CENTRAL VALUES OF DERIVATIVES OF DIRICHLET L-FUNCTIONS

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Abstract. Let $\mathcal{C}_q^+$ be the set of even, primitive Dirichlet characters (mod $q$). Using the mollifier method we show that $L(\frac{1}{2}, \chi) \neq 0$ for at least half of the characters $\chi \in \mathcal{C}_q^+$. Here, $L(s, \chi)$ is the Dirichlet $L$-function associated to the character $\chi$. This result was previously known to hold for a third of the $\chi \in \mathcal{C}_q^+$. In addition, we show that almost all the characters $\chi \in \mathcal{C}_q^+$ satisfy $L^{(k)}(\frac{1}{2}, \chi) \neq 0$ when $k$ and $q$ are large.

1. Introduction & Statement of the Main Result

An important topic in number theory is the behavior of families of $L$-functions and their derivatives inside the critical strip. In particular, questions concerning the order of vanishing of $L$-functions at special points on the critical line have received a great deal of attention. In the case of Dirichlet $L$-functions, it is widely believed that $L(\frac{1}{2}, \chi) \neq 0$ for all primitive characters $\chi$. For quadratic characters $\chi$, this appears to have been first conjectured by Chowla; he states this as problem 3 in chapter 8 of [3]. Though a proof of the non-vanishing of Dirichlet $L$-functions at the central point $s = 1/2$ has remained elusive, there has been considerable progress in showing that $L(\frac{1}{2}, \chi)$ is very often non-zero within various families of characters $\chi$. In [10], Iwaniec and Sarnak show that at least 1/3 of Dirichlet $L$-functions in the family of primitive characters, to a large modulus $q$, do not vanish at the central point. This improves upon earlier work of Balasubramanian and Murty [1]. Soundararajan [15] has shown that at least 7/8 of the central values in the family of quadratic Dirichlet $L$-functions are non-zero. More recently, Baier and Young [2] consider the family of Dirichlet $L$-functions associated to cubic and sextic characters and show that infinitely many (though not a positive proportion) of these functions are not zero at the central point.

In [14], Michel and VanderKam consider the behavior of the derivatives of completed Dirichlet $L$-functions, $\Lambda(s, \chi)$, at the central point. (See §3, below, for a definition.) In particular, they show that for $\varepsilon > 0$ and $q$ sufficiently large depending on $\varepsilon$, the inequality

$$\sum_{\chi \equiv \chi_0 \pmod{q}} \Lambda^{(k)}(\frac{1}{2}, \chi) \neq 0$$

holds, where the proportion

$$P_k = \frac{2}{3} - \frac{1}{36k^2} - \frac{c}{k^4}$$

for some absolute constant $c > 0$. As $k$ tends to infinity, the proportion $P_k$ approaches two thirds. This is analogous to a result of Conrey [4], who shows that almost all of

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the zeros of the $k$-th derivative of the Riemann $\xi$-function are on the critical line, and to a result of Kowalski, Michel and VanderKam [13] who show that almost half of the set $\{\Lambda^{(k)}(\frac{1}{2},f)\}$ is non-zero, where $f$ runs over the set of primitive Hecke eigenforms of weight 2 relative to $\Gamma_0(q)$. This last result is best possible because half of these forms are even and half are odd. However, unlike the results in [1] and [13], the inequality in (1.1) is not best possible since it is expected that $P_k = 1$ for every positive integer $k$.

In contrast to [14], we study the behavior of the functions $L^{(k)}(s,\chi)$, the derivatives of Dirichlet $L$-functions, at $s = \frac{1}{2}$. When $k$ and $q$ are sufficiently large, we show that $L^{(k)}(\frac{1}{2},\chi) \neq 0$ for almost all of the even, primitive characters $\chi$. As is the case in [4] and [13], our result is asymptotically best possible as $k$ tends to infinity.

**Theorem 1.1.** Let $k \in \mathbb{N}$. Then, for $\varepsilon > 0$ and $q$ sufficiently large (depending on $\varepsilon$), we have

$$\sum_{\chi \pmod{q}}^{+} 1 \geq \left(P_k^* - \varepsilon\right) \cdot \sum_{\chi \pmod{q}}^{+} 1,$$

where the proportion

$$P_k^* = 1 - \frac{1}{16k^2} - \frac{c}{k^4}$$

for some absolute constant $c > 0$. In particular, $P_1^* \geq .7544$, $P_2^* \geq .9083$, $P_3^* \geq .9642$, $P_4^* \geq .9853$, $P_5^* \geq .9935$, and $P_{25}^* \geq .9999$.

Theorem 1.1 confirms a prediction of Conrey and Snaith which arises from the $L$-functions Ratios Conjectures (see §8.1 of [8]). Their heuristic is based upon studying the behavior of the mollified moments of the derivatives of the Riemann zeta-function in $t$-aspect which they conjecture should behave similarly to the mollified moments of the derivatives of Dirichlet $L$-functions at the central point in $q$-aspect. This is in agreement with the conjectures of Keating and Snaith [11] [12] that suggest that both of these families of $L$-functions, the Riemann zeta-function in $t$-aspect and Dirichlet $L$-functions in $q$-aspect, should have the same underlying “unitary” symmetry and so their (mollified) moments should behave similarly. See [5] for a detailed discussion of these ideas. In particular, our Proposition 2.2 is a $q$-analogue of a result of Conrey and Ghosh [1] who computed the mollified moments of the derivatives of the Riemann zeta-function on the critical line.

