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Zeros of Derivatives of Riemann's ξ-Function on the Critical Line

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Explicit lower bounds for the proportion of zeros of the derivatives of Riemann's ξ-function on the critical line are given. In particular, it is shown that the proportion tends to one as the order of the derivative tends to infinity.

1. INTRODUCTION

The Riemann ξ-function is given by $\xi(s) = H(s)\,\zeta(s)$, where $\zeta(s)$ is the Riemann ζ-function and $H(s) = \frac{1}{2}s(s-1)\,\pi^{-s/2}\Gamma(s/2)$. The ξ-function has the same zeros as the ζ-function in the critical strip $0 < \sigma < 1$ and the Riemann hypothesis is the conjecture that all these zeros have real part $\frac{1}{2}$. It can be shown that the Riemann hypothesis implies that all of the zeros of $\xi^{(m)}(s)$, the mth derivative of the ξ-function, have real part $\frac{1}{2}$ for any m. The object of this paper is to give explicit lower bounds for α_m, the "proportion" of zeros of $\xi^{(m)}(s)$ which have real part $\frac{1}{2}$. We define α_m as follows. Let T be a (large) positive number and set $L = \log T/2\pi$ and $U = T/L^{10}$. Let $N_m(T)$ be the number of zeros of $\xi^{(m)}(\frac{1}{2} + it)$ with $0 < t < T$ and let

$$\alpha_m = \varliminf_{T\to\infty} \frac{N_m(T+U) - N_m(T)}{UL/(2\pi)}.$$

(It follows from Lemma 2 that the zeros of $\xi^{(m)}(s)$ lie in the strip $0 < \sigma < 1$ and that the number of them in the rectangle $0 < \sigma < 1$, $T < t < T+U$ is asymptotically $UL/(2\pi)$.)

Levinson [8, 6] has obtained the bounds $\alpha_0 > 0.3474$ and $\alpha_1 > 0.71$. We prove the following

THEOREM. *Let $\phi(x)$ be any real, continuously differentiable function on*

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$[0,1]$ *which satisfies* $\phi(0)=1$ *and* $\phi'(x)=\phi'(1-x)$. *Let* $\phi_m(x)=\phi(x)(1-2x)^m$ *and let*

$$F_m(R)=2\Phi\Lambda\coth\Lambda+(e^{2R}\phi(1)^2+1)/2,$$

where $\Phi=\int_0^1 e^{2Rx}\phi_m(x)^2\,dx$, $\Phi'=\int_0^1 e^{2Rx}\phi_m'(x)^2\,dx$, $\Lambda^2=[\Phi'+R(e^{2R}\phi(1)^2-1)-R^2\Phi]/(4\Phi)$, *and* $\Lambda\geqslant 0$. *Then*

$$\alpha_m\geqslant 1-\frac{\log F_m(R)}{R}$$

for any $R\geqslant 0$.

As a consequence of this Theorem we deduce the

COROLLARY. *With* α_m *defined as above we have* $\alpha_0>0.3658$, $\alpha_1>0.8137$, $\alpha_2>0.9584$, $\alpha_3>0.9873$, $\alpha_4>0.9948$, *and* $\alpha_5>0.9970$. *Furthermore, as* $m\to\infty$ *we have* $\alpha_m=1+O(m^{-2})$.

In the analysis which follows we treat m, R, ϕ, and $\hbar$ as fixed; implicit constants may depend on them. Also, we use A to denote a positive absolute constant, not necessarily the same at each occurrence.

2. Sketch of Proof

We first prove an identity

$$\xi^{(m)}(s)=Q_m(s)+(-1)^m\,\overline{Q_m(1-\bar{s})}$$

which implies that $\xi^{(m)}(\frac{1}{2}+it)=0$ when $\arg\,Q_m(\frac{1}{2}+it)\equiv((m+1)/2)\,\pi \bmod \pi$. (Many such identities are possible since Q_m depends on $\phi(x)$ which is constrained only as described in the Theorem.) We put $Q_m(s)=H(s)\,V(s)$. Since $\arg H(\frac{1}{2}+it)$ changes quickly enough by itself to supply all the zeros of $\xi^{(m)}(s)$, it is sufficient to bound $-\Delta\arg V(\frac{1}{2}+it)|_T^{T+U}$. By the argument principle, the latter is bounded by $2\pi N+O(L)$, where N is the number of zeros of $V(s)$ with $\sigma>\frac{1}{2}$ and $T<t<T+U$. We estimate N by using Littlewood's lemma on a rectangle with left side $\sigma=a$, where $\frac{1}{2}-a=R/L$ for some fixed $R>0$. Littlewood's lemma is applied to ψV, rather than V, where ψ is entire and is chosen to "mollify" V. We find that

$$2\pi N\leqslant\frac{1}{1/2-a}\int_T^{T+U}\log|\psi V(a+it)|\,dt+O(U),$$

$$\leqslant\frac{UL}{2R}\log\left(\frac{1}{U}\int_T^{T+U}|\psi V(a+it)|^2\,dt\right)+O(U).$$

If ψ is chosen properly, then the latter integral can be shown to be asymptotic to U times a function which depends only on m, R, ϕ, and ψ. We specify ψ to obtain the Theorem, and choose R and ϕ to obtain the Corollary.

3. Basic Lemmas

In this section we include lemmas that are needed for the proof of our Theorem.

