

## CENTRAL VALUES OF DERIVATIVES OF DIRICHLET *L*-FUNCTIONS

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Let  $\mathscr{C}_q^+$  be the set of even, primitive Dirichlet characters (mod q). Using the mollifier method, we show that  $L^{(k)}(\frac{1}{2},\chi) \neq 0$  for almost all the characters  $\chi \in \mathscr{C}_q^+$  when k and q are large. Here  $L(s,\chi)$  is the Dirichlet *L*-function associated to the character  $\chi$ .

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## 1. Introduction and 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 (see [3, Chap. 8]).

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 even 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 [16] 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 [15], Michel and VanderKam consider the behavior of the derivatives of completed Dirichlet *L*-functions,  $\Lambda(s, \chi)$ , at the central point. (See Sec. 2, below, for a definition.) In particular, they show that for  $\varepsilon > 0$  and *q* sufficiently large depending on  $\varepsilon$ , the inequality

$$\sum_{\substack{\chi \in \mathscr{C}_q^+ \\ \Lambda^{(k)}(\frac{1}{2},\chi) \neq 0}} 1 \geq (P_k - \varepsilon) \cdot \sum_{\chi \in \mathscr{C}_q^+} 1$$
(1.1)

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 the zeros of the kth derivative of the Riemann  $\xi$ -function are on the critical line, and to a result of Kowalski *et al.* [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 [4, 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 [15], 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, 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

$$\sum_{\substack{\chi \in \mathscr{C}_q^+ \\ L^{(k)}(\frac{1}{2},\chi) \neq 0}} 1 \ge (P_k^* - \varepsilon) \cdot \sum_{\chi \in \mathscr{C}_q^+} 1,$$
(1.2)

where the proportion

$$P_k^* = 1 - \frac{1}{16k^2} - \frac{c}{k^4} \tag{1.3}$$

for some absolute constant c > 0. In particular,  $P_1^* \ge 0.7544, P_2^* \ge 0.9083, P_3^* \ge 0.9642, P_4^* \ge 0.9853, P_5^* \ge 0.9935, and P_{25}^* \ge 0.9999.$ 

Theorem 1.1 confirms a prediction of Conrey and Snaith which arises from the L-functions Ratios Conjectures (see [8, §8.1]). 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<sup>a</sup> 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 [15]. 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 $_{\chi}$ ) 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. Under the RH $_{\chi}$ , one can prove that all the zeros of  $\Lambda^{(k)}(s,\chi)$  lie on the line Re  $s = \frac{1}{2}$ . In contrast, it can be shown that all but possibly a finite number of the non-real zeros of  $L^{(k)}(s,\chi)$  are forced to lie in the half-plane Re  $s \ge \frac{1}{2}$  and it is very likely the case that none of these zeros lie on the critical line.<sup>b</sup> In particular, it is reasonable to conjecture that  $L^{(k)}(\frac{1}{2},\chi) \ne 0$  for all primitive characters  $\chi$  and all  $k \in \mathbb{N}$ . However, if  $\chi$  is an even, real-valued, primitive (i.e. quadratic) 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 values of k and infinitely many characters  $\chi$ .

## 1.1. Notation and conventions

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

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

the proof of this appears in Lemma 4.1, below. It is not difficult to show that  $|\mathscr{C}_q^+| = \varphi^+(q) + O(1)$ . In addition, we write  $\sum_{\chi \pmod{q}}^+$  to indicate that the summation is restricted to  $\chi \in \mathscr{C}_q^+$  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.

<sup>&</sup>lt;sup>a</sup>See [6, Eq. (7)].

<sup>&</sup>lt;sup>b</sup>We can show that if q is sufficiently large, then the only zeros of  $L'(s, \chi)$  on the critical line are the multiple zeros of  $L(s, \chi)$ . However, it is believed that the zeros of  $L(s, \chi)$  are simple.

# 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  $\chi \in \mathscr{C}_q^+$  and then we use Cauchy's inequality.

For  $\chi \in \mathscr{C}_q^+$ , the Dirichlet L-function  $L(s,\chi)$  satisfies the functional equation

$$\Lambda(s,\chi) := \left(\frac{q}{\pi}\right)^{s/2} \Gamma\left(\frac{s}{2}\right) L(s,\chi) = \varepsilon_{\chi} \Lambda(1-s,\overline{\chi}), \qquad (2.1)$$

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

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

Note that  $|\varepsilon_{\chi}| = 1$  and, since  $\chi$  is even,  $\overline{\tau(\chi)} = \tau(\overline{\chi})$ . For each  $\chi \in \mathscr{C}_q^+$ , we let

$$M(\chi) = M(\chi, P, y) := \sum_{n \le y} \frac{\mu(n)\chi(n)}{\sqrt{n}} P\left(\frac{\log y/n}{\log y}\right),\tag{2.2}$$