We remark that Theorem 1.1 does not improve upon the main result of [14]. In fact, for $k \in \mathbb{N}$, the zeros of the functions $L^{(k)}(s,\chi)$ and $\Lambda^{(k)}(s,\chi)$ are expected to behave quite differently. To illustrate this point, let $\chi$ be a primitive character and assume that the Riemann Hypothesis (RH) holds for the function $L(s,\chi)$. Then all the non-trivial zeros of $L(s,\chi)$ and all the zeros of $\Lambda(s,\chi)$ lie on the critical line $\Re s = \frac{1}{2}$. In addition, $L(s,\chi)$ has an infinite number of trivial zeros on the negative real axis. Since both $L(s,\chi)$ and $\Lambda(s,\chi)$ are entire functions, this distinction has a profound effect on the distribution of the zeros of their derivatives. The reason for this is the following classical result from the theory of entire functions: *If $F(s)$ is an entire function, then the zeros of $F'(s)$ lie within the convex hull of the zeros of $F(s)$. Under the RH for $L(s,\chi)$, this implies that all the zeros of $\Lambda^{(k)}(s,\chi)$ lie on the line $\Re s = \frac{1}{2}$*. In contrast, the zeros of $L^{(k)}(s,\chi)$ are forced to lie in the half-plane $\Re s \leq \frac{1}{2}$ and it is very likely the case that

\[^1\text{See equation (7) of [6].}\]

none of these zeros lie on the critical line. In particular, it is reasonable to conjecture that $L^{(k)}(\frac{1}{2}, \chi) \neq 0$ for all primitive characters $\chi$ and all $k \in \mathbb{N}$. However, if $\chi$ is an even, real-valued (i.e. quadratic), primitive character, then the functional equation for $L(s, \chi)$ states that $\Lambda(s, \chi) = \Lambda(1 - s, \chi)$. It follows from this that $\Lambda^{(k)}(\frac{1}{2}, \chi) = 0$ whenever $k$ is odd. Thus, the analogous conjecture for $\Lambda^{(k)}(\frac{1}{2}, \chi)$ fails for infinitely many characters $\chi$.

1.1. **Notation & Conventions.** We say a Dirichlet character $\chi \pmod{q}$ is even if $\chi(-1) = 1$. We let $\mathcal{C}_q$ denote the set of primitive characters $\pmod{q}$ and let $\mathcal{C}_q^+$ denote the subset of characters in $\mathcal{C}_q$ which are even. We put $\varphi^+(q) = \frac{1}{2} \varphi(q)$ where

$$\varphi^*(q) = \sum_{k \leq q} \varphi(k) \mu\left(\frac{q}{k}\right) = |\mathcal{C}_q|;$$

the proof of this appears in Lemma 4.1, below. It is not difficult to show that $|\mathcal{C}_q^+| = \varphi^+(q) + O(1)$. In addition, we write $\sum_{\chi \pmod{q}}^*$ to indicate that the summation is restricted to $\chi \in \mathcal{C}_q^+$ and we write $\sum_{a \pmod{q}}^*$ and $\sum_n^*$ to indicate that the summation is restricted to the residues $a \pmod{q}$ which are coprime to $q$ and to $n$ which are relatively prime to $q$, respectively.

2. **The Mollified Moments of $L^{(k)}(\frac{1}{2}, \chi)$**

As may be expected, we prove Theorem 1.1 by computing certain mollified first and second moments of $L^{(k)}(\frac{1}{2}, \chi)$ over the characters $\chi \in \mathcal{C}_q^+$ and then we use Cauchy’s inequality.

To each character $\chi \in \mathcal{C}_q^+$ we associate the function

$$M(\chi) = M(\chi, P, y) := \sum_{n \leq y} \mu(n) \chi(n) \frac{P\left(\frac{\log y/n}{\log y}\right)}{\sqrt{n}}, \tag{2.1}$$

where $P$ is an arbitrary polynomial satisfying the conditions $P(0) = 0$ and $P(1) = 1$. The purpose of the function $M(\chi)$ is to smooth out or “mollify” the large values of $L^{(k)}(\frac{1}{2}, \chi)$ as we average over the $\chi \in \mathcal{C}_q^+$. If we let

$$S_1(k, q) = \sum_{\chi \pmod{q}}^+ L^{(k)}(\frac{1}{2}, \chi) M(\chi) \tag{2.2}$$

and

$$S_2(k, q) = \sum_{\chi \pmod{q}}^+ |L^{(k)}(\frac{1}{2}, \chi)|^2 |M(\chi)|^2, \tag{2.3}$$

then Cauchy’s inequality implies that

$$\sum_{\chi \pmod{q}}^+ 1 \geq \frac{|S_1(k, q)|^2}{S_2(k, q)}. \tag{2.4}$$

Thus, we require a lower bound for $|S_1(k, q)|$ and an upper bound for $S_2(k, q)$. Such estimates are provided by the following propositions.

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\[\text{We can show that if } q \text{ is sufficiently large, then the only zeros of } L'(s, \chi) \text{ on the critical line are the multiple zeros of } L(s, \chi). \text{ However, it is believed that the zeros of } L(s, \chi) \text{ are simple.}\]
Proposition 2.1. Let $k$ be a positive integer. Then, for $y = q^\vartheta$ and $0 < \vartheta < 1$, we have

$$S_1(k, q) = (-1)^k \varphi^+(q) P(1) \log^k q \left(1 + O\left(\frac{1}{\log q}\right)\right),$$

where the implied constant depends on $\vartheta$ and $k$.

Proposition 2.2. Let $k$ be a positive integer and $\varepsilon > 0$ be arbitrary. Then, for $y = q^\vartheta$ and $0 < \vartheta < \frac{1}{2}$, we have

$$S_2(k, q) = C_k(\vartheta) \varphi^+(q) \log^k q \left(1 + O\left(\frac{1}{\log q}^{1-\varepsilon}\right)\right),$$

where

$$C_k(\vartheta) = \vartheta - \frac{1}{2k+1} \int_0^1 P'(x)^2 \, dx + \frac{1}{2} + \vartheta - \frac{1}{2k-1} \int_0^1 P(x)^2 \, dx,$$

and the implied constant depends on $\vartheta$, $\varepsilon$, and $k$.

