + (s/2)) \tag{36}$$

and thus

$$b(\chi) = -\log\frac{q}{2\pi} + \gamma - \frac{L'}{L}(1, \overline{\chi}) \qquad (\mathfrak{a} = 0) \tag{37}$$

as desired. $\qquad\square$

Lemma 8.2. *We have*

$$C(q, a) = -C_0(q, a) - \frac{\gamma}{\varphi(q)} + \frac{1}{\varphi(q)} \sum_{\substack{d|q, \\ d>1}} \sum_{\chi \bmod^* d} \chi(a)\left(b(\chi) + \log\frac{d}{2\pi} - \gamma\right).$$

Appealing to Lemma 8.2, we can now examine computationally

$$\max_{q \leq Q} \max_{q \leq x \leq X} \max_{a \bmod^* q} \sqrt{x}\left|\tilde{\psi}(x; q, a) - \frac{x}{\varphi(q)} - C(q, a)\right|.$$

Theorem 8.1. *Let $X = 10^5$ and $Q = 10^3$. Then*

$$\max_{q \leq Q} \max_{q \leq x \leq X} \max_{a \bmod^* q} \sqrt{x}\left|\tilde{\psi}(x; q, a) - \frac{x}{\varphi(q)} - C(q, a)\right| \in (0.8533, 0.8534)$$

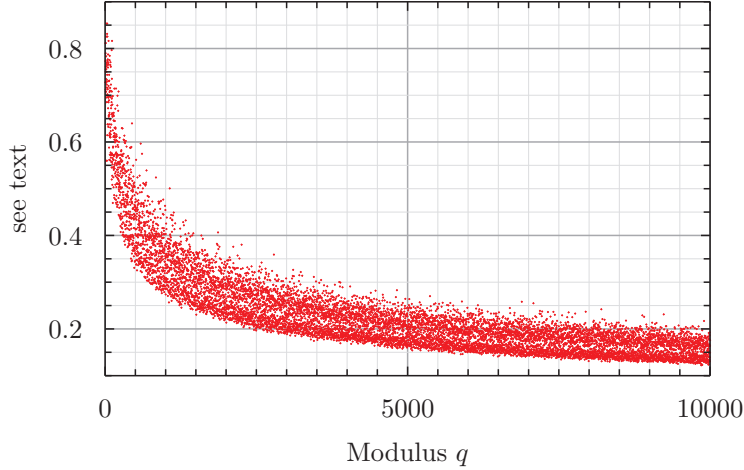*and the maximum is attained with $q = 17$, $x = 606$ and $a = 12$.*

Figure 6: $\displaystyle\max_{q \leq x \leq 10^5} \max_{a \bmod^* q} \sqrt{x}\left|\tilde{\psi}(x; q, a) - \frac{x}{\varphi(q)} - C(q, a)\right|$ vs. q

9 The sum over the zeros; proof of Theorems 1.2 and 1.1

We recall the following lemma of [21] in the notation of [31, Lemma 4.1.1]. See also [40].

Lemma 9.1 (McCurley). *If χ is a Dirichlet character of conductor q, if $T \geq 1$ is a real number, and if $N(T, \chi)$ denotes the number of zeros $\beta + i\gamma$ of $L(s, \chi)$ in the rectangle $0 < \beta < 1$, $|\gamma| \leq T$, then*

$$\left| N(T, \chi) - \frac{T}{\pi} \log\left(\frac{qT}{2\pi e}\right) \right| \leq C_2 \log(qT) + C_3$$

with $C_2 = 0.9185$ and $C_3 = 5.512$.

Once again, the reader should be wary of the change of indexes in C_1, C_2 and C_3 between [21] and [31].