LEMMA 1. *Let* $H(s) = \frac{1}{2}s(s-1)\,\pi^{-s/2}\Gamma(s/2), \chi(s) = H(1-s)/H(s)$, *and* $F(s) = H'(s)/H(s)$. *Then*

$$\text{(a)} \quad \arg H\left(\frac{1}{2} + it\right) = \frac{t}{2}\log\frac{|t|}{2\pi} - \frac{t}{2} + O(1),$$

where arg $H(3) = 0$ *and* arg $H(s)$ *is obtained by letting* arg *vary continuously on the straight line path from* 3 *to* s;

$$\text{(b)} \quad F(s) = \frac{1}{2}\log\frac{s}{2\pi} + O(|t|^{-1})$$

and

$$F^{(k)}(s) \ll |t|^{-k}$$

for $|t| \geqslant 1$ *and* $k \geqslant 1$;

$$\text{(c)} \quad H^{(k)}(s) = H(s)(F(s)^k + O(t^{-1}\log^{k-1} t))$$

for $0 \leqslant \sigma < A\log L$ *and* $t > 10$;

$$\text{(d)} \quad \chi(s) = \left(\frac{t}{2\pi}\right)^{1/2-\sigma} \exp\left(\frac{\pi i}{4} - it\log\frac{t}{2\pi e}\right)\left(1 + O\left(\frac{\log^2 L}{T}\right)\right)$$

for $0 < \sigma < A\log L$ *and* $T \leqslant t \leqslant T + U$.

The statements here are easily proved using the well-known formula for the log of the Γ-function

$$\log\Gamma(s) = \tfrac{1}{2}\log(2\pi) + (s - \tfrac{1}{2})\log s - s - \Omega(s),$$

where $\Omega(s) \ll 1/|t|$, and if $|t| \leqslant \sigma$ then $\Omega(s) \ll 1/\sigma$. (For a proof of this, see Rademacher [12, Sect. 21].)

LEMMA 2. *Any zero of $\xi^{(m)}(s)$ satisfies $0 < \sigma < 1$. If $N^{(m)}(T)$ denotes the number of zeros of $\xi^{(m)}(s)$ with $0 < t < T$, then*

$$N^{(m)}(T) = \frac{T}{2\pi}\log\frac{T}{2\pi} - \frac{T}{2\pi} + O_m(\log T).$$

We prove the first statement by induction on m. We apply Hadamard's factorization theorem to $\xi^{(m)}(s)$ which is entire and of order one since $\xi(s)$ is. Then by logarithmic differentiation of the product and use of the symmetry of the zeros about the real axis and about the line $\sigma = \frac{1}{2}$ (which follows from the functional equation $\xi^{(m)}(s) = (-1)^m \xi^{(m)}(1-s)$) we conclude that $\mathrm{Re}(\xi^{(m+1)}(s)/\xi^{(m)}(s))$ cannot vanish unless $0 < \sigma < 1$.

The second statement of the Lemma can be proven by the argument principle and parts (a), (b), and (c) of Lemma 1. The proof is similar to Backlund's proof of the assertion in the case $m = 0$ (see Titchmarsh [14, Sect. 9.3]).

LEMMA 3. *Let $0 \swarrow\!\!\!\nearrow 1$ signify a straight line path of slope 1 which crosses the real axis between 0 and 1. Then*

$$\xi(s) = H(s) f(s) + H(1-s)\,\overline{f(1-\bar{s})},$$

where

$$f(s) = \int_{0 \nearrow 1} \frac{z^{-s} e^{\pi i z^2}}{2i \sin \pi z}\,dz.$$

This is the Riemann–Siegel integral formula as stated by Siegel [13, Sect. 3]. Note that

$$\overline{f(1-\bar{s})} = \int_{0 \searrow 1} \frac{z^{s-1} e^{\pi i z^2}}{2i \sin \pi z}\,dz,$$

where $0 \searrow 1$ signifies a straight line path of slope -1.

LEMMA 4. *Suppose that $h(z)$ is regular in the z-plane slit along the negative real axis and $|h(z)| \ll |\log z|^j$ for $|z| > 10$ and some $j > 0$. Let $0 \leqslant \sigma < A \log L$, $T \leqslant t \leqslant T + U$, and $\eta = (t/2\pi)^{1/2}$. Then for any $\varepsilon > 0$,*

$$\int_{0 \nearrow 1} \frac{z^{-s} e^{\pi i z^2}}{2i \sin \pi z}\,h(z)\,dz = \sum_{n \leqslant \eta} h(n)\,n^{-s} + O_\varepsilon(T^{\varepsilon - \sigma/2})$$

and

$$\int_{0 \searrow 1} \frac{z^{s-1} e^{-\pi i z^2}}{2i \sin \pi z}\,h(z)\,dz = \sum_{n < \eta} h(n)\,n^{s-1} + O_\varepsilon(T^{\varepsilon + (\sigma - 1)/2}).$$

Proof. We move the paths of integration so that they pass through η and use Cauchy's theorem. The main terms arise from the residues at integers $\leqslant \eta$. The integrals on the new paths are easily estimated to give the above error terms. (Siegel [13, Sect. 4] has estimated similar integrals.)

LEMMA 5. *Let $f_n(t)$ be a complex-valued function defined on $[T_1, T_2]$ such that $|f_n(t)| \leqslant \delta$ and* var $f_n(t)|_{T_1}^{T_2} \leqslant \delta$. *Then for any complex numbers a_n,*

$$\int_{T_1}^{T_1} \left| \sum_{n=1}^{N} a_n f_n(t)\, n^{-it} \right|^2 dt = \sum_{n=1}^{N} |a_n|^2 \int_{T_1}^{T_2} |f_n(t)|^2\, dt + O\left(\delta^2 N(\log N) \sum_{n=1}^{N} |a_n|^2\right).$$

The implicit constant is absolute.