It is clear from (2.4) and the propositions that in order to prove Theorem 1.1 we need to choose the polynomial $P$, for each $k \geq 1$, which minimizes the constant $C_k(\vartheta)$. This is done in §6. It turns out that except for a term which is exponentially small (as a function of $k$), the optimal choice of $P$ is independent of the choice of $\vartheta$. This is not surprising, since similar phenomena have been observed when mollifying high derivatives of the Riemann zeta-function and the Riemann $\xi$-function on the critical line, and also when mollifying high derivatives of families of $L$-functions at the central point (see [4, 6, 13, 14]).

3. Proof of Proposition 2.1

In this section we establish Proposition 2.1. For $\chi \in \mathcal{C}_q^+$, the Dirichlet $L$-function, $L(s, \chi)$, associated to $\chi$ satisfies the functional equation

$$\Lambda(s, \chi) := \left(\frac{q}{\pi}\right)^{s/2} \Gamma\left(\frac{s}{2}\right) L(s, \chi) = \varepsilon_\chi \Lambda(1-s, \overline{\chi}),$$

where $\varepsilon_\chi = \tau(\chi) q^{-1/2}$ and $\tau(\chi)$ is the Gauss sum

$$\tau(\chi) = \sum_{a \pmod{q}} \chi(a) e\left(\frac{a}{q}\right) ; \quad e(x) = e^{2\pi ix}.$$

Note that $|\varepsilon_\chi| = 1$ and, since $\chi$ is even, $\overline{\tau(\chi)} = \tau(\overline{\chi})$.

The result we require is implicit in [14] (see §3, page 135) where it is shown that

$$\sum_{\chi \pmod{q}}^\chi \Lambda^{(k)}(\frac{1}{2}, \chi) M(\chi) = \varphi^+(q) P(1) \Gamma(\frac{1}{2}) q^{1/2} \log^k q \left(1 + O\left(\frac{1}{\log q}\right)\right)$$

It follows from the functional equation for $\Lambda(s, \chi)$ that the quantity $\mathcal{L}(P_k)$ in §3 of [14] is equal to

$$2 \sum_{\chi \pmod{q}}^\chi \Lambda^{(k)}(\frac{1}{2}, \chi) M(\chi).$$
for \( k \in \mathbb{N} \) and \( 0 < \vartheta < 1 \). Here \( \hat{q} = \sqrt{q/\pi} \) and the implied constant depends on \( \vartheta \).

From (3.1), we see that

\[
L(s, \chi) = H_q(s) \Lambda(s, \chi), \quad \text{where } H_q(s) = \frac{\hat{q}^{-s}}{\Gamma(\frac{s}{2})},
\]

(3.3)

A straightforward calculation shows that

\[
H_q^{(k)}(\frac{1}{2}) = (-1)^k \hat{q}^{-1/2} \log^k \hat{q} \left( 1 + O_k\left(\frac{1}{\log \hat{q}}\right)\right)
\]

(3.4)

for each \( k \in \mathbb{N} \). Now, combining (3.2), (3.3), (3.4) and using the Leibniz formula for differentiation, it follows that

\[
\sum_{\chi \pmod{q}}^{+} L^{(k)}(\frac{1}{2}, \chi) M(\chi) = \sum_{\ell=0}^{k} \binom{k}{\ell} \sum_{\chi \pmod{q}}^{+} H_q^{(\ell)}(\frac{1}{2}) \Lambda^{(k-\ell)}(\frac{1}{2}, \chi) M(\chi)
\]

\[
= (-1)^k 2^k \varphi^+(q) P(1) \log^k \hat{q} \left( 1 + O\left(\frac{1}{\log \hat{q}}\right)\right),
\]

where the implied constant depends on \( \vartheta \) and \( k \). Since \( 2 \log \hat{q} = \log q + O(1) \), we can conclude that

\[
\sum_{\chi \pmod{q}}^{+} L^{(k)}(\frac{1}{2}, \chi) M(\chi) = (-1)^k \varphi^+(q) P(1) \log^k q \left( 1 + O\left(\frac{1}{\log q}\right)\right),
\]

This establishes Proposition 2.1.

### 4. Some Preliminary Results

In this section we collect some preliminary results which we will use to establish Proposition 2.2. In what follows, \( q \) is a large positive integer and \( \alpha, \beta \in \mathbb{C} \) are taken to be small shifts satisfying \( |\alpha|, |\beta| \leq 2(\log q)^{-1} \).

Our first lemma concerns the orthogonality of primitive characters.

**Lemma 4.1.** For \((mn, q) = 1\) we have

\[
\sum_{\chi \pmod{q}}^{+} \chi(m) \chi(n) = \frac{1}{2} \sum_{\substack{d \mid m \pm n \atop r \mid d}} \mu(d) \varphi(r),
\]

where the sums for the different signs \( \pm \) are to be taken separately.

**Proof.** Let

\[
f(h) = \sum_{\chi \pmod{h}}^{*} \chi(m) \chi(n)
\]

where \( \sum^{*} \) denotes summation over primitive characters \( \chi \). Then for \((mn, q) = 1\) we have

\[
\sum_{h \mid q} f(h) = \sum_{\chi \pmod{q}} \chi(m) \chi(n) = \left\{ \begin{array}{ll} \varphi(q) & \text{if } m \equiv n \pmod{q} \\ 0 & \text{otherwise.} \end{array} \right.
\]
Using the Möbius inversion we obtain
\[ \sum_{\chi \mod q}^{*} \chi(m)\overline{\chi}(n) = f(q) = \sum_{h \mid q}^{\perp} \varphi(h)\mu(q/h). \]

It follows from this identity that
\[ |\mathcal{C}_q| = \sum_{\chi \mod q}^{*} 1 = \sum_{h \mid q} \varphi(k)\mu(\tfrac{q}{k}), \]
which justifies an above remark. Our lemma now follows by noting that
\[ \sum_{\chi \mod q}^{*} \chi(m)\overline{\chi}(n) = \sum_{\chi \mod q}^{*} \left[ 1 + \frac{\chi(-1)}{2} \right] \chi(m)\overline{\chi}(n). \]
\[ \square \]