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  $\chi \in \mathscr{C}_q^+$ . Since  $|\varepsilon_{\chi}L^{(k)}(\frac{1}{2},\bar{\chi})| = |L^{(k)}(\frac{1}{2},\chi)|$ , if we let

$$S_1(k,q) = \sum_{\chi \pmod{q}}^+ \varepsilon_{\chi} L^{(k)}\left(\frac{1}{2}, \bar{\chi}\right) M(\chi)$$
(2.3)

and

$$S_2(k,q) = \sum_{\chi \pmod{q}}^+ \left| L^{(k)}\left(\frac{1}{2},\chi\right) \right|^2 \left| M(\chi) \right|^2,$$
(2.4)

then Cauchy's inequality implies that

$$\sum_{\substack{\chi \pmod{q} \\ L^{(k)}(\frac{1}{2},\chi) \neq 0}}^{+} 1 \ge \frac{\left|S_1(k,q)\right|^2}{S_2(k,q)}.$$
(2.5)

Thus, we require a lower bound for  $|S_1(k,q)|$  and an upper bound for  $S_2(k,q)$ . The following propositions provide such estimates.

**Proposition 2.1.** Let  $k \in \mathbb{N}$ . Then, for  $y = q^{\vartheta}$  and  $0 < \vartheta < 1$ , we have

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

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

$$S_2(k,q) = \mathcal{C}_k(\vartheta) \ \varphi^+(q) \log^{2k} q(1 + O((\log q)^{-1+\varepsilon})),$$

where

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

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

It is clear from (2.5) 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 Sec. 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, 15]).

#### 3. Proof of Proposition 2.1

In this section we establish Proposition 2.1. The result we require is implicit in  $[15, \S3, p. 135]$  where it is shown that<sup>c</sup>

$$\sum_{\chi \pmod{q}} {}^{+} \Lambda^{(k)}\left(\frac{1}{2}, \chi\right) M(\chi) = \varphi^{+}(q) \Gamma\left(\frac{1}{4}\right) \hat{q}^{1/2} \log^{k} \hat{q} (1 + O((\log q)^{-1}))$$
(3.1)

for  $k \in \mathbb{N}$  and  $0 < \vartheta < 1$ . Here  $\hat{q} = \sqrt{q/\pi}$  and the implied constant depends on  $\vartheta$ . From (2.1), we see that

$$\varepsilon_{\chi}L(s,\bar{\chi}) = H_q(s)\Lambda(1-s,\chi), \quad \text{where } H_q(s) = \frac{\hat{q}^{-s}}{\Gamma\left(\frac{s}{2}\right)}.$$
 (3.2)

Using well-known estimates for the gamma function, it follows that

$$H_q^{(k)}\left(\frac{1}{2}\right) = (-1)^k \frac{\hat{q}^{-1/2}}{\Gamma\left(\frac{1}{4}\right)} \log^k \hat{q}(1 + O_k((\log q)^{-1}))$$
(3.3)

for each  $k \in \mathbb{N}$ . Now, combining (3.1)–(3.3) and using the Leibniz formula for differentiation, we find that

$$\sum_{\chi \pmod{q}}^{+} \varepsilon_{\chi} L^{(k)} \left(\frac{1}{2}, \bar{\chi}\right) M(\chi)$$
$$= \sum_{\chi \pmod{q}}^{+} \sum_{\ell=0}^{k} \binom{k}{\ell} H_{q}^{(\ell)} \left(\frac{1}{2}\right) (-1)^{k-\ell} \Lambda^{(k-\ell)} \left(\frac{1}{2}, \chi\right) M(\chi)$$

<sup>c</sup>It follows from the functional equation for  $\Lambda(s,\chi)$  that the quantity  $\mathscr{L}(P_k)$  in [15, §3] is equal to  $2\sum_{\chi \pmod{q}}^+ \Lambda^{(k)}(\frac{1}{2},\chi)M(\chi)$ .

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$$= \sum_{\ell=0}^{k} \binom{k}{\ell} (-1)^{k-\ell} H_q^{(\ell)} \left(\frac{1}{2}\right) \sum_{\chi \pmod{q}} {}^+ \Lambda^{(k-\ell)} \left(\frac{1}{2}, \chi\right) M(\chi)$$
  
$$= (-1)^k \sum_{\ell=0}^{k} \binom{k}{\ell} \varphi^+(q) \log^k \hat{q} (1 + O((\log q)^{-1}))$$
  
$$= (-1)^k 2^k \varphi^+(q) \log^k \hat{q} (1 + O((\log q)^{-1})),$$

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

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

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  $|\alpha|, |\beta| \leq (\log q)^{-1}$ .

Our first lemma concerns the orthogonality of primitive characters.