Proof of Theorem 1.2. We first note that the quantities we are interested (namely $\widetilde{\psi}(x; q, a)$) are real numbers. We can thus replace the sum over the zeros by

$$J_m(\chi, x) = \frac{1}{2}\left(\sum_{\rho \in Z(\chi)} \frac{x^{\rho-1} c_m(\kappa, \rho)}{\rho(\rho-1)} + \sum_{\rho \in Z(\overline{\chi})} \frac{x^{\rho-1} c_m(\kappa, \rho)}{\rho(\rho-1)} \right).$$

The advantage is the symmetry that results from the following remark: when $\rho \in Z(\chi)$, then $1 - \overline{\rho} \in Z(\overline{\chi})$. We continue by assuming that every non-trivial zero $\rho = \beta + i\gamma$ of $L(s, \chi)$ of imaginary part γ not more than H in absolute value lies on the line $\Re s = 1/2$. We get

$$|J_m(\chi, x)| \leq \frac{1}{2}\left(\sum_{\substack{\rho \in Z(\chi), \\ |\gamma| \leq H}} \frac{2x^{-1/2}|c_m(\kappa, \rho)|}{|\rho(1-\rho)|} + \sum_{\substack{\rho \in Z(\chi), \\ |\gamma| > H}} \frac{(x^{-1/2} + 1)|c_m(\kappa, \rho)|}{|\rho(1-\rho)|} \right)$$

since one of $x^{\beta-1}$ or $x^{-\beta}$ is not more than $x^{-1/2}$. We use $|c_m(\kappa, \rho)| \leq 1$ for the first sum, getting a contribution that adds up, when summing over all characters, to $\varphi(q)U(q, H)$. We use (16) to bound $|c_m(\kappa, \rho)|$ in the second summand, together with Lemma 9.1 to write:

$$\sum_{\substack{\rho \in Z(\chi), \\ |\gamma| > H}} \frac{1}{|\gamma|^{m+2}} \leq (m+2) \int_H^\infty (N(t, \chi) - N(H, \chi)) \frac{dt}{t^{m+3}}$$

$$\leq -\frac{\log\left(\frac{qH}{2\pi e}\right)}{\pi H^{m+1}} + \frac{C_2 \log(qH) + C_3}{H^{m+2}}$$
$$+ (m+2) \int_H^\infty \left(\frac{t}{\pi} \log\left(\frac{qt}{2\pi e}\right) + C_2 \log(qt) + C_3\right) \frac{dt}{t^{m+3}}$$

20

After some integration by parts and some shuffling, we reach the upper bound

$$\frac{\log\left(\frac{qH}{2\pi e}\right)}{(m+1)\pi H^{m+1}} + \frac{2C_2\log(qH) + 2C_3 + C_2 + \frac{m+2}{\pi(m+1)^2}}{H^{m+2}}.$$

As a consequence, we find that, under $\mathrm{GRH}(q,H)$, we have

$$\frac{1}{\varphi(q)}\sum_{\chi \bmod q}|J_m(\chi,x)| \leq \frac{U(q,H)}{\sqrt{x}} + e^{\frac{1}{24m}}\frac{\sqrt{2\kappa+2}}{H^2}\left(\frac{4(1+\kappa^{-1})m}{eH}\right)^m$$

$$\times (1 + x^{-1/2})\left(\frac{H\log\left(\frac{qH}{2\pi e}\right)}{(m+1)\pi} + 2C_2\log(qH) + 2C_3 + C_2 + \frac{m+2}{\pi(m+1)^2}\right).$$

We select
$$m = H/(4(1+\kappa^{-1})) \geq 10. \tag{38}$$

The Theorem follows readily.

$\square$

Proof of Theorem 1.1. We follow the above scheme but we have to bound

$$\sum_{|\gamma|\leq H}\frac{x^\beta}{|\rho(1-\rho)|}$$

differently. We select $H = \log x + \mathcal{O}(1)$ in such a way that the parameter m defined by (38) is an integer greater than 10. When there is no exceptional zero, we use the zero-free region for $L(s,\chi)$ to write

$$x^\beta \leq \exp\frac{-c\log x}{\log(qH+10)}$$

for some positive constant c. The sum over the zeros is at most $\mathcal{O}((\log q)^2)$. Hence Theorem 1.1 in this case (with a different contant c to take care of the sum over the zeros). If there is an exceptional zero, the contribution of the other zeros can still be evaluated in the same fashion, but we do have to take the contribution of this zero into account. From (17), we see that when $\rho = \beta$ is close to 1, $c_m(\kappa,\rho)$ is also close to 1: this contribution should simply be incorporated into the main term to get the same error term. $\square$

10 Proof of Theorem 1.4

We have split the proof in several lemmas.