**Lemma 4.2.** Let \( G(s) \) be an even, entire function with rapid decay as \( |s| \to \infty \) in any fixed vertical strip \( A \leq \sigma \leq B \) and with \( G(0) = 1 \). Let
\[ W_{\alpha,\beta}^\pm(x) = \frac{1}{2\pi i} \int_{(1)} G(s)H(s)g_{\alpha,\beta}^\pm(s)x^{-s}\frac{ds}{s}, \] (4.1)
where
\[ g_{\alpha,\beta}^+(s) = \frac{\Gamma(\frac{1}{2}+\alpha+s)}{\Gamma(\frac{1}{2}+\alpha)} \frac{\Gamma(\frac{1}{2}+\beta+s)}{\Gamma(\frac{1}{2}+\beta)}, \quad g_{\alpha,\beta}^-(s) = \frac{\Gamma(\frac{1}{2}-\alpha+s)}{\Gamma(\frac{1}{2}+\alpha)} \frac{\Gamma(\frac{1}{2}+\beta+s)}{\Gamma(\frac{1}{2}+\beta)}, \]
and
\[ H(s) = \frac{(\alpha+\beta)^2 - s^2}{(\frac{n+\beta}{2})^2} \quad (\alpha + \beta \neq 0). \]
Then for \( \chi_1, \chi_2 \in \mathcal{C}_q^+, \alpha \neq -\beta \) we have that
\[ L(\frac{1}{2} + \alpha, \chi_1)L(\frac{1}{2} + \beta, \chi_2) = \sum_{m,n}^{\chi_1(m)\chi_2(n)} \frac{\chi_1(m)\chi_2(n)}{m^{1/2+\alpha}n^{1/2+\beta}} W_{\alpha,\beta}^+(\frac{\pi mn}{q}) \]
\[ + \varepsilon_{\chi_1}(\varepsilon_{\chi_2} \frac{q}{\pi})^{-\alpha-\beta} \sum_{m,n}^{\chi_1(m)\chi_2(n)} \frac{\chi_1(m)\chi_2(n)}{m^{1/2-\alpha}n^{1/2-\beta}} W_{\alpha,\beta}^-(\frac{\pi mn}{q}). \]

**Some Remarks.**

(1) An admissible choice of \( G \) in the above lemma is \( G(s) = \exp(s^2) \).

(2) The purpose of the function \( H(s) \) in the above lemma is to cancel the poles of the functions \( \zeta_q(1 \pm (\alpha + \beta) + 2s) \) at \( s = \mp(\alpha + \beta)/2 \) which appear in the next lemma. This substantially simplifies our later calculations. A similar effect has been previously observed by Conrey, Iwaniec and Soundararajan (see §3 of [7]).

**Proof.** Consider the integral
\[ I_{\alpha,\beta} = \frac{1}{2\pi i} \int_{1-i\infty}^{1+i\infty} G(s)H(s) \frac{\Lambda(1/2 + \alpha + s, \chi_1)\Lambda(1/2 + \beta + s, \chi_2)}{\Gamma(\frac{1}{2}+\alpha)\Gamma(\frac{1}{2}+\beta)} \frac{ds}{s}. \]
Shifting the line of integration to \( \text{Re} \, s = -1 \) and using Cauchy’s theorem we obtain
\[
I_{\alpha, \beta} = R_0 + \frac{1}{2\pi i} \int_{-1-i\infty}^{-1+i\infty} G(s) H(s) \frac{\Lambda(1/2 + \alpha + s, \chi_1)\Lambda(1/2 + \beta + s, \chi_2)}{\Gamma(\frac{1/2 + \alpha}{2})\Gamma(\frac{1/2 + \beta}{2})} \frac{ds}{s},
\]
where \( R_0 \) is the term arising from the residue of the integrand at \( s = 0 \). Evidently,
\[
R_0 = \left( \frac{q}{\pi} \right)^{(1+\alpha+\beta)/2} L(\frac{1}{4} + \alpha, \chi_1)L(\frac{1}{4} + \beta, \chi_2).
\]
By making the change of variables \( s \) to \(-s\) and using \((3.1)\), we have that
\[
R_0 = I_{\alpha, \beta} + \frac{1}{2\pi i} \int_{1-i\infty}^{1+i\infty} G(s) H(s) \frac{\Lambda(1/2 - \alpha + s, \chi_1)\Lambda(1/2 - \beta + s, \chi_2)}{\Gamma(\frac{1/2 + \alpha}{2})\Gamma(\frac{1/2 + \beta}{2})} \frac{ds}{s}.
\]
The lemma now follows by using \((3.1)\) to express the \( \Lambda \)-functions as Dirichlet series and then integrating term-by-term.

**Lemma 4.3.** Let
\[
S_{\alpha, \beta}^+(x) = \sum_{n=1 \atop (n,q)=1}^\infty \frac{W_{\alpha, \beta}(n^2/x)}{n^{1+\alpha+\beta}} \quad \text{and} \quad S_{\alpha, \beta}^-(x) = \sum_{n=1 \atop (n,q)=1}^\infty \frac{W_{\alpha, \beta}(n^2/x)}{n^{1-\alpha-\beta}}.
\]
Then, for any \( \varepsilon > 0 \) and \( \alpha \neq -\beta \), we have that
\[
S_{\alpha, \beta}^+(x) = \zeta_q(1 + \alpha + \beta) + O(\tau(q)x^{-1/2+\varepsilon})
\]
and
\[
S_{\alpha, \beta}^-(x) = g_{\alpha, \beta}^-(0)\zeta_q(1 - \alpha - \beta) + O(\tau(q)x^{-1/2+\varepsilon}),
\]
where \( \tau(q) \) is the number of divisors of \( q \) and the function \( \zeta_q(s) \) is defined by
\[
\zeta_q(s) = \zeta(s) \prod_{p|q} \left( 1 - \frac{1}{p^s} \right).
\]