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

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

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

**Proof.** Let

$$f(h) = \sum_{\chi \pmod{h}}^{*} \chi(m)\overline{\chi}(n)$$

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

$$\sum_{h|q} f(h) = \sum_{\chi \pmod{q}} \chi(m)\overline{\chi}(n) = \begin{cases} \varphi(q), & \text{if } m \equiv n \pmod{q}, \\ 0, & \text{otherwise.} \end{cases}$$

Using Möbius inversion we obtain

$$\sum_{\chi \pmod{q}}^{*} \chi(m) \overline{\chi}(n) = f(q) = \sum_{\substack{h \mid q \\ h \mid m-n}} \varphi(h) \mu\left(\frac{q}{h}\right).$$

It follows from this identity that

$$\left|\mathscr{C}_{q}\right| = \sum_{\chi \pmod{q}}^{*} 1 = \sum_{k|q} \varphi(k) \mu\left(\frac{q}{k}\right),$$

which justifies an above remark. Our lemma now follows by noting that

$$\sum_{\substack{\chi(\text{mod }q)\\\chi(-1)=1}}^{*} \chi(m)\overline{\chi}(n) = \sum_{\chi(\text{mod }q)}^{*} \left[\frac{1+\chi(-1)}{2}\right] \chi(m)\overline{\chi}(n).$$

**Lemma 4.2.** Let G(s) be an even, entire function with rapid decay as  $|s| \to \infty$  in any fixed vertical strip  $A \le \sigma \le B$  and with G(0) = 1. Let

$$W_{\alpha,\beta}^{\pm}(x) = \frac{1}{2\pi i} \int_{1-i\infty}^{1+i\infty} G(s)H(s)g_{\alpha,\beta}^{\pm}(s)x^{-s}\frac{ds}{s},$$
(4.1)

where

$$g_{\alpha,\beta}^{+}(s) = \frac{\Gamma\left(\frac{1/2 + \alpha + s}{2}\right)\Gamma\left(\frac{1/2 + \beta + s}{2}\right)}{\Gamma\left(\frac{1/2 + \alpha}{2}\right)\Gamma\left(\frac{1/2 + \beta}{2}\right)},$$
$$g_{\alpha,\beta}^{-}(s) = \frac{\Gamma\left(\frac{1/2 - \alpha + s}{2}\right)\Gamma\left(\frac{1/2 - \beta + s}{2}\right)}{\Gamma\left(\frac{1/2 + \alpha}{2}\right)\Gamma\left(\frac{1/2 + \beta}{2}\right)},$$

and

$$H(s) = \frac{\left(\frac{\alpha+\beta}{2}\right)^2 - s^2}{\left(\frac{\alpha+\beta}{2}\right)^2} \quad (for \ \alpha+\beta\neq 0).$$

Then for  $\chi_1, \chi_2 \in \mathscr{C}_q^+$  and  $\alpha \neq -\beta$  we have that

$$L\left(\frac{1}{2} + \alpha, \chi_1\right) L\left(\frac{1}{2} + \beta, \chi_2\right)$$
  
=  $\sum_{m,n} \frac{\chi_1(m)\chi_2(n)}{m^{1/2+\alpha}n^{1/2+\beta}} W^+_{\alpha,\beta}\left(\frac{\pi mn}{q}\right)$   
+  $\varepsilon_{\chi_1}\varepsilon_{\chi_2}\left(\frac{q}{\pi}\right)^{-\alpha-\beta} \sum_{m,n} \frac{\overline{\chi_1}(m)\overline{\chi_2}(n)}{m^{1/2-\alpha}n^{1/2-\beta}} W^-_{\alpha,\beta}\left(\frac{\pi mn}{q}\right).$ 

**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 proof of the next lemma. This substantially simplifies our later calculations. A similar effect has been observed by Conrey *et al.* (see [7, §3]).

**Proof.** Consider the integral

$$I_{\alpha,\beta} = \frac{1}{2\pi i} \int_{1-i\infty}^{1+i\infty} G(s)H(s) \frac{\Lambda(1/2 + \alpha + s, \chi_1)\Lambda(1/2 + \beta + s, \chi_2)}{\Gamma\left(\frac{1/2 + \alpha}{2}\right)\Gamma\left(\frac{1/2 + \beta}{2}\right)} \frac{ds}{s}$$

Shifting the line of integration to Re s = -1 and using Cauchy's theorem, it follows that

$$I_{\alpha,\beta} = R_0 + \frac{1}{2\pi i} \int_{-1-i\infty}^{-1+i\infty} G(s)H(s) \frac{\Lambda(1/2 + \alpha + s, \chi_1)\Lambda(1/2 + \beta + s, \chi_2)}{\Gamma\left(\frac{1/2 + \alpha}{2}\right)\Gamma\left(\frac{1/2 + \beta}{2}\right)} \frac{ds}{s},$$

where  $R_0$  is the residue of the integrand at s = 0. Evidently,

$$R_0 = \left(\frac{q}{\pi}\right)^{(1+\alpha+\beta)/2} L\left(\frac{1}{2}+\alpha,\chi_1\right) L\left(\frac{1}{2}+\beta,\chi_2\right).$$