10.1 Some technical steps

Lemma 10.1. *When $1 \leq X, q$, we have*

$$\sum_{q < p} \frac{\log p}{p} e^{-p/X} \ll \frac{X \log q}{q} e^{-q/X}$$

Proof. We simply write

$$\sum_{q < p} \frac{\log p}{p} e^{-p/X} \ll \frac{\log q}{q} e^{-q/X} \sum_{k \geq 0} e^{-k/X} \ll \frac{X \log q}{q} e^{-q/X}.$$

$\square$

Lemma 10.2. *Let $Y > 0$. We have*

$$\sum_{1 \leq n} \frac{\Lambda(n)}{n} e^{-n/Y} \ll \log(2 + Y).$$

Proof. We use an integration by parts

$$\sum_{n \geq 1} \frac{\Lambda(n)}{n} e^{-n/Y} = \sum_{n \geq 1} \frac{\Lambda(n)}{n} \frac{1}{Y} \int_n^\infty e^{-t/Y} dt = \frac{1}{Y} \int_1^\infty \sum_{n \leq t} \frac{\Lambda(n)}{n} e^{-t/Y} dt$$

$$\ll \frac{1}{Y} \int_1^\infty (\log t) e^{-t/Y} dt = \int_{1/Y}^\infty \log(uY) e^{-u} du$$

$$\ll \left[-\log(uY) e^{-u} \right]_{1/Y}^\infty + \int_{1/Y}^\infty e^{-u} \frac{du}{u}.$$

When $1/Y \geq 1$, we forget the $1/u$, while, when $1/Y < 1$, we separate the integration from $1/Y$ to 1, which we bound above by $\log Y$, and integration from 1 to ∞, which we bound above by 1. The total contribution is $\mathcal{O}(\log(2 + Y))$. $\square$

Lemma 10.3. *Let Q and X be two real parameters larger than 1. We have*

$$\sum_{\substack{1 \leq n, \\ p \geq 2}} \frac{\Lambda(n)}{n} \sum_{\substack{k \geq 2, \\ p^k \geq Q}} \frac{\log p}{p^k} e^{-np^k/X} \ll e^{-Q/X} \log(2X)/\sqrt{Q}.$$

Proof. Indeed, when n and p are fixed, we bound above $e^{-np^k/X}$ by $e^{-nQ/X}$. Further, let k_0 be the first integer larger than 2 such that $p^{k_0} \geq Q$. The remaining sum over k is $\frac{1}{p^{k_0}(1 - \frac{1}{p})}$ which is $\leq 2/\max(Q, p^2)$. Next we use

$$\sum_{p \geq 2} \frac{\log p}{\max(Q, p^2)} = \sum_{p \leq \sqrt{Q}} \frac{\log p}{Q} + \sum_{p > \sqrt{Q}} \frac{\log p}{p^2} \ll \frac{1}{\sqrt{Q}}.$$

Concerning the summation upon n, we use Lemma 10.2. The lemma follows readily. $\qquad\square$

Lemma 10.4. *When $1 \le X, q$, we have*

$$\sum_{\substack{1 \le n < p, \\ p \equiv n[q]}} \frac{\Lambda(n)}{n} \frac{\log p}{p} e^{-np/X} \ll \frac{(\log q)^2}{\varphi(q)}.$$

The summation above carries over both n and p.