**Proof.** From \((4.1)\) we observe that
\[
S_{\alpha, \beta}^+(x) = \frac{1}{2\pi i} \int_{(1)} G(s) H(s) g_{\alpha, \beta}(s)x^s \zeta_q(1 + \alpha + \beta + 2s) \frac{ds}{s}.
\]
We now move the line of integration to \( \text{Re} \, s = -1/2 + \varepsilon \), encountering only a simple pole of the integrand at \( s = 0 \). We note that the simple pole of \( \zeta_q(1 + \alpha + \beta + 2s) \) at \( s = -(\alpha + \beta)/2 \) is canceled by a zero \( H(s) \). The residue of the integrand at \( s = 0 \) is \( \zeta_q(1 + \alpha + \beta) \). Also, the integral along the new contour is trivially \( \ll \tau(q)x^{-1/2+\varepsilon} \). This implies the first claim of the lemma. The second claim can be proved in a similar manner.

**Lemma 4.4.** Assume \( \alpha \neq -\beta \) and let
\[
\mathcal{B}(m_1, n_1; \alpha, \beta) = \sum_{\chi \pmod{q}}^+ L(\frac{s}{2} + \alpha, \chi)L(\frac{s}{2} + \beta, \chi)\chi(m_1)\overline{\chi}(n_1).
\]
Then for \((m_1, n_1) = 1\) and \((m_1n_1, q) = 1\) we have
\[
\mathcal{B}(m_1, n_1; \alpha, \beta) = \frac{\varphi^+(q)}{\sqrt{m_1n_1}} \left( \frac{\zeta_q(1 + \alpha + \beta)}{m_1^{\beta/2}n_1^{\alpha/2}} + \left( \frac{q}{\pi} \right)^{-\alpha-\beta} g_{\alpha, \beta}^-(0)\zeta_q(1 - \alpha - \beta) \right)
+ O(\beta(m_1, n_1) + q^{1/2+\varepsilon}),
\]
where $\beta(m_1, n_1)$ satisfies
\[
\sum_{m_1,n_1 \leq y} \frac{\beta(m_1, n_1)}{\sqrt{m_1n_1}} \ll y^{1/2+\varepsilon}.
\]

**Proof.** With $\chi_1 = \chi$, $\chi_2 = \overline{\chi}$, Lemma 4.1 and Lemma 4.2 imply that
\[
\mathcal{B}(m_1, n_1; \alpha, \beta) = \frac{1}{2} \sum_{q \mid d \tau r} \mu(d) \varphi(r) \sum_{r \mid mn_1 \pm nn_1} W_{\alpha,\beta}^+ \left( \frac{\pi mn}{q} \right) m_1^{1/2+\alpha} n_1^{1/2+\beta} + \frac{1}{2} \sum_{q \mid d \tau r} \mu(d) \varphi(r) \sum_{r \mid mn_1 \pm nn_1} W_{\alpha,\beta}^- \left( \frac{\pi mn}{q} \right) m_1^{1/2-\alpha} n_1^{1/2-\beta}, \tag{4.2}
\]
where $\sum^*$ denotes summation over all $(mn, q) = 1$. The main contribution to $\mathcal{B}(m_1, n_1; \alpha, \beta)$ comes from the diagonal terms $mn_1 = n_1$ and $mn_1 = nn_1$ in the first and second sums on the right-hand side of (4.2), respectively. For $(m_1, n_1) = 1$, this contribution is
\[
\varphi^+(q) \left( \sum_{mn_1 = n_1} W_{\alpha,\beta}^+ \left( \frac{\pi mn}{q} \right) m_1^{1/2+\alpha} n_1^{1/2+\beta} + \frac{1}{2} \frac{1}{\pi} \sum_{mn_1 = n_1} W_{\alpha,\beta}^- \left( \frac{\pi mn}{q} \right) m_1^{1/2-\alpha} n_1^{1/2-\beta} \right) + O(q^{1/2+\varepsilon}).
\]
All the other terms in (4.2) contribute at most
\[
\beta(m_1, n_1) = \sum_{mn_1 \neq n_1} \frac{(mn_1 \pm nn_1, q)}{\sqrt{mn}} \left| W_{\alpha,\beta}^\pm \left( \frac{\pi mn}{q} \right) \right|.
\]
Using the estimate $|W_{\alpha,\beta}^\pm(x)| \ll (1 + x)^{-1}$ one can show that (see [10], Section 4)
\[
\sum_{m_1,n_1 \leq y} \frac{\beta(m_1, n_1)}{\sqrt{m_1n_1}} \ll y^{1/2+\varepsilon} \log y q^4.
\]
The lemma now follows from the above estimates. \hfill \square

**Lemma 4.5.** For $d \leq y$ and $(d, q) = 1$, let
\[
S_j(d) = \sum_{n \leq y/d} \frac{\mu(n)}{n} (\log n)^j \left( \frac{\log y}{dn} \right) P \left( \frac{\log y}{dn} \right).
\]
Then $S_j(d) = M_j(d) + O(E_j(d))$ where
\[
M_0(d) = \frac{dq}{\varphi(dq) \log y} P^r \left( \frac{\log y/d}{\log y} \right), \quad M_1(d) = -\frac{dq}{\varphi(dq) \log y} P \left( \frac{\log y/d}{\log y} \right), \quad M_j(d) = 0 \ (j \geq 2),
\]
and
\[
E_j(d) = (\log y)^{j-2} (\log \log y)^4 \left( 1 + \frac{d^q \log y}{y^q} \right) \prod_{p \mid dq} \left( 1 + \frac{1}{p^{l-2d}} \right)^2.
\]
with \( \theta \gg 1 / \log \log y \) and \( \delta = 1 / \log \log y \).