Note that by taking $f_n = 0$ or 1 we can deal with Dirichlet polynomials in which the range of summation varies with t. In the special case $f_n(t) = 1$ for all n and t Montgomery and Vaughan [10] have shown that

$$\int_{T_1}^{T_2} \left| \sum_{n=1}^{\infty} a_n n^{-it} \right|^2 dt = \sum_{n=1}^{\infty} |a_n|^2 (T_2 - T_1 + O(n)).$$

Proof. By homogeneity we may suppose that $\delta = 1$. We square out and integrate term-by-term. Thus it suffices to show that

$$\sum_{m \neq n} |a_m a_n| \left| \int_{T_1}^{T_2} f_m(t)\, \overline{f_n(t)} \left(\frac{n}{m}\right)^{it} dt \right| \ll N(\log N) \sum_{n=1}^{N} |a_n|^2.$$

By integration by parts we see that

$$i(\log y) \int_a^b f(t)\, y^{it}\, dt = f(t)\, y^{it} \Big|_a^b - \int_a^b y^{it}\, df(t) \ll \max |f| + \operatorname{var} f \Big|_a^b.$$

We apply this with $f = f_m \overline{f_n}$. Note that $|f| \leqslant 1$, while

$$\operatorname{var} f \leqslant (\max |f_m|) \operatorname{var} f_n + (\max |f_n|) \operatorname{var} f_m \leqslant 2.$$

Thus it suffices to show that

$$\sum_{m \neq n} \frac{|a_m a_n|}{|\log m/n|} \ll N(\log N) \sum_{n=1}^{N} |a_n|^2.$$

This is well-known (see Titchmarsh [14, Sect. 7.2] for the proof of a similar result).

The next four lemmas appear in Levinson's work [5].

LEMMA 6 [5, Lemma 3.2]. *Let* $1 \leqslant \kappa_1, \kappa_2 \leqslant T^{1/2}$ *with* $(\kappa_1, \kappa_2) = 1$. *Suppose that* $a = 1/2 + O(1/\log T)$. *Then*

$$\sum_{\substack{j_1, j_2 \leqslant T^{1/2} \\ j_1 \kappa_1 \neq j_2 \kappa_2}} \sum \frac{j_1^{-a} j_2^{-a}}{|\log(j_1 \kappa_1 / j_2 \kappa_2)|} \ll T^{1/2} \log T.$$

LEMMA 7 [5, Lemma 3.4]. *Define*

$$I(r) = \int_T^{T+U} \exp\left(it \log \frac{t}{2\pi r e}\right) dt.$$

Then

$$I(r) = 2\pi r^{1/2} e^{\pi i/4} e(-r) + O(E(r))$$

for $T/2\pi \leqslant r \leqslant (T+U)/2\pi$, *where* $e(x) = \exp(2\pi i x)$ *and*

$$E(r) = 1 + T/(|T - r| + T^{1/2}) + (T+U)/(|T + U - r| + (T+U)^{1/2}).$$

If $r < T/2\pi$ *or* $r > (T+U)/2\pi$ *then* $I(r) \ll E(r)$.

LEMMA 8 [5, (8.2) *and* (8.5)–(8.8)]. *With* $E(r)$ *defined as in the previous lemma*,

$$\sum_{k_1, k_2 \leqslant y} \sum k_1^{-1/2} k_2^{-1/2} \sum_{j_1, j_2 \leqslant \tau} \sum j_1^{-1/2} j_2^{-1/2} E(r) \ll U L^{-6},$$

where $\tau = (T/2\pi)^{1/2}$ *and* $y = T^{1/2} L^{-20}$.

LEMMA 9 [5, Lemma 3.6]. *Let* $1 \leqslant k_1, k_2 \leqslant y$ *and let* $k = \gcd(k_1, k_2)$. *Then* $\sum k\, k_1^{-1} k_2^{-1} \ll \log^3 y$.

LEMMA 10. *Let* $\hbar$ *be a real polynomial with* $\hbar(0) = 0$, *and let*

$$G_j(\beta) = \sum_{\substack{n \leqslant y/j \\ (n,j)=1}} \frac{\mu(n)}{n^\beta} \hbar\left(\frac{\log y/nj}{\log y}\right).$$

Then

$$G_j^{(i)}(\beta) = M_{i,j}(\beta) + O(E_{i,j})$$

uniformly for $j \leqslant y$ *and* $0 < |\beta - 1| \ll 1/\log y$, *where*

$$M_{0,j}(\beta) = \frac{1}{F(j,\beta)} \left[(\beta - 1)\hbar\left(\frac{\log y/j}{\log y}\right) + \frac{1}{\log y} \hbar'\left(\frac{\log y/j}{\log y}\right)\right],$$

$$M_{1,j}(\beta) = \frac{1}{F(j,\beta)} \hbar\left(\frac{\log y/j}{\log y}\right),$$

$$M_{i,j}(\beta) = 0 \qquad \text{for } i \geqslant 2,$$

and

$$E_{i,j}(\beta) = (\log y)^{i-2}(\log\log y)^2(1 + (\log y)(j/y)^b)\,F_1(j, 1-2\delta).$$

Here we define $F(j,s) = \prod_{p|j}(1-p^{-s})$, $F_1(j,s) = \prod_{p|j}(1+p^{-s})$, $\delta = 1/\log\log y$, *and* $b = 1/(M\log\log y)$, *where* M *is a (sufficiently large) absolute constant. (The products are over primes p which divide j.)*