Proof. We separate the treatment according to whether $p < n + 2q$ (i.e. $p = n + q$) or not. In the second case, we notice when n is fixed, with $Y = X/n$ and on using the Brun-Titchmarsh Theorem, that

$$\sum_{\substack{n+2q \le p, \\ p \equiv n[q]}} \frac{\log p}{p} e^{-p/Y} \ll \int_{n+2q}^{\infty} \sum_{\substack{p \le t, \\ p \equiv n[q]}} \log p \left(\frac{e^{-t/Y}}{Yt} + \frac{e^{-t/Y}}{t^2} \right) dt$$

$$\ll \int_{n+2q}^{\infty} \frac{t \log t}{\varphi(q) \log(t/q)} \left(\frac{e^{-t/Y}}{Yt} + \frac{e^{-t/Y}}{t^2} \right) dt$$

$$\ll \frac{\log(n+2q)}{\varphi(q) \log(2 + (n/q))} \int_{n+2q}^{\infty} \left(\frac{1}{Y} + \frac{1}{t} \right) e^{-t/Y} dt$$

$$\ll \frac{\log(n+2q)}{\varphi(q) \log(2 + (n/q))} \int_{(n+2q)/Y}^{\infty} \left(1 + \frac{1}{x} \right) e^{-x} dx$$

and, on recalling the value of Y, this quantity is finally majorized up to a multiplicative constant by

$$\frac{\log q}{\varphi(q)} \left(1 + \frac{X}{n(n+q)} \right) e^{-nq/X} \ll \frac{\log q}{\varphi(q)} \left(1 + \frac{X}{nq} \right) e^{-nq/X}. \tag{39}$$

For the summation over n, and as far as the first summand of $1 + X/(nq)$ is concerned, we employ Lemma 10.2 getting $\mathcal{O}((\log q)(\log X)/\varphi(q))$. When it comes to the second summand we discuss according to whether $n > X/q$ or not. When $n \le X/q$, the contribution is

$$\ll \frac{\log q}{\varphi(q)} \sum_{n \ge 1} \frac{\Lambda(n)}{n^2} \frac{X}{q} e^{-X/q} \ll \frac{\log q}{\varphi(q)}.$$

When $n > X/q$, the contribution is

$$\ll \frac{\log q}{\varphi(q)} \frac{q}{X} \int_{X/q}^{\infty} \sum_{X/q < n \le t} \frac{\Lambda(n)}{n} e^{-qt/X} dt$$

$$\ll \frac{\log q}{\varphi(q)} \frac{q}{X} \int_{X/q}^{\infty} (1 + \log \frac{t}{X/q}) e^{-qt/X} dt \ll \frac{\log q}{\varphi(q)}.$$

Let us now consider the case when $p = n + q$. The contribution is

$$\ll \sum_{n \geq 1} \frac{\Lambda(n) \log(n + q)}{n(n + q)} e^{-n(n+q)/X} \ll \sum_{n \leq q} \frac{\Lambda(n) \log q}{nq} + \sum_{n > q} \frac{\Lambda(n) \log n}{n^2}$$

$$\ll \frac{(\log q)^2}{q} + \frac{\log q}{q}.$$

We could use, in the first sum, the fact that n is a prime power such that $n + q$ is also a prime, but the saving would be irrelevant in our subsequent application. $\square$

We follow the idea of [31, beginning of section 4.3] that dispenses with the transition from characters to primitive ones.

Lemma 10.5. *Let m and n be two positive integers. Let $q(mn)$ be the largest divisor of q that is prime to mn. We have*

$$\frac{1}{\varphi(q)} \sum_{\mathfrak{f}|q} \sum_{\chi \bmod^* \mathfrak{f}} \chi(m)\overline{\chi(n)} = \begin{cases} \frac{\varphi(q(mn))}{\varphi(q)} & \text{when } m \equiv n[q(mn)], \\ 0 & \text{otherwise.} \end{cases}$$

Proof. We repeat the proof, as it is a two-liner: we simply have that

$$\sum_{\mathfrak{f}|q} \sum_{\chi \bmod^* \mathfrak{f}} \chi(m)\overline{\chi(n)} = \sum_{\mathfrak{f}|q(mn)} \sum_{\chi \bmod^* \mathfrak{f}} \chi(m)\overline{\chi(n)}$$

$$= \sum_{\chi \bmod q(mn)} \chi(m)\overline{\chi(n)}$$

as required. $\square$

10.2 Analytical material

We start with a classical lemma. Its proof and statement has taken some years to find a proper shape. One can find traces of it in [19] of Landau, between equations (92) and (93), see the definition of F. It will evolve until [20, Lemma 1] to yield a bound on $\zeta'/\zeta(s)$ next to the line $\Re s = 1$. At the time, Gronwall and Landau were improving each other's bound. See also [39, section 3.9, Lemma α].