**Proof.** This is Lemma 10 of Conrey [4]. \( \square \)

**Lemma 4.6.** Given that \( f(d) = \prod_{p \mid d} f(p) \) with \( f(p) = 1 + O(p^{-c}) \) for \( c > 0 \) and
\[
\mu(d)^2 \frac{d}{f(d)} \left( \frac{\log y}{d} \right)^j.
\]

Then we have
\[
J_j(y) = \frac{1}{j+1} \prod_p \left( 1 - \frac{1}{p} \right) \left( 1 + \frac{f(p)}{p} \right) \prod_{p \nmid q} \left( 1 + \frac{f(p)}{p} \right)^{-1} (\log y)^{j+1} + O((\log y)^j).
\]

**Proof.** This is Lemma 11 of Conrey [4]. \( \square \)

5. **Proof of Proposition 2.2**

In this section, we prove Proposition 2.2. Throughout the proof, we let \( y = q^\vartheta \) and assume that \( 0 < \vartheta < \frac{1}{2} \). We begin by considering the mollified “shifted” second moment
\[
J_{\alpha,\beta}(q) = \sum_{\chi \pmod{q}} + L(\frac{1}{2} + \alpha, \chi) L(\frac{1}{2} + \beta, \overline{\chi}) M(\chi)^2,
\]
where \( \alpha, \beta \in \mathbb{C} \) are small shifts satisfying \( |\alpha|, |\beta| \leq (\log q)^{-1} \) and \( \alpha \neq -\beta \). Applying Lemma 4.4, we have that
\[
J_{\alpha,\beta}(q) = \sum_{m,n \leq y} \sum_{\chi \pmod{q}} \mu(m) \mu(n) P\left( \frac{\log y/m}{\log y} \right) P\left( \frac{\log y/n}{\log y} \right) \mathcal{B}(m, n; \alpha, \beta)
\]
\[
= \Sigma_1(\alpha, \beta) + \Sigma_2(\alpha, \beta) + O\left( yq^{1/2+\varepsilon} \right),
\]
where
\[
\Sigma_1(\alpha, \beta) = \varphi^+(q) \zeta_q(1 + \alpha + \beta) \sum_{d \leq y} \sum_{m,n,y/d} \mu(dm) \mu(dn) d^{1+\beta} n^{1+\alpha} P\left( \frac{\log y/dm}{\log y} \right) P\left( \frac{\log y/dn}{\log y} \right)
\]
and
\[
\Sigma_2(\alpha, \beta) = \varphi^+(q) \left( \frac{q}{\pi} \right)^{-\alpha-\beta} \sum_{d \leq y} \sum_{m,n,y/d} \mu(dm) \mu(dn) d^{1-\alpha} n^{1-\beta} P\left( \frac{\log y/dm}{\log y} \right) P\left( \frac{\log y/dn}{\log y} \right).
\]

We can remove the restriction \( (m, n) = 1 \) by writing \( K_{\alpha,\beta}(q) := \Sigma_1(\alpha, \beta) + \Sigma_2(\alpha, \beta) \) as
\[
\varphi^+(q) \sum_{c,d \leq y} \frac{\mu(c) \mu(cd)^2}{c^2 d} \times
\sum_{m,n,c,d} \frac{\mu(m) \mu(n)}{mn} P\left( \frac{\log y/cdm}{\log y} \right) P\left( \frac{\log y/cdn}{\log y} \right) Z_{q,\alpha,\beta}(m, n, c),
\]
where

\[ Z_{q, \alpha, \beta}(m, n, c) = \frac{\zeta_q(1 + \alpha + \beta)}{c^2m^2n^{\alpha}} + \left( \frac{q}{\pi} \right)^{-\alpha - \beta} g_{\alpha, \beta}^-(0) \frac{\zeta_q(1 - \alpha - \beta)}{c^{-\alpha - \beta - a}m^{-a}n^{-\beta}}. \] (5.4)

Though the function \( \zeta_q(s) \) has a simple pole at \( s = 1 \), we note that \( Z_{q, \alpha, \beta}(m, n, c) \) is holomorphic in both \( \alpha \) and \( \beta \) for certain constants \( \alpha \) at \( C \). Thus, by computing the Laurent series expansion of each of the terms on the right-hand side of (5.4) about \( \alpha = \beta = 0 \). Therefore, the expressions in (5.1) and (5.3) provide an analytic continuation of the function \( J_{\alpha, \beta}(q) - K_{\alpha, \beta}(q) \) to the region \( |\alpha|, |\beta| \leq (\log q)^{-1} \); the function \( K_{0,0}(q) \) must be defined in terms of the limit

\[ Z_{q,0,0}(m, n, c) = \lim_{\alpha \to 0} \frac{q}{\pi} \left( \frac{q}{c^2mn} \right)^{\alpha} \frac{\zeta_q(1 - 2\alpha)}{m^{2\alpha}n^{-\alpha}}. \]

Moreover, by the maximum modulus principle and (5.2), we see that

\[ |J_{\alpha, \beta}(q) - K_{\alpha, \beta}(q)| \ll \varepsilon yq^{1/2+\varepsilon} \]

uniformly for \( |\alpha|, |\beta| \leq (\log q)^{-1} \). Hence, by Cauchy’s Integral Theorem,

\[ \frac{d^{2k}}{d\alpha^k d\beta^k} \left[ J_{\alpha, \beta}(q) - K_{\alpha, \beta}(q) \right]_{\alpha=\beta=0} = \frac{(k!)^2}{(2\pi)^2} \int_{\gamma\alpha} \int_{\gamma\beta} \frac{J_w, w_\beta(q) - K_{w_\alpha, w_\beta}(q)}{(w_\alpha w_\beta)^{k+1}} dw_\alpha dw_\beta \ll k, \varepsilon yq^{1/2+\varepsilon}, \]

where \( \gamma\alpha \) (resp. \( \gamma\beta \)) denotes the positively oriented circle in the complex plane centered at \( \alpha = 0 \) (resp. \( \beta = 0 \)) with radius \( (\log q)^{-1} \). Thus, we have shown that

\[ S_2(k, q) = \frac{d^{2k}}{d\alpha^k d\beta^k} K_{\alpha, \beta}(q) \bigg|_{\alpha=\beta=0} = O_k, \varepsilon (yq^{1/2+\varepsilon}). \] (5.5)