By making the change of variables s to -s and using (2.1), we have that

$$R_0 = I_{\alpha,\beta} + \frac{1}{2\pi i} \int_{1-i\infty}^{1+i\infty} G(s)H(s) \frac{\Lambda(1/2 - \alpha + s, \overline{\chi_1})\Lambda(1/2 - \beta + s, \overline{\chi_2})}{\Gamma\left(\frac{1/2 + \alpha}{2}\right)\Gamma\left(\frac{1/2 + \beta}{2}\right)} \frac{ds}{s}.$$

The lemma now follows by using (2.1) to express the  $\Lambda$ -functions in terms of Dirichlet series and then integrating term-by-term.

#### Lemma 4.3. Let

$$S^{+}_{\alpha,\beta}(x) = \sum_{\substack{n=1\\(n,q)=1}}^{\infty} \frac{W^{+}_{\alpha,\beta}(n^{2}/x)}{n^{1+\alpha+\beta}} \quad and \quad S^{-}_{\alpha,\beta}(x) = \sum_{\substack{n=1\\(n,q)=1}}^{\infty} \frac{W^{-}_{\alpha,\beta}(n^{2}/x)}{n^{1-\alpha-\beta}}.$$

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

$$S^+_{\alpha,\beta}(x) = \frac{1}{2\pi i} \int_{1-i\infty}^{1+i\infty} G(s)H(s)g^+_{\alpha,\beta}(s)x^s \zeta_q(1+\alpha+\beta+2s)\frac{ds}{s}$$

We now shift the line of integration left to 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

$$\mathscr{B}(m_1, n_1; \alpha, \beta) = \sum_{\chi \pmod{q}}^+ L\left(\frac{1}{2} + \alpha, \chi\right) L\left(\frac{1}{2} + \beta, \overline{\chi}\right) \chi(m_1) \overline{\chi}(n_1).$$

Then for  $(m_1, n_1) = 1$  and  $(m_1n_1, q) = 1$  we have

$$\mathscr{B}(m_1, n_1; \alpha, \beta) = \frac{\varphi^+(q)}{\sqrt{m_1 n_1}} \left( \frac{\zeta_q (1 + \alpha + \beta)}{m_1^\beta n_1^\alpha} + \left(\frac{q}{\pi}\right)^{-\alpha - \beta} g_{\alpha, \beta}^-(0) \frac{\zeta_q (1 - \alpha - \beta)}{m_1^{-\alpha} n_1^{-\beta}} \right) + O(\beta(m_1, n_1) + q^{1/2 + \varepsilon}),$$

where  $\beta(m_1, n_1)$  satisfies

$$\sum_{m_1,n_1 \le y} \frac{\beta(m_1,n_1)}{\sqrt{m_1 n_1}} \ll y q^{1/2+\varepsilon}.$$

**Proof.** With  $\chi_1 = \chi$ ,  $\chi_2 = \overline{\chi}$ , Lemmas 4.1 and 4.2 imply that

$$\mathscr{B}(m_1, n_1; \alpha, \beta) = \frac{1}{2} \sum_{q=dr} \mu(d) \varphi(r) \sum_{r|mm_1 \pm nn_1}^{\star} \frac{W_{\alpha, \beta}^+ \left(\frac{\pi mn}{q}\right)}{m^{1/2 + \alpha} n^{1/2 + \beta}} + \frac{1}{2} \left(\frac{q}{\pi}\right)^{-\alpha - \beta} \sum_{q=dr} \mu(d) \varphi(r) \sum_{r|mn_1 \pm nm_1}^{\star} \frac{W_{\alpha, \beta}^- \left(\frac{\pi mn}{q}\right)}{m^{1/2 - \alpha} n^{1/2 - \beta}}, \quad (4.2)$$

where  $\sum^{\star}$  denotes summation over all (mn, q) = 1. The main contribution to  $\mathscr{B}(m_1, n_1; \alpha, \beta)$  comes from the diagonal terms  $mm_1 = nm_1$  and  $mn_1 = nm_1$  in the first and second sums on the right-hand side of (4.2), respectively. For  $(m_1, n_1) = 1$ ,