Lemma 10.6. *Let M be an upper bound for the holomorphic function F in $|s - s_0| \leq R$. Assume we know of a lower bound $m > 0$ for $|F(s_0)|$. Then*

$$\frac{F'(s)}{F(s)} = \sum_{|\rho - s_0| \leq R/2} \frac{1}{s - \rho} + \mathcal{O}^*\left(16 \frac{\log(M/m)}{R}\right)$$

for every s such that $|s - s_0| \leq R/4$ and where the summation variable ρ ranges the zeros ρ of F in the region $|\rho - s_0| \leq R/2$, repeated according to multiplicity.

Lemma 10.7. *There is a constant c such that, for any non-principal character χ modulo q, we have*

$$\frac{L'}{L}(s, \chi) \ll \log q$$

provided that

$$\Re s \geq 1 - \frac{c}{\log q}, \quad |t| \leq q$$

except for at most one of them, which we call exceptional, *and for which we have $\frac{L'}{L}(s, \chi) \ll_\varepsilon q^\varepsilon$ in the above region.*

We define, for a primitive character χ modulo q:

$$N(T, \sigma, \chi) = \#\big\{ \rho \mid L(\rho, \chi) = 0, \ |\Im \rho| \leq T, \ \Re \rho \geq \sigma \big\}. \tag{40}$$

We recall another classical lemma from [12] (better results are available).

Lemma 10.8. *We have, when $\sigma > 4/5$ and for any $\varepsilon > 0$,*

$$\sum_{\mathfrak{f} \mid q} \sum_{\chi \bmod^* \mathfrak{f}} N(T, \chi, \sigma) \ll_\varepsilon (qT)^{2(1-\sigma)+\varepsilon}.$$

10.3 Proof of Theorem 1.4

Proof of Theorem 1.4. We consider the function

$$G_q(s) = \sum_{\mathfrak{f} \mid q} \sum_{\chi \bmod^* \mathfrak{f}} \frac{L'}{L}(s, \chi) \frac{L'}{L}(s, \overline{\chi}) \tag{41}$$

where χ ranges the primitive characters modulo $\mathfrak{f}$. When $\Re s > 1$, the series converges absolutely. The proof relies on two distinct evaluations of the quantity:

$$S_q(X) = \frac{1}{2i\pi} \int_{2-i\infty}^{2+i\infty} G_q(s) X^{s-1} \Gamma(s-1) ds \tag{42}$$

where $X \geq 2$ is a parameter at our disposal. We shall select $X = q^{3/2}$ at the end of the proof.

The first evaluation is elementary and relies on the Cahen-Mellin formula $e^{-y} = \frac{1}{2i\pi} \int_{2-i\infty}^{2+i\infty} y^{-s} \Gamma(s) ds$ (valid for positive y). On using Lemma 10.5, we readily find that

$$S_q(X) = \sum_{\substack{m,n \geq 1, \\ m \equiv n [q(mn)]}} \varphi(q(mn)) \frac{\Lambda(m)\Lambda(n)}{mn} e^{-mn/X}, \tag{43}$$

which we decompose in $S_q(X) = D_q(X) + 2S_q^*(X)$, with

$$D_q(X) = \sum_{m \geq 1} \varphi(q(m)) \frac{\Lambda(m)^2}{m^2} e^{-m^2/X} \tag{44}$$

and

$$S_q^*(X) = \sum_{\substack{1 \leq n < m, \\ m \equiv n [q(mn)]}} \varphi(q(mn)) \frac{\Lambda(m)\Lambda(n)}{mn} e^{-mn/X}. \tag{45}$$