Writing

\[ \frac{d^{2k}}{d\alpha^k d\beta^k} Z_{q, \alpha, \beta}(m, n, c) \bigg|_{\alpha=\beta=0} = \sum_{h+i+j \leq 2k+1} \left( a_{h, i, j}(\log c)^h + b_{h, i, j}(\log q/c)^h \right) (\log m)^i (\log n)^j \]

for certain constants \( a_{h, i, j} \) and \( b_{h, i, j} \), we see that

\[ \frac{d^{2k}}{d\alpha^k d\beta^k} K_{\alpha, \beta}(q) \bigg|_{\alpha=\beta=0} = \varphi^+(q) \sum_{h+i+j \leq 2k+1} \sum_{cd \leq y}^* \left( a_{h, i, j}(\log c)^h + b_{h, i, j}(\log cq)^h \right) \frac{\mu(c)\mu(cd)^2}{c^2d} S_i(cd) S_j(cd), \] (5.6)

where \( S_i \) and \( S_j \) are defined in Lemma 4.5. It follows from Lemma 4.5 that

\[ S_i(cd) \ll_i \frac{cdq}{\varphi(cdq)} (\log y)^{i-1}, \]
from which it can be seen that the contribution of the terms with \( h + i + j \leq 2k \) to the sum on the right-hand side of (5.6) is

\[
\ll_k (\log q)^{2k-1} q \varphi^+(q)/\varphi(q) \ll_{k, \varepsilon} \varphi^+(q)(\log q)^{2k-1+\varepsilon}
\]

since \( q/\varphi(q) \ll \log \log q \). It remains to consider the contribution of the terms with \( h + i + j = 2k + 1 \). In the notation of Lemma 4.5, it can be shown that

\[
\sum_{cd \leq y}^* \frac{S_i(cd)E_j(cd)}{c^2d} \ll_{i,j,\varepsilon} (\log y)^{i+j-2+\varepsilon}
\]

and

\[
\sum_{cd \leq y}^* \frac{E_i(cd)E_j(cd)}{c^2d} \ll_{i,j,\varepsilon} (\log y)^{i+j-3+\varepsilon}.
\]

Hence the contribution of the error terms \( E_i \) and \( E_j \), arising from Lemma 4.5, to the terms in (5.6) with \( h + i + j = 2k + 1 \) is \( \ll_{k, \varepsilon} \varphi^+(q)(\log q)^{2k-1+\varepsilon} \). Thus,

\[
\frac{d^{2k}}{d\alpha^k d\beta^k} K_{\alpha,\beta}(q) \bigg|_{\alpha=\beta=0} = \varphi^+(q) \sum_{h+i+j=2k+1} \sum_{cd \leq y}^* \left( a_{h,i,j}(\log c)^h + b_{h,i,j}(\log cq)^h \right) \frac{\mu(c)\mu(cd)^2}{c^2d} M_i(cd) M_j(cd)
\]

\[+ O_{k,\varepsilon} (\varphi^+(q)(\log q)^{2k-1+\varepsilon}). \]

Since \( M_i(cd) = 0 \) for \( i > 1 \), we need only to consider the terms with \( 0 \leq i, j \leq 1 \). Moreover, the terms involving powers of \( \log c \) can be ignored, as they contribute (due to the presence of \( c^{-2} \) in the sum) an amount which is \( \ll_{k, \varepsilon} (\log q)^{2k-1+\varepsilon} \). Therefore, the above expression simplifies to

\[
\frac{d^{2k}}{d\alpha^k d\beta^k} K_{\alpha,\beta}(q) \bigg|_{\alpha=\beta=0} = T_1 + 2T_2 + T_3 + O_{k,\varepsilon} \left( \varphi^+(q)(\log q)^{2k-1+\varepsilon} \right),
\]

where

\[
T_1 = \varphi^+(q) \sum_{cd \leq y}^* b_{2k+1,0,0}(\log q)^{2k+1} \frac{\mu(c)\mu(cd)^2}{c^2d} M_0(cd)^2
\]

\[
T_2 = \varphi^+(q) \sum_{cd \leq y}^* b_{2k,1,0}(\log q)^{2k} \frac{\mu(c)\mu(cd)^2}{c^2d} M_0(cd) M_1(cd)
\]

and

\[
T_3 = \varphi^+(q) \sum_{cd \leq y}^* b_{2k-1,1,1}(\log q)^{2k-1} \frac{\mu(c)\mu(cd)^2}{c^2d} M_1(cd)^2.
\]

We first evaluate \( T_1 \). Using Lemma 4.5 we have that

\[
T_1 = \varphi^+(q) \frac{b_{2k+1,0,0}q^2(\log q)^{2k+1}}{\varphi(q)^2(\log y)^2} \sum_{cd \leq y}^* \frac{\mu(c)\mu(cd)^2d}{\varphi(cd)} P' \left( \frac{\log y/cd}{\log y} \right)^2
\]

\[= \varphi^+(q) \frac{b_{2k+1,0,0}q^2(\log q)^{2k+1}}{\varphi(q)^2(\log y)^2} \sum_{n \leq y}^* \frac{\mu(n)^2}{\varphi(n)} P' \left( \frac{\log y/n}{\log y} \right)^2.
\]
Now Lemma 4.6 implies that
\[ \sum_{n \leq y} \frac{\mu(n)^2}{n} P\left( \frac{\log n}{\log y} \right)^2 = \frac{\varphi(q)}{q} \varphi(q) \log y \frac{\varphi(q)}{\varphi(q) \log y} \int_0^1 P'(x)^2 \, dx. \]