this contribution is

$$\varphi^{+}(q) \left( \sum_{mm_{1}=nn_{1}}^{\star} \frac{W_{\alpha,\beta}^{+}\left(\frac{\pi mn}{q}\right)}{m^{1/2+\alpha}n^{1/2+\beta}} + \left(\frac{q}{\pi}\right)^{-\alpha-\beta} \sum_{mn_{1}=nm_{1}}^{\star} \frac{W_{\alpha,\beta}^{-}\left(\frac{\pi mn}{q}\right)}{m^{1/2-\alpha}n^{1/2-\beta}} \right)$$
$$= \varphi^{+}(q) \left( \frac{S_{\alpha,\beta}^{+}\left(\frac{q}{\pi m_{1}n_{1}}\right)}{n_{1}^{1/2+\alpha}m_{1}^{1/2+\beta}} + \left(\frac{q}{\pi}\right)^{-\alpha-\beta} \frac{S_{\alpha,\beta}^{-}\left(\frac{q}{\pi m_{1}n_{1}}\right)}{m_{1}^{1/2-\alpha}n_{1}^{1/2-\beta}} \right),$$

where  $S^{\pm}_{\alpha,\beta}(x)$  are defined in Lemma 4.3. By Lemma 4.3, the above expression is equal to

$$\frac{\varphi^+(q)}{\sqrt{m_1 n_1}} \left( \frac{\zeta_q (1+\alpha+\beta)}{m_1^\beta n_1^\alpha} + \left(\frac{q}{\pi}\right)^{-\alpha-\beta} g_{\alpha,\beta}^-(0) \frac{\zeta_q (1-\alpha-\beta)}{m_1^{-\alpha} n_1^{-\beta}} \right) + O(q^{1/2+\varepsilon}).$$

All the other terms in (4.2) contribute at most

$$\beta(m_1, n_1) = \sum_{mm_1 \neq nn_1} \frac{(mm_1 \pm nn_1, q)}{\sqrt{mn}} \left| W_{\alpha, \beta}^{\pm} \left( \frac{\pi mn}{q} \right) \right|$$

Using the estimate  $|W_{\alpha,\beta}^{\pm}(x)| \ll (1+|x|)^{-1}$  one can show that (see [10, Sec. 4])

$$\sum_{m_1, n_1 \le y} \frac{\beta(m_1, n_1)}{\sqrt{m_1 n_1}} \ll y q^{1/2 + \varepsilon} (\log y q)^4.$$

The lemma now follows from the above estimates.

## Lemma 4.5. Let

$$S_j(d) = \sum_{\substack{n \le y/d \\ (n,dq)=1}} \frac{\mu(n)}{n} (\log n)^j P\left(\frac{\log y/dn}{\log y}\right).$$

Then  $S_j(d) = M_j(d) + O(E_j(d))$  uniformly for  $d \leq y$ , where

$$M_0(d) = \frac{dq}{\varphi(dq)\log y} P'\left(\frac{\log y/d}{\log y}\right), \quad M_1(d) = -\frac{dq}{\varphi(dq)} P\left(\frac{\log y/d}{\log y}\right),$$

 $M_j(d) = 0$  (for  $j \ge 2$ ), and

$$E_j(d) = (\log y)^{j-2} (\log \log y)^2 (1 + (d/y)^{\theta} \log y) \prod_{p|dq} \left( 1 + \frac{1}{p^{1-2\delta}} \right)$$

with  $\theta \gg 1/\log \log y$  and  $\delta = 1/\log \log y$ .

**Proof.** Consider the Dirichlet polynomial

$$G(z) = \sum_{\substack{n \le y/d \\ (n,dq)=1}} \frac{\mu(n)}{n^{1+z}} P\left(\frac{\log y/dn}{\log y}\right).$$

Since, for  $n \leq y/d$ , we have

$$P\left(\frac{\log y/dn}{\log y}\right) = \sum_{\ell \ge 1} \frac{a_\ell}{(\log y)^\ell} (\log y/dn)^\ell = \sum_{\ell \ge 1} \frac{a_\ell \ell!}{(\log y)^\ell} \frac{1}{2\pi i} \int_{2-i\infty}^{2+i\infty} \left(\frac{y}{dn}\right)^s \frac{ds}{s^{\ell+1}},$$

we can express G(z) as

$$G(z) = \sum_{\ell \ge 1} \frac{a_{\ell} \ell!}{(\log y)^{\ell}} \frac{1}{2\pi i} \int_{2-i\infty}^{2+i\infty} \left(\frac{y}{d}\right)^s A(s+z) \frac{ds}{\zeta(1+z+s)s^{\ell+1}}$$

where

$$A(s) = \prod_{p|dq} \left(1 - \frac{1}{p^{1+s}}\right)^{-1}$$

We note that G(z) is precisely  $G_j(1+z)$  in Lemma 10 of Conrey [4] (see the first expression in the proof), with x being replaced by y/d and 1/F(j, s) being replaced by A(s-1). Using this, we obtain that

$$G^{(j)}(z) = M_j(d; z) + O(E_j(d))$$
(4.3)