The study of $S_q^*(X)$ is tedious and is concluded at the level of inequalities (46). We decompose $S_q^*(X)$ as follows:

$$S_q^*(X) = \sum_{\substack{1 \leq n < m \leq q, \\ m \equiv n [q(mn)]}} \varphi(q(mn)) \frac{\Lambda(m)\Lambda(n)}{mn} e^{-mn/X}$$

$$+ \sum_{\substack{1 \leq n < m, \\ m > q, \\ \omega(m) \geq 2, \\ m \equiv n [q(mn)]}} \varphi(q(mn)) \frac{\Lambda(m)\Lambda(n)}{mn} e^{-mn/X}$$

$$+ \sum_{\substack{1 \leq n < m, \\ m > q, \\ \omega(m) = 1, \\ m \equiv n [q(mn)]}} \varphi(q(mn)) \frac{\Lambda(m)\Lambda(n)}{mn} e^{-mn/X}.$$

The second sum is dealt with by majorising $\varphi(q(mn))$ by $\varphi(q)$, forgetting the congruence condition and appealing to Lemma 10.3 with $Q = q$. In the third one, m is prime to q (it is a prime number $> q$). Thus Lemma 10.4 takes care of the n that are coprime with q; the joint contribution is $\mathcal{O}(\varphi(q)q^{-1/2}\log X +$

$(\log q)^2)$ which simplifies to $\mathcal{O}(\varphi(q)q^{-1/2}\log X)$. Finally

$$S_q^*(X) = \sum_{\substack{1 \le n < m \le q, \\ m \equiv n[q(mn)]}} \varphi(q(mn)) \frac{\Lambda(m)\Lambda(n)}{mn} e^{-mn/X}$$

$$+ \sum_{p^a \| q} \frac{\varphi(q)}{p^{a-1}(p-1)} \sum_{k \ge 1} \frac{\log p}{p^k} \sum_{\substack{1 \le p^k < m, \\ m > q, \\ \omega(m)=1, \\ m \equiv p^k[q/p^a]}} \frac{\Lambda(m)}{m} e^{-mp^k/X}.$$

$$+ \mathcal{O}\big(\varphi(q)q^{-1/2}\log X\big).$$

We can reuse (39) for the inner summation, of the second term above, with q/p^a instead of q. This shows that this sum is

$$\ll \sum_{p^a \| q} \frac{\log q}{p^{a-1}(p-1)} \sum_{k \ge 1} \frac{\log p}{p^k}\Big(1 + \frac{Xp^a}{qp^k}\Big) e^{-p^{k-a}q/X}$$

$$\ll \sum_{p^a \| q} \frac{\log q}{p^{a-1}(p-1)} \frac{\log p}{p}\Big(1 + \frac{Xp^a}{q}\Big) \ll \log q + \frac{X\log^2 q}{q}.$$

In the (temporary) main term of $S_q^*(X)$, at least one of m or n has a non-trivial gcd with q. The contribution of m prime to q is, once n is fixed,

$$\ll \log q \sum_{1 \le k \le q/q(n)} \frac{1}{n + kq(n)} \ll \frac{\log^2 q}{q(n)},$$

and thus $S_q^*(X)$ is equal to

$$\sum_{\substack{1 \le n < m \le q, \\ m \equiv n[q(mn)], \\ (m,q)>1}} \varphi(q(mn)) \frac{\Lambda(m)\Lambda(n)}{mn} e^{-mn/X} + \mathcal{O}\Big(\frac{\varphi(q)}{q^{1/2}}\log X + \log^3 q + \frac{X}{q}\log^2 q\Big).$$

We bound above the coefficient $e^{-mn/X}$ by 1 in the first sum. We next check

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that:

$$\sum_{\substack{1\le n<m\le q, \\ m\equiv n[q(m)], \\ (m,q)>1,(n,q)=1}} \varphi(q(m))\frac{\Lambda(m)\Lambda(n)}{mn} \ll \sum_{p^a\|q}\frac{\varphi(q)\log p}{p^{a-1}(p-1)}\sum_{\substack{k\ge 1, \\ p^k\le q}}\sum_{\substack{1\le n<p^k, \\ m\equiv n[q/p^a], \\ (n,q)=1}}\frac{\Lambda(n)}{np^k}$$