Proof. We expand $\not{h}$ in a MacLaurin series and express the sum over n as an integral. Then

$$G_j(\beta) = \sum_{l\geqslant 1} \frac{\not{h}^{(l)}(0)}{\log^l y} \cdot \frac{1}{2\pi i}\int_{2-i\infty}^{2+i\infty} \frac{x^{s-\beta}}{\zeta(s)\,F(j,s)(s-\beta)^{l+1}}\,ds,$$

where $x = y/j$. The integrand has a pole of order $l+1$ at $s=\beta$. We move the path of integration and apply Cauchy's Theorem. Let $R_0(\beta)$ be the residue from the pole at $s=\beta$; let $R_1(\beta)$ be the integral on $s = 1+it$, $-\infty < t \leqslant -(\log y)^{10}$; let $R_2(\beta)$ be the integral on $s = \sigma - i(\log y)^{10}$, $1-b \leqslant \sigma \leqslant 1$; let $R_3(\beta)$ be the integral on $s = (1-b)+it$, $-(\log y)^{10} \leqslant t \leqslant (\log y)^{10}$; let $R_4(\beta)$ and $R_5(\beta)$ be the integrals on paths conjugate to the paths of $R_2(\beta)$ and $R_1(\beta)$, respectively. Then

$$G_j^{(i)}(\beta) = \sum_{l\geqslant 1} \frac{\not{h}^{(l)}(0)}{\log^l y}\,\frac{1}{2\pi i}\left(2\pi i\,R_0^{(i)}(\beta) + \sum_{m=1}^{5} R_m^{(i)}(\beta)\right).$$

The main term of $G_j^{(i)}(\beta)$ will result from the residue $R_0^{(i)}(\beta)$. To estimate the error terms we recall (see Titchmarsh [14, p. 53]) that

$$\frac{1}{\zeta(1+it)} \ll \log|t|$$

for s on the paths of R_1 and R_5 and if M is sufficiently large,

$$\frac{1}{\zeta(s)} < M\log y$$

for s on the paths of R_2, R_3, and R_4. We also observe that $1/F(j,s) \ll F_1(j, 1-2\delta)$ for s anywhere on the new path of integration. Further, if we apply Cauchy's theorem on a circle of radius $1/\log y$, we see that

$$\left(\frac{\partial}{\partial\beta}\right)^i \left(\frac{x^{s-\beta}}{(s-\beta)^{l+1}}\right) \ll \frac{(\log y)^i\,x^{\sigma-1}}{((\sigma-1)^2+t^2)^{(l+1)/2}}.$$

From these estimates we obtain

$$R_5^{(i)}(\beta) \ll F_1(j, 1-2\delta)(\log y)^{i-9}$$

and similarly for $R_1^{(i)}(\beta)$,

$$R_4^{(i)}(\beta) \ll F_1(j, 1-2\delta)(\log y)^{i-20}$$

and similarly for $R_2^{(i)}(\beta)$, and

$$R_3^{(i)}(\beta) \ll F_1(j, 1-2\delta)(\log y)^i (\log\log y)^{l+1}(j/y)^b.$$

Hence

$$G_j^{(i)}(\beta) = \sum_{l \geq 1} \frac{h^{(l)}(0)}{\log^l y} R_0^{(i)}(\beta) + O(E_{i,j}).$$

Clearly, the ith derivative of the residue is given by

$$R_0^{(i)}(\beta) = \frac{1}{l!} \sum_{q=0}^{l} \binom{l}{q} (\log x)^{l-q} Z^{(q+i)}(\beta),$$

where $Z(s) = 1/(\zeta(s)\, F(j, s))$. Now

$$\frac{F'}{F}(j, s) = \sum_{p \mid j} \frac{\log p}{p^s - 1} \ll \sum_{p \mid j} \frac{\log p}{p} \ll \log\log j$$

for $|s-1| \ll \delta$. Hence

$$\begin{aligned} Z(\beta) &= [(\beta - 1) + O(|\beta - 1|^2)]/F(j, \beta), \\ Z'(\beta) &= -((F'/F)(j, \beta) + (\zeta'/\zeta)(\beta))/(F(j, \beta)\, \zeta(\beta)) \\ &= 1/F(j, \beta) + O(F_1(j, 1-2\delta)\, |\beta - 1| \log\log y), \end{aligned}$$

and by Cauchy's theorem,

$$Z^{(k)}(\beta) \ll F_1(j, 1-2\delta)(\log\log y)^{k-1}.$$

Therefore,

$$\sum_{l \geq 1} \frac{h^{(l)}(0)}{\log^l y} R_0^{(i)}(\beta) = M_{i,j}(\beta) + O(E_{i,j})$$

as was required to prove.

LEMMA 11. *Suppose that* $f(p) = 1 + O(p^{-c})$ *for primes* p *and some* $c > 0$. *Define* $f(r) = \prod_{p \mid r} f(p)$, *and*

$$J_d(x) = \sum_{r \leq x} \frac{\mu^2(r)}{r} f(r) \left(\log \frac{x}{r}\right)^d$$

for d, a non-negative integer. Then

$$J_d(x) = \left(\prod_p \left(1 + \frac{f(p) - 1}{p + 1}\right)(1 - p^{-2})\right) \frac{\log^{d+1} x}{d+1} + O(\log^d x),$$

where the implicit constant depends on c and d.

Note that the product is absolutely convergent.

For $d = 0$ this lemma has been proved by Levinson [5, Lemma 3.11]. For $d > 0$ the lemma is easily demonstrated by expressing $J_d(x)$ as a complex integral

$$J_d(x) = \frac{d!}{2\pi i} \int_{3 - i\infty}^{3 + i\infty} \frac{A(s)\, x^{s-1}}{(s-1)^{d+1}}\, ds,$$

where $A(s) = \sum_{n=1}^{\infty} \mu^2(n) f(n)\, n^{-s}$, and using Cauchy's theorem to shift the path of integration to the line $s = 1 - c/2 + it$, $-\infty < t < \infty$. On the new path of integration the estimate $A(s) \ll (1 + |t|)^{1/2}$ is valid and the result follows.