,

uniformly for  $0 < |z| \ll 1/\log y$ , where

$$M_0(d;z) = A(z) \left[ z P\left(\frac{\log y/d}{\log y}\right) + \frac{1}{\log y} P'\left(\frac{\log y/d}{\log y}\right) \right]$$
$$M_1(d;z) = A(z) P\left(\frac{\log y/d}{\log y}\right), \text{ and }$$
$$M_j(d;z) = 0 \quad \text{for } j \ge 2.$$

Since G(z) and  $M_j(d; z)$  are both holomorphic in z, (4.3) also holds for z = 0. Observing that  $S_j(d) = (-1)^j G^{(j)}(0)$  and  $A(0) = dq/\varphi(dq)$ , the lemma follows.  $\Box$ 

**Lemma 4.6.** Suppose that  $f(d) = \prod_{p|d} f(p)$  with  $f(p) = 1 + O(p^{-c})$  for some c > 0 and that

$$J_j(y) = \sum_{d \le y}^* \frac{\mu(d)^2}{d} f(d) \left(\log \frac{y}{d}\right)^j.$$

Then we have

$$J_j(y) = \frac{1}{j+1} \prod_p \left(1 - \frac{1}{p}\right) \left(1 + \frac{f(p)}{p}\right) \prod_{p|q} \left(1 + \frac{f(p)}{p}\right)^{-1} (\log y)^{j+1} + O((\log y)^j).$$

**Proof.** We consider only the case where  $j \ge 1$ . The case j = 0 can be handled by following [14, proof of Lemma 3.11]. We first express  $J_j(y)$  as a complex integral, namely

$$J_j(y) = \frac{j!}{2\pi i} \int_{2-i\infty}^{2+i\infty} \sum_{(d,q)=1} \frac{\mu(d)^2 f(d)}{d^{1+s}} y^s \frac{ds}{s^{j+1}}.$$

The sum over d is

$$\prod_{p \nmid q} \left( 1 + \frac{f(p)}{p^{1+s}} \right) = B(s)\zeta(1+s),$$

where

$$B(s) = \prod_{p} \left[ \left( 1 - \frac{1}{p^{1+s}} \right) \left( 1 + \frac{f(p)}{p^{1+s}} \right) \right] \prod_{p|q} \left( 1 + \frac{f(p)}{p^{1+s}} \right)^{-1}.$$

Since  $f(p) = 1 + O(p^{-c})$  for some c > 0, B(s) is absolutely and uniformly convergent in some half-plane containing the origin. We now shift the line of integration left to Re  $s = -\delta$ , crossing a pole of order j + 2 at s = 0. Here  $\delta > 0$  is some small, fixed constant chosen so that the arithmetical factor B(s) converges absolutely for Re  $s \ge -\delta$ . Using Cauchy's theorem and the bound  $\zeta(s) \ll (1 + |t|)^{1/2+\delta}$  on the new line of integration, we obtain the estimate

$$J_j(y) = \frac{1}{j+1} B(0) (\log y)^{j+1} + O((\log y)^j).$$

The lemma now follows.

## 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

$$J_{\alpha,\beta}(q) = \sum_{\chi \pmod{q}}^{+} L\left(\frac{1}{2} + \alpha, \chi\right) L\left(\frac{1}{2} + \beta, \overline{\chi}\right) |M(\chi)|^2, \tag{5.1}$$

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

$$J_{\alpha,\beta}(q) = \sum_{m,n \le y} \frac{\mu(m)\mu(n)}{\sqrt{mn}} P\left(\frac{\log y/m}{\log y}\right) P\left(\frac{\log y/n}{\log y}\right) \mathscr{B}(m,n;\alpha,\beta)$$
$$= \Sigma_1(\alpha,\beta) + \Sigma_2(\alpha,\beta) + O(yq^{1/2+\varepsilon}), \tag{5.2}$$

where

$$\Sigma_1(\alpha,\beta) = \varphi^+(q) \, \zeta_q(1+\alpha+\beta) \sum_{d \le y}^* \sum_{\substack{m,n \le y/d \\ (m,n)=1}}^* \frac{\mu(dm)\mu(dn)}{dm^{1+\beta}n^{1+\alpha}}$$
$$\times P\left(\frac{\log y/dm}{\log y}\right) P\left(\frac{\log y/dn}{\log y}\right)$$

and

$$\Sigma_{2}(\alpha,\beta) = \varphi^{+}(q) \left(\frac{q}{\pi}\right)^{-\alpha-\beta} g_{\alpha,\beta}^{-}(0)\zeta_{q}(1-\alpha-\beta)$$
$$\times \sum_{d \leq y} * \sum_{\substack{m,n \leq y/d \\ (m,n)=1}} * \frac{\mu(dm)\mu(dn)}{dm^{1-\alpha}n^{1-\beta}} P\left(\frac{\log y/dm}{\log y}\right) P\left(\frac{\log y/dn}{\log y}\right).$$