$$\ll \sum_{p^a\|q}\frac{\varphi(q)\log p}{p^{a-1}(p-1)}\sum_{\substack{k\ge 1, \\ p^k\le q}}\sum_{\substack{1\le n<p^k, \\ m\equiv n[q/p^a], \\ (n,q)=1}}\frac{\Lambda(n)}{n(n+qp^{-a})}$$

$$\ll \sum_{p^a\|q}\frac{\varphi(q)\log p}{qp^{-1}(p-1)}\sum_{\substack{k\ge 1, \\ p^k\le q}}\sum_{1\le n<p^k}\frac{\Lambda(n)}{n} \ll \log^2 q.$$

We are left with the contribution of n that have a non-trivial gcd with q. We start with the case $(m,n)=1$. We find that

$$\sum_{\substack{p_1^a\|q, \\ p_2^b\|q, \\ p_1\ne p_2}}\frac{\varphi(q)\log p_1\log p_2}{p_1^{a-1}p_2^{b-1}(p_2-1)(p_1-1)}\sum_{\substack{k\ge 1, \\ p_1^k\le q}}\sum_{\substack{\ell\ge 1, \\ p_2^\ell\le q, \\ p_1^k\equiv p_2^\ell[qp_1^{-a}p_2^{-b}]}}\frac{1}{p_2^\ell p_1^k}$$

$$\ll \sum_{\substack{p_1^a\|q, \\ p_2^b\|q, \\ p_1\ne p_2}}\frac{\varphi(q)\log p_1\log p_2}{p_1^{a-1}p_2^{b-1}(p_2-1)(p_1-1)}\sum_{\substack{k\ge 1\ \ell\ge 1 \\ p_2^\ell<p_1^k\le q, \\ p_1^k\equiv p_2^\ell[qp_1^{-a}p_2^{-b}]}}\sum\frac{1}{p_2^\ell qp_1^{-a}p_2^{-b}} \ll (\log q)^3.$$

The contribution with $p_2=p_1$ is even smaller. Thus

$$S_q^*(X) \ll (\log q)^3 + q\varphi(q)X^{-1}\log q + \varphi(q)q^{-1/2}\log X + Xq^{-1}\log^2 X. \quad (46)$$

With $X=q^{3/2}$, we find that $S_q^*(q^{3/2}) \ll \sqrt{q}\log^2 q$. The main term $D_q(X)$, with $X=q^{3/2}$, is much easier to simplify:

$$D_q(X) = \sum_{m\le\sqrt{q}}\varphi(q(m))\frac{\Lambda(m)^2}{m^2}e^{-m^2/X} + \mathcal{O}(\varphi(q)q^{-1/2})$$

$$= \sum_{m\le\sqrt{q}}\varphi(q(m))\frac{\Lambda(m)^2}{m^2} + \mathcal{O}(\varphi(q)q^{-1/2})$$

$$= \sum_{m\ge 1}\varphi(q(m))\frac{\Lambda(m)^2}{m^2} + \mathcal{O}(\varphi(q)q^{-1/2}).$$

The second evaluation of $S_q(X)$ is analytical and runs as follows.

On selecting $\sigma = 9/10$, $\varepsilon = 1/10$ and $T = q$ in Lemma 10.8, we see that at most $\mathcal{O}(q^{3/5})$ characters modulo a divisor of q have a zero in the region

$$|\Im\rho| \leq q, \ \Re\rho \geq 9/10. \tag{47}$$

We call these characters *bad* and the other set, the one of *good* characters. We shift the line of integration in (42)

- To $\Re s = 9/10$ and $|\Im s| \leq q$ when χ belongs to the good set;

- To $\Re s = 1 - c/\log q$ and $|\Im s| \leq q$ when χ belongs to the bad set; Here c is the constant from Lemma 10.7.