Hence
\[ T_1 = \varphi^+(q) \frac{b_{2k+1,0} q (\log q)^{2k+1}}{\varphi(q) \log y} \int_0^1 P'(x)^2 \, dx + O_{k,\varepsilon}(\varphi^+(q)(\log q)^{2k-1+\varepsilon}). \quad (5.8) \]

Similarly, it can be shown that
\[ T_2 = -\varphi^+(q) \frac{b_{2k,1} q (\log q)^{2k}}{\varphi(q) \log y} \int_0^1 P'(x) P(x) \, dx + O_{k,\varepsilon}(\varphi^+(q)(\log q)^{2k-1+\varepsilon}) \]
\[ = -\frac{b_{2k,1} q (\log q)^{2k}}{2\varphi(q) \log y} + O_{k,\varepsilon}(\varphi^+(q)(\log q)^{2k-1+\varepsilon}), \quad (5.9) \]

and that
\[ T_3 = \varphi^+(q) \frac{b_{2k-1,1} q (\log q)^{2k-1} \log y}{\varphi(q) \log y} \int_0^1 P(x)^2 \, dx + O_{k,\varepsilon}(\varphi^+(q)(\log q)^{2k-1+\varepsilon}). \quad (5.10) \]

Thus, combining \([5.5], [5.7], [5.8], [5.9], [5.10]\) and noting that
\[ b_{2k+1,0,0} = \frac{\varphi(q)}{q(2k+1)}, \quad b_{2k,0,1} = -\frac{\varphi(q)}{2q}, \quad \text{and} \quad b_{2k-1,1,1} = \frac{\varphi(q) k^2}{2q(2k-1)}, \]

it follows that, for \(y = q^\vartheta\) and \(0 < \vartheta < \tfrac{1}{2}\),
\[ S_2(k, q) = \left( \frac{\vartheta^{-1}}{2k+1} \int_0^1 P'(x)^2 \, dx + \frac{1}{2} + \frac{\vartheta k^2}{2k-1} \int_0^1 P(x)^2 \, dx \right) \varphi^+(q)(\log q)^{2k} \]
\[ + O_{k,\varepsilon}(\varphi^+(q)(\log q)^{2k-1+\varepsilon}). \]

This completes the proof of Proposition 2.2.

6. Completing the Proof of Theorem 1.1: Optimizing the Mollifier

We are now in a position to complete the proof of Theorem 1. By Proposition 2.1 and Proposition 2.2, for \(0 < \vartheta < \frac{1}{2}\), we see that
\[ P_k^* \geq \left[ \frac{\vartheta^{-1}}{2k+1} \int_0^1 P'(x)^2 \, dx + \frac{1}{2} + \frac{\vartheta k^2}{2k-1} \int_0^1 P(x)^2 \, dx \right]^{-1}. \quad (6.1) \]

For each choice of \(k \in \mathbb{N}\), we wish to find a polynomial \(P\) satisfying \(P(0) = 1\) and \(P(1) = 0\) that maximizes the expression on the right-hand side of the above inequality. Equivalently, we wish to minimize the expression
\[ F_k(P) := \frac{\vartheta^{-1}}{2k+1} \int_0^1 P'(x)^2 \, dx + \frac{\vartheta k^2}{2k-1} \int_0^1 P(x)^2 \, dx. \quad (6.2) \]

This optimization problem is solved explicitly in §7 of [14] (and, independently, in [6]; see the remarks on page 97). We recall the argument given by Michel and Vanderkam in [14].

Using a standard approximation argument, the polynomial \(P\) can be replaced by any infinitely differentiable function with a rapidly convergent Taylor series on \([0, 1]\). In this
case, using the calculus of variations, the optimization problem can be explicitly solved and, for \( k > 0 \), the optimal choice of \( P \) is

\[
P(t) = \frac{\sinh(\Lambda t)}{\sinh(\Lambda)}, \quad \text{where} \quad \Lambda = \vartheta k \sqrt{\frac{2k+1}{2k-1}}.
\]

With this choice of \( P \), it follows that

\[
F_k(P) = \frac{\Lambda \coth \Lambda}{\vartheta (2k+1)} = \frac{k \coth \Lambda}{\sqrt{4k^2-1}}.
\]

As \( k \) gets large, the function \( \coth \Lambda \to 1 \) and so asymptotically (as \( k \to \infty \))

\[
F_k(P) = \frac{1}{2} + \frac{1}{16k^2} + O\left(\frac{1}{k^4}\right).
\]

When combined with (6.1) and (6.2), this asymptotic formula is enough to establish the estimate for \( P_k^* \) in (1.3) and, thus, completes the proof of Theorem 1.1.

### Table 1

In the table below, lower bounds for the proportions \( P_k \) and \( P_k^* \), defined in equations (1.1) and (1.2), respectively. These calculations were performed by using the expression for \( F_k(P) \) given in (6.3) with \( \vartheta = \frac{1}{2} - 1 \times 10^{-8} \).

| \( k \) | Lower bound for \( P_k \) | Lower bound for \( P_k^* \) |
|------|-----------------|-----------------|
| 1    | \( \frac{2}{3} \times 0.8216 \ldots \) | 0.7544 \ldots |
| 2    | \( \frac{2}{3} \times 0.9369 \ldots \) | 0.9083 \ldots |
| 3    | \( \frac{2}{3} \times 0.9758 \ldots \) | 0.9642 \ldots |
| 4    | \( \frac{2}{3} \times 0.9901 \ldots \) | 0.9853 \ldots |
| 5    | \( \frac{2}{3} \times 0.9956 \ldots \) | 0.9935 \ldots |
| 10   | \( \frac{2}{3} \times 0.9995 \ldots \) | 0.9993 \ldots |
| 15   | \( \frac{2}{3} \times 0.9997 \ldots \) | 0.9997 \ldots |
| 20   | \( \frac{2}{3} \times 0.9998 \ldots \) | 0.9998 \ldots |
| 25   | \( \frac{2}{3} \times 0.9999 \ldots \) | 0.9999 \ldots |

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