4. An Identity for $\xi^{(m)}(s)$

Let ϕ be a real polynomial which satisfies $\phi(0) = 1$ and $\phi(z) + \phi(1 - z) = K$ for some constant $K \neq 0$. Let $c(z) = \phi(L^{-1} \log z)$ and $d(z) = \phi(1 - L^{-1} \log z)$. Then by Lemma 3,

$$K\xi(s) = Q(s) + \overline{Q(1 - \bar{s})},$$

where

$$Q(s) = H(s) \int_{0 \swarrow 1} \frac{z^{-s} e^{\pi i z^2} c(z)}{2i \sin \pi z}\, dz + H(1 - s) \int_{0 \searrow 1} \frac{z^{s-1} e^{-\pi i z^2} d(z)}{2i \sin \pi z}\, dz.$$

This may be differentiated m times with respect to s to obtain

$$K\xi^{(m)}(s) = Q_m(s) + (-1)^m \overline{Q_m(1 - \bar{s})}, \tag{1}$$

where

$$\begin{aligned} Q_m(s) = & \sum_{k=0}^{m} \binom{m}{k} H^{(k)}(s) \int_{0 \swarrow 1} \frac{z^{-s} e^{\pi i z^2}}{2i \sin \pi z} (-\log z)^{m-k} c(z)\, dz \\ & + \sum_{k=0}^{m} \binom{m}{k} H^{(k)}(1 - s) \int_{0 \searrow 1} \frac{z^{s-1} e^{-\pi i z^2}}{2i \sin \pi z} (\log z)^{m-k} d(z)\, dz. \end{aligned}$$

This identity expresses $\xi^{(m)}(\frac{1}{2}+it)$ as a sum (m even) or a difference (m odd) of complex conjugates. Hence $\xi^{(m)}(\frac{1}{2}+it)=0$ precisely when

$$\text{(a)}\quad \arg Q_m(\tfrac{1}{2}+it) \equiv \frac{m+1}{2}\pi \pmod{\pi}$$

or

$$\text{(b)}\quad Q_m(\tfrac{1}{2}+it)=0.$$

These conditions do not depend on how we define $\arg Q_m(\frac{1}{2}+it)$. We suppose that $Q_m(\frac{1}{2}+iT) \neq 0 \neq Q_m(\frac{1}{2}+i(T+U))$ and define $\arg Q_m(\frac{1}{2}+it)$ for $T \leqslant t \leqslant T+U$ by continuous variation along the line $\sigma=\frac{1}{2}$ once $\arg Q_m(\frac{1}{2}+iT)$ is defined. If $\frac{1}{2}+it_0$ is a zero of Q_m of multiplicity n we define

$$\arg Q_m(1/2+it_0^+) = \arg Q_m(1/2+it_0^-) + n\pi.$$

By (1), such a point is a zero of $\xi^{(m)}(s)$ of multiplicity at least n. Hence

$$N_m(T+U) - N_m(T) \geqslant 1/\pi(\arg Q^{(m)}(1/2+i(T+U)) \\ - \arg Q^{(m)}(1/2+iT)) - 1.$$

Since our identity (1) is different from Levinson's [5, (1.8)], it is not clear that we are counting only simple zeros (see Heath-Brown [2]).

It follows from Lemmas 1 (part (a)) and 2 that

$$1/\pi(\arg H(1/2+i(T+U)) - \arg H(1/2+iT)) \\ = N^{(m)}(T+U) - N^{(m)}(T) + O_m(\log T).$$

Therefore,

$$N_m(T+U) - N_m(T) \geqslant N^{(m)}(T+U) - N^{(m)}(T) + O_m(\log T) \\ - (1/\pi)(\arg V(1/2+i(T+U)) - \arg V(1/2+iT)), \tag{2}$$

where $V(s) = Q_m(s)/H(s)$.

We obtain a simpler expression for $V(s)$. By Lemma 4,

$$Q_m(s) = \sum_{k=0}^{m} \binom{m}{k} H^{(k)}(s) \left(\sum_{n \leqslant \eta} (-\log n)^{m-k} c(n)\, n^{-s} + O(T^{\varepsilon-\sigma/2}) \right) \\ + \sum_{k=0}^{m} \binom{m}{k} H^{(k)}(1-s) \left(\sum_{n \leqslant \eta} (\log n)^{m-k} d(n)\, n^{s-1} + O(T^{\varepsilon+(\sigma-1)/2}) \right).$$

for $T \leqslant t \leqslant T+U$ and $0 \leqslant \sigma \leqslant A \log L$. Then by Lemma 1(c) we can replace $H^{(k)}(s)$ by $H(s)\,F(s)^k$ with a small error; we use the estimate of Lemma 1(d) and obtain

$$V(s) = C(s) + \chi(s)\,D(s) + O(T^{\varepsilon-\sigma/2} + T^{\varepsilon-1/2})$$

for $T \leqslant t \leqslant T+U$ and $0 \leqslant \sigma \leqslant A \log L$, where

$$C(s) = \sum_{n \leqslant \eta} c(n)(F(s) - \log n)^m n^{-s}$$

and

$$D(s) = \sum_{n \leqslant \eta} d(n)(\log n - F(1-s))^m n^{s-1}.$$

We apply the argument principle to V on the rectangle $\mathscr{D}$ with vertices $\frac{1}{2}+iT$, σ_0+iT, $\sigma_0+i(T+U)$, and $\frac{1}{2}+i(T+U)$, where $3 \leqslant \sigma_0 = \sigma_0(m)$. On the left side of $\mathscr{D}$ the argument of V is determined as it was for Q_m above. Let $l = \log(t/2\pi)$. Then on the right side of $\mathscr{D}$, since $c(1) = 1$,

$$|V(s) - (l/2)^m| < A\,2^{-\sigma_0}(L/2)^m$$

by Lemmas 1(b) and (d). Hence

$$|\Delta \arg V(\sigma_0 + it)|_T^{T+U}| < \pi$$

if σ_0 is large enough. By Jensen's theorem, $\Delta \arg V(s) \ll L$ on horizontal parts of the contour. Thus

$$(1/\pi)\,\Delta \arg V(1/2 + it)|_T^{T+U} = -2N + O(L), \tag{3}$$

where N is the number of zeros of V inside or on $\mathscr{D}$.