For a bad character, Lemma 10.7 gives the necessary material, even for the exceptional one. For a good character, Lemma 10.6 gives us that

$$L'/L(s, \chi) \ll \log q \tag{48}$$

when $\sigma \geq 9/10$ and $|t| \leq q$. A line shifting gives us that

$$S_q^*(X) = \sum_{1 < \mathfrak{f}|q} \sum_{\chi \bmod^* \mathfrak{f}} \left| \frac{L'}{L}(1, \chi) \right|^2$$
$$+ \mathcal{O}\left((\log X)^2 + q^{3/5} \log^2 q + \varphi(q) X^{-1/10} (\log q)^2 \right). \tag{49}$$

(The $\mathcal{O}((\log X)^2)$ comes from the principal character; the exponential decay on the Γ-function in vertical strips ensures that the contribution of the vertical segments is negligible).

We have reached

$$\sum_{1 < \mathfrak{f}|q} V_2^\flat(\mathfrak{f}) = \sum_{m \geq 1} \varphi(q(m)) \frac{\Lambda(m)^2}{m^2} + \mathcal{O}(q^{17/20} \log q).$$

and we reduce $\mathcal{O}(q^{17/20} \log q)$ to $\mathcal{O}(q^{9/10})$ since we anyway did not try to minimize the exponent of q. To ease typographical work, we momentarily define

$$C_0 = \sum_{m \geq 1} \frac{\Lambda(m)^2}{m^2}.$$

An easy discussion leads to

$$\sum_{m \geq 1} \varphi(q(m)) \frac{\Lambda(m)^2}{m^2} = \varphi(q) C_0 - \varphi(q) \sum_{p^a \| q} \left(1 - \frac{1}{p^a - p^{a-1}} \right) \frac{\log^2 p}{p^2 - 1}$$
$$= \varphi(q) C_0 - \varphi(q) \sum_{p^a \| q} \frac{p^a - p^{a-1} - 1}{p^a - p^{a-1}} \frac{\log^2 p}{p^2 - 1}.$$

Moebius inversion formula gives us

$$V_2^{\flat}(q) = \varphi(q)^* C_0 - \sum_{\mathfrak{f}|q} \mu(q/\mathfrak{f})\varphi(\mathfrak{f}) \sum_{p^b\|\mathfrak{f}} \frac{p^b - p^{b-1} - 1}{p^b - p^{b-1}} \frac{\log^2 p}{p^2 - 1}.$$

$$= \varphi(q)^* C_0 - \sum_{p^b|q} \frac{\log^2 p}{p^2 - 1} \sum_{p^b\|\mathfrak{f}|q} \mu(q/\mathfrak{f})\varphi(\mathfrak{f}) \frac{p^b - p^{b-1} - 1}{p^b - p^{b-1}}.$$

Concerning this last summand, we distinguish two cases according to whether $p^2|q$ or not. Let $a \geq 1$ be the power of p in q. When $a = 1$, we have forcibly $b = 1$ above and the sum over $\mathfrak{f}$ is

$$\sum_{p|\mathfrak{f}|q} \mu(q/\mathfrak{f})\varphi(\mathfrak{f}/p)(p - 2) = (p - 2)\varphi^*(q/p) = \varphi^*(q).$$

When $a \geq 2$, we have either $b = a - 1$ or $b = a$ and writing $\mathfrak{f} = p^b\mathfrak{f}'$ and $q = p^a q'$, the sum over $\mathfrak{f}$ is

$$-\sum_{\mathfrak{f}'|q'} \mu(q'/\mathfrak{f}')\varphi(\mathfrak{f}'p^{a-1}) \frac{p^{a-1} - p^{a-2} - 1}{p^{a-1} - p^{a-2}} + \sum_{\mathfrak{f}'|q'} \mu(q'/\mathfrak{f}')\varphi(\mathfrak{f}'p^a) \frac{p^a - p^{a-1} - 1}{p^a - p^{a-1}}$$

$$= \varphi^*(q')(p^a - p^{a-2}) = \varphi^*(q)\frac{p^2 - 1}{(p-1)^2} = \varphi^*(q)\frac{p+1}{p-1}$$

since $\varphi^*(p^a) = p^{a-2}(p - 1)^2$ as soon as $a \geq 2$. Our result is proved. $\qquad\square$

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