We can remove the restriction (m,n) = 1 by writing  $K_{\alpha,\beta}(q) := \Sigma_1(\alpha,\beta) + \Sigma_2(\alpha,\beta)$  as

$$\varphi^{+}(q) \sum_{cd \leq y}^{\star} \frac{\mu(c)\mu(cd)^{2}}{c^{2}d} \times \sum_{\substack{m,n \leq y/cd \\ (mn,cdq)=1}} \frac{\mu(m)\mu(n)}{mn} P\left(\frac{\log y/cdm}{\log y}\right) P\left(\frac{\log y/cdn}{\log y}\right) Z_{q,\alpha,\beta}(m,n,c), \quad (5.3)$$

where

$$Z_{q,\alpha,\beta}(m,n,c) = \frac{\zeta_q(1+\alpha+\beta)}{c^{\alpha+\beta}m^{\beta}n^{\alpha}} + \left(\frac{q}{\pi}\right)^{-\alpha-\beta} g_{\alpha,\beta}^-(0) \frac{\zeta_q(1-\alpha-\beta)}{c^{-\alpha-\beta}m^{-\alpha}n^{-\beta}}.$$
 (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  $\beta$  in a small neighborhood of  $\alpha = \beta = 0$  (as can be seen, for instance, 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

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

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,

$$\frac{d^{2k}}{d\alpha^k d\beta^k} [J_{\alpha,\beta}(q) - K_{\alpha,\beta}(q)] \bigg|_{\alpha=\beta=0}$$
  
=  $\frac{(k!)^2}{(2\pi i)^2} \int_{\mathscr{C}_{\alpha}} \int_{\mathscr{C}_{\beta}} \frac{J_{w_{\alpha},w_{\beta}}(q) - K_{w_{\alpha},w_{\beta}}(q)}{(w_{\alpha}w_{\beta})^{k+1}} dw_{\alpha} dw_{\beta}$   
 $\ll_{k,\varepsilon} yq^{1/2+2\varepsilon},$ 

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

$$S_2(k,q) = \left. \frac{d^{2k}}{d\alpha^k d\beta^k} K_{\alpha,\beta}(q) \right|_{\alpha=\beta=0} + O_{k,\varepsilon}(yq^{1/2+2\varepsilon}).$$
(5.5)

Writing

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

for certain constants  $a_{h,i,j}$  and  $b_{h,i,j}$ , we see that

$$\frac{d^{2k}}{d\alpha^k d\beta^k} K_{\alpha,\beta}(q) \Big|_{\alpha=\beta=0}$$

$$= \varphi^+(q) \sum_{h+i+j\leq 2k+1} \sum_{cd\leq y} (a_{h,i,j}(\log c)^h + b_{h,i,j}(\log cq)^h) \frac{\mu(c)\mu(cd)^2}{c^2 d} S_i(cd) S_j(cd),$$
(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  $h + i + j \le 2k$  to the sum on the right-hand side of (5.6) is

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

The last estimate holds 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

$$\sum_{cd \le y} \star \frac{S_i(cd)E_j(cd)}{c^2d} \ll_{i,j,\varepsilon} (\log y)^{i+j-2+\varepsilon}$$

and

$$\sum_{cd \le y} \star \frac{E_i(cd)E_j(cd)}{c^2 d} \ll_{i,j,\varepsilon} (\log y)^{i+j-3+\varepsilon}$$

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,

$$\frac{d^{2k}}{d\alpha^k d\beta^k} K_{\alpha,\beta}(q) \Big|_{\alpha=\beta=0} = \varphi^+(q) \sum_{h+i+j=2k+1} \sum_{cd \le y} (a_{h,i,j}(\log c))^h + b_{h,i,j}(\log cq)^h) \frac{\mu(c)\mu(cd)^2}{c^2 d} M_i(cd) M_j(cd) + O_{k,\varepsilon}(\varphi^+(q)(\log q)^{2k-1+\varepsilon}).$$