We obtain an upper bound for N by applying Littlewood's lemma (see Titchmarsh [14, Sect. 9.9]) to $2^m L^{-m} V(s)\,\psi(s)$ on the rectangle $\mathscr{E}$ with vertices $a+iT$, σ_1+iT, $\sigma_1+i(T+U)$, and $a+i(T+U)$. Here $\sigma_1 = \log L$ and $(\frac{1}{2}-a) = R/L$ for a number $R > 0$ which will be considered fixed. The mollifier ψ is a Dirichlet polynomial

$$\psi(s) = \sum_{k \leqslant y} b(k)\,k^{-s}$$

with $b(1)=1$, $b(k)\ll 1$, and $y=T^{1/2}L^{-20}$. Then

$$2\pi\sum_{\mathscr{E}}(\beta-a)=\int_T^{T+U}\log\left|\left(\frac{2}{L}\right)^m\psi V(a+it)\right|dt$$
$$-\int_T^{T+U}\log\left|\left(\frac{2}{L}\right)^m\psi V(\sigma_1+it)\right|dt$$
$$+\int_a^{\sigma_1}\arg\left(\frac{2}{L}\right)^m\psi V(\sigma+i(T+U))\,d\sigma$$
$$-\int_a^{\sigma_1}\arg\left(\frac{2}{L}\right)^m\psi V(\sigma+iT)\,d\sigma,$$

where $\sum_{\mathscr{E}}$ runs over all zeros $\beta+i\gamma\in\mathscr{E}$ of $V(s)\,\psi(s)$. The last two integrals are $\ll L$ by the usual application of Jensen's formula. Also

$$|(2/L)^m V(s)-1|<A2^{-\sigma_1}\ll L^{-1},$$

and similarly $|\psi(s)-1|\ll L^{-1}$ for s on the right side of $\mathscr{E}$. Hence the second integral is $\ll UL^{-1}$. The zeros of $\psi(s)\,V(s)$ inside $\mathscr{E}$ include the zeros of $V(s)$ inside or on $\mathscr{D}$, and if $\beta+i\gamma\in\mathscr{D}$ then $\beta-a\geqslant\frac{1}{2}-a$. Hence

$$\sum_{\mathscr{E}}(\beta-a)\geqslant(\tfrac{1}{2}-a)\,N.$$

By the arithmetic-geometric mean inequality,

$$\int_T^{T+U}\log\left|\left(\frac{2}{L}\right)^m\psi V(a+it)\right|dt\leqslant U\log(I/U),$$

where

$$I=\int_T^{T+U}|(2/L)^m\psi V(a+it)|\,dt.$$

Hence

$$2N\leqslant(UL/\pi R)\log(I/U)+O(U). \tag{4}$$

We can simplify the integrand of I. By Lemma 1(b),

$$C(s)=\sum_{n\leqslant n}c(n)\left(\frac{l}{2}+\frac{\pi i}{4}-\log n\right)^m n^{-s}+O(T^{-1/2}L^{m-1})$$

for $\sigma = a$, $T \leqslant t \leqslant T + U$. Thus

$$
\begin{aligned}
|(2/L)^m C(s)| &= C_1(s) \\
&\quad + \sum_{n \leqslant \tau} c(n) \left(\left(\frac{l}{L} + \frac{i\pi}{2L} - \frac{2 \log n}{L} \right)^m - \left(1 + \frac{i\pi}{2L} - \frac{2 \log n}{L} \right)^m \right) n^{-s} \\
&\quad + \sum_{\tau < n \leqslant \eta} c(n) \left(\frac{l}{L} + \frac{i\pi}{2L} - \frac{2 \log n}{L} \right)^m n^{-s} + O(T^{-1/2} L^{-1}) \\
&= C_1(s) + C_2(s) + C_3(s) + O(T^{-1/2} L^{-1}),
\end{aligned}
$$

where $\tau = (T/2\pi)^{1/2}$ and

$$
C_1(s) = \sum_{n \leqslant \tau} c(n) \left(1 + \frac{\pi i}{2L} - \frac{2 \log n}{L} \right)^m n^{-s}.
$$

We now apply Lemma 5 several times. With $\delta \ll (\log(T+U)/T) \ll L^{-10}$ the lemma gives

$$
\int_T^{T+U} |C_2(a+it)|^2 \, dt \ll L^{-20} U \sum \frac{|c(n)|^2}{n} \ll UL^{-19}.
$$

With $\delta \ll 1$, and $\tau_1 = ((T+U)/2\pi)^{1/2}$, we have

$$
\int_T^{T+U} |C_3(a+it)|^2 \, dt \ll U \sum_{\tau < n \leqslant \tau_1} \frac{|c(n)|^2}{n} \ll UL^{-10}.
$$

We treat $D_2(s)$ and $D_3(s)$ in a similar way, where

$$
(2/L)^m D(s) = D_1(s) + D_2(s) + D_3(s) + O(T^{-1/2} L^{-1})
$$

with D_2 and D_3 similar to C_2 and C_3 and with

$$
D_1(s) = \sum_{n \leqslant \eta} d(n) \left(\frac{2 \log n}{L} + \frac{\pi i}{2L} - 1 \right)^m n^{s-1}.
$$

Also by Lemma 5,

$$
\int_T^{T+U} |\psi(a+it)|^2 \, dt \ll U \sum \frac{|b(k)|^2}{k} \ll UL.
$$

Let $\chi^*(t) = (T/2\pi)^{1/2-a} \exp(\pi i/4 - it \log t/2\pi e)$. Then by Lemma 1(d),

$$
\chi(a+it) - \chi^*(t) \ll L^{-11}
$$

for $T \leqslant t \leqslant T+U$. Hence by Lemma 5,

$$\int_T^{T+U} |\chi(a+it) - \chi^*(t)|\, |D_1 \psi(a+it)|\, dt$$

$$\ll L^{-11} \left(\int_T^{T+U} |D_1|^2 \right)^{1/2} \left(\int_T^{T+U} |\psi|^2 \right)^{1/2} \ll UL^{-10}.$$

Now by several applications of the triangle and Cauchy–Schwarz inequalities we conclude that

$$I = \int_T^{T+U} |V^* \psi(a+it)|\, dt + O(UL^{-9/2}),$$

where $V^*(s) = C_1(s) + \chi^*(t)\, D_1(s)$.

Let

$$J = \int_T^{T+U} |V^* \psi(a+it)|^2\, dt.$$

Then by the Cauchy–Schwarz inequality,

$$I \leqslant U^{1/2} J^{1/2} + O(UL^{-9/2}).$$

The left side of (4) is non-negative so $I \gg U$. Hence $J \gg U$ and by (4) we see that

$$2N \leqslant \frac{UL}{2\pi} \frac{\log(J/U)}{R} + O(U).$$

It now follows from (2), (3), and Lemma 2 that

$$\alpha_m \geqslant 1 - R^{-1} \log(J/U). \tag{5}$$

5. Simplification of J

To evaluate J we use the same basic techniques as Levinson [5] but we make use of Pan's simplifications [11]. We square out to see that

$$J = J_1 + 2 Re\, J_2 + J_3, \tag{6}$$

where $J_1 = \int_T^{T+U} |\psi C_1(a+it)|^2\, dt$, $J_2 = \int_T^{T+U} |\psi|^2\, C_1 \overline{\chi^* D_1}(a+it)\, dt$, and $J_3 = \int_T^{T+U} |\psi D_1(a+it)|^2\, dt$. By Lemma 5 with $\delta \ll 1$,

$$J_1 = U(1 + O(L^{-10})) \sum_{n \leqslant \tau y} \frac{1}{n^{2a}} \left| \sum_{d \mid n} c_*(n)\, b(n/d) \right|^2,$$

and since $|\chi^*(t)|^2 = (T/2\pi)^{1/2-a} = \tau^{2-4a}$,

$$J_3 = U\tau^{2-4a}(1+O(L^{-10})) \sum_{n\leqslant\tau y} \frac{1}{n^{2-2a}} \left| \sum_{d|n} d_*(n)\, b(n/d) \right|^2,$$

where $c_*(n) = c(n)(1-2(\log n)/L + \pi i/2L)^m$ and $d_*(n) = d(n)(2(\log n)/L - 1 + \pi i/2L)^m$. The inner sums on n are $\ll L^5$. We rearrange the order of summation and obtain

$$J_1 = U \sum_{k_1,k_2}\sum \frac{b(k_1)\, b(k_2)}{k_1^{2a}\, k_2^{2a}} k^{2a} \sum_{j\leqslant\tau/\kappa_M} c_*(j\kappa_1)\, \overline{c_*(j\kappa_2)} j^{-2a} + O(UL^{-5}) \quad (7)$$

and

$$J_3 = U\tau^{2-4a} \sum_{k_1,k_2}\sum \frac{b(k_1)\, b(k_2)}{k_1 k_2} k^{2-2a} \sum_{j\leqslant\tau/\kappa_M} d_*(j\kappa_1)\, \overline{d_*(j\kappa_2)}\, j^{2a-2} + O(UL^{-5}), \quad (8)$$

where $\gcd(k_1, k_2) = k$, $k_1 = \kappa_1 k$, $k_2 = \kappa_2 k$, $\kappa_M = \max\{\kappa_1, \kappa_2\}$, and $\kappa_m = \min\{\kappa_1, \kappa_2\}$. Unless otherwise indicated, sums on k_1 and k_2 are for $1 \leqslant k_1, k_2 \leqslant y$ and sums on j_1 and j_2 are for $1 \leqslant j_1, j_2 \leqslant \tau$.

Clearly

$$J_2 = \tau^{1-2a} e^{-\pi i/4} \sum_{k_1,k_2}\sum \frac{b(k_1)\, b(k_2)}{k_1^a k_2^a} \sum_{j_1,j_2}\sum \frac{c_*(j_1)\, \overline{d_*(j_2)}}{j_1^a j_2^{1-a}} I(r),$$

where $r = j_1 j_2 k_1/k_2$ and $I(r)$ is defined in Lemma 7. By Lemmas 7 and 8,

$$J_2 = J_{21} + O(UL^{-6}), \quad (9)$$

where

$$J_{21} = 2\pi\tau^{1-2a} \sum_{k_1,k_2}\sum \frac{b(k_1)\, b(k_2)}{k_1^{a-1/2}\, k_2^{a+1/2}} \sum_{\substack{j_1,j_2 \\ \tau^2\leqslant r\leqslant\tau_1^2}}\sum \frac{c_*(j_1)\, \overline{d_*(j_2)}}{j_1^{a-1/2} j_2^{1/2-a}} e(-r).$$