Since  $M_i(cd) = 0$  for i > 1, we need only to consider the terms with  $0 \le i, j \le 1$ . 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

$$\frac{d^{2k}}{d\alpha^k d\beta^k} K_{\alpha,\beta}(q) \Big|_{\alpha=\beta=0} = T_1 + 2T_2 + T_3 + O_{k,\varepsilon}(\varphi^+(q)(\log q)^{2k-1+\varepsilon}), \tag{5.7}$$

where

$$T_{1} = \varphi^{+}(q) \sum_{cd \leq y} {}^{\star} b_{2k+1,0,0} (\log q)^{2k+1} \frac{\mu(c)\mu(cd)^{2}}{c^{2}d} M_{0}(cd)^{2},$$
  
$$T_{2} = \varphi^{+}(q) \sum_{cd \leq y} {}^{\star} b_{2k,1,0} (\log q)^{2k} \frac{\mu(c)\mu(cd)^{2}}{c^{2}d} M_{0}(cd) M_{1}(cd)$$

and

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

We first evaluate  $T_1$ . Using Lemma 4.5, we have that

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

Now Lemma 4.6 implies that

$$\sum_{n \le y} \frac{\mu(n)^2}{\varphi(n)} P'\left(\frac{\log y/n}{\log y}\right)^2 = \frac{\varphi(q)}{q} (\log y + O(1)) \int_0^1 P'(x)^2 dx.$$

Hence

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

Similarly, it can be shown that

$$T_{2} = -\varphi^{+}(q) \frac{b_{2k,1,0}q(\log q)^{2k}}{\varphi(q)} \int_{0}^{1} P'(x)P(x)dx + O_{k,\varepsilon}(\varphi^{+}(q)(\log q)^{2k-1+\varepsilon})$$
$$= -\varphi^{+}(q) \frac{b_{2k,1,0}q(\log q)^{2k}}{2\varphi(q)} + O_{k,\varepsilon}(\varphi^{+}(q)(\log q)^{2k-1+\varepsilon})$$
(5.9)

and that

$$T_{3} = \varphi^{+}(q) \frac{b_{2k-1,1,1}q(\log q)^{2k-1}\log y}{\varphi(q)} \int_{0}^{1} P(x)^{2} dx + O_{k,\varepsilon}(\varphi^{+}(q)(\log q)^{2k-1+\varepsilon}).$$
(5.10)

Thus, combining (5.5), (5.7)–(5.10), and noting that

$$b_{2k+1,0,0} = \frac{\varphi(q)}{q(2k+1)}, \quad b_{2k,0,1} = -\frac{\varphi(q)}{2q} \text{ and } b_{2k-1,1,1} = \frac{\varphi(q)k^2}{q(2k-1)},$$

it follows that, for  $y = q^{\vartheta}$  and  $0 < \vartheta < \frac{1}{2}$ ,

$$S_2(k,q) = \left(\frac{\vartheta^{-1}}{2k+1} \int_0^1 P'(x)^2 dx + \frac{1}{2} + \frac{\vartheta k^2}{2k-1} \int_0^1 P(x)^2 dx\right) \varphi^+(q) (\log q)^{2k} + O_{k,\varepsilon}(\varphi^+(q)(\log q)^{2k-1+\varepsilon}).$$

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 1.1. By Propositions 2.1 and 2.2, for  $0 < \vartheta < \frac{1}{2}$ , we see that

$$P_k^* \ge \left[\frac{\vartheta^{-1}}{2k+1} \int_0^1 P'(x)^2 dx + \frac{1}{2} + \frac{\vartheta k^2}{2k-1} \int_0^1 P(x)^2 dx\right]^{-1}.$$
 (6.1)

For each choice of  $k \in \mathbb{N}$ , we wish to find a polynomial P satisfying P(0) = 0and P(1) = 1 that maximizes the expression on the right-hand side of the above inequality. Equivalently, we wish to minimize the expression

$$F_k(P) := \frac{\vartheta^{-1}}{2k+1} \int_0^1 P'(x)^2 dx + \frac{\vartheta k^2}{2k-1} \int_0^1 P(x)^2 dx.$$
(6.2)

This optimization problem is solved explicitly in [15, Sec. 7] and, independently, in [6, p. 97]. We recall the argument given by Michel and Vanderkam in [15].

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

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

Table 1. In the table, lower bounds for the proportions  $P_k$  and  $P_k^*$ , defined in Eqs. (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	$\frac{2}{3} \times 0.8216$	0.7544
2	$\frac{2}{3} \times 0.9369 \dots$	0.9083
3	$\frac{2}{3} \times 0.9758$	0.9642
4	$\frac{2}{3} \times 0.9901$	0.9853
5	$\frac{2}{3} \times 0.9956 \dots$	0.9935
10	$\frac{2}{3} \times 0.9995 \dots$	0.9993
15	$\frac{2}{3} \times 0.9997 \dots$	0.9997
20	$\frac{2}{3} \times 0.9998 \dots$	0.9998
25	$\frac{2}{3} \times 0.9999 \dots$	0.9999

With this choice of P, it follows that

$$F_k(P) = \frac{\Lambda \coth \Lambda}{\vartheta(2k+1)} = \frac{k \coth \Lambda}{\sqrt{4k^2 - 1}}.$$
(6.3)

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

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

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.

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