We have used $\tau_1^2 = (T+U)/2\pi$. (Recall, also, that $\tau^2 = T/2\pi$.) We take the sum over j_1 inside. If $k_2 \nmid j_2 k_1$ then the sum over j_1 is $\ll (\sin \pi(j_2 k_1/k_2))^{-1} \ll \|j_2 k_1/k_2\|^{-1}$ (see [14; Sect. 5.2]), where $\|\theta\|$ is the distance from θ to the nearest integer. The sum of this quantity over j_2, $j_2 \not\equiv 0 (\mathrm{mod}\; k_2/(k_1, k_2))$, is $\ll (\tau + k_2) L$. Thus the total contribution of these terms to J_{21} is $\ll \tau y L^2 + y^2 L \ll UL^{-8}$. Hence

$$J_{21} = 2\pi\tau^{1-2a} \sum_{k_1,k_2}\sum \frac{b(k_1)\, b(k_2)}{k_1^{a-1/2}\, k_2^{a+1/2}} \sum_{j_1,j_2}\sum \frac{c_*(j_1)\, \overline{d_*(j_2)}}{j_1^{a-1/2} j_2^{1/2-a}} + O(UL^{-8}),$$

where the sum on j_1 and j_2 is for $j_1, j_2 \leqslant \tau$, $\tau^2 \leqslant r \leqslant \tau_1^2$, and $j_2 \equiv 0 \bmod \kappa_2$. (Recall that $\kappa_2 = k_2/(k_1, k_2)$.) In this sum let $j_2 = j\kappa_2$. Then the conditions of summation may be written

$$\frac{\tau}{\kappa_1} \leqslant j \leqslant \frac{\tau}{\kappa_2}, \frac{\tau^2}{j\kappa_1} \leqslant j_1 \leqslant \min\left(\tau, \frac{\tau_1^2}{j\kappa_1}\right).$$

If we drop the restraint $j_1 \leqslant \tau$ then we introduce $\ll UL^{-10}\kappa_1^{-1}$ additional terms to the sum on j_1, j_2. Thus

$$J_{21} = 2\pi\tau^{1-2a} \sum_{k_1, k_2}\sum \frac{b(k_1)\, b(k_2)}{k_1^{a-1/2}\, k_2^{a+1/2}} (\Sigma_1 + O(UL^{-10}\kappa_1^{-1})) + O(UL^{-8}), \quad (10)$$

where

$$\Sigma_1 = \sum_{\tau/\kappa_1 \leqslant j \leqslant \tau/\kappa_2} \overline{d_*(j_2)}\, j^{a-1/2} \sum_{\tau^2/j\kappa_1 \leqslant j_1 \leqslant \tau_1^2/j\kappa_1} c_*(j_1)\, j_1^{1/2-a}.$$

The terms of the inner sum on j_1 here are almost constant since $(d/dn)(c_*(n)\, n^{1/2-a}) \ll 1/Ln$. Thus the inner sum is

$$= \frac{1}{2\pi} c_*\left(\frac{\tau^2}{j\kappa_1}\right) U\tau^{1-2a}(j\kappa_1)^{-3/2+a} + O(1) + O(UL^{-11}\kappa_1^{-1}j^{-1}),$$

so that

$$\Sigma_1 = \frac{U\tau^{1-2a}}{2\pi} \kappa_1^{a-3/2} \sum_{\tau/\kappa_1 \leqslant j \leqslant \tau/\kappa_2} d_*(j\kappa_1)\, \overline{d_*(j\kappa_2)}\, j^{2a-2} + O(T^{1/2})$$
$$+ O\left(\frac{UL^{-10}}{\kappa_1}\right).$$

(We have used the fact that $c_*(\tau^2/x) = d_*(x)$.) We substitute this in (10) and use Lemma 9 to find that

$$J_{21} = U\tau^{2-4a} \sum_{k_1, k_2}\sum \frac{b(k_1)\, b(k_2)}{k_1 k_2} k^{2-2a} \sum_{\tau/\kappa_1 \leqslant j \leqslant \tau/\kappa_2} d_*(j\kappa_1)\, \overline{d_*(j\kappa_2)}\, j^{2a-2}$$
$$+ O(UL^{-7}).$$

Thus, the main term of $2 \operatorname{Re} J_2$ is

$$= U\tau^{2-4a} \sum_{k_1, k_2}\sum \frac{b(k_1)\, b(k_2)}{k_1 k_2} k^{2-2a} \sum_{\tau/\kappa_M \leqslant j \leqslant \tau/\kappa_m} d_*(j\kappa_1)\, \overline{d_*(j\kappa_2)}\, j^{2a-2},$$

which combines nicely with the main term of J_3 in (8). Hence

$$J/U = J_4 + J_5 + O(L^{-7}), \tag{11}$$

where

$$J_4 = \sum_{k_1, k_2}\sum \frac{b(k_1)\, b(k_2)}{k_1^{2a} k_2^{2a}} k^{2a} \sum_{j \leqslant \tau/\kappa_M} c_*(j\kappa_1)\, \overline{c_*(j\kappa_2)}\, j^{-2a}$$

and

$$J_5 = \tau^{2-4a} \sum_{k_1, k_2}\sum \frac{b(k_1)\, b(k_2)}{k_1 k_2} k^{2-2a} \sum_{j \leqslant \tau/\kappa_m} d_*(j\kappa_1)\, \overline{d_*(j\kappa_2)}\, j^{2a-2}.$$

We now estimate the innermost sums in J_4 and J_5. If $h(u)$ has a continuous first derivative, then

$$\sum_{n \leqslant x} h(n) = \int_1^x h(u)\, du + h(1) - h(x)\{x\} + \int_1^x \{u\}\, h'(u)\, du.$$

If $|h'(u)| \leqslant M/u^2$ for $u \leqslant X$, where $x \leqslant X$, then the above is

$$= \int_1^x h(u)\, du + c + \frac{2\theta M}{x} \qquad (|\theta| \leqslant 1),$$

where $c = h(1) + \int_1^X \{u\}\, h'(u)\, du$. Hence with $X = \tau$, $x = \tau/\kappa_M$, and $h(u) = c_*(u\kappa_1)\, \overline{c_*(u\kappa_2)}\, u^{-2a}$ we see that the innermost sum of J_4 is

$$= \int_1^{\tau/\kappa_M} c_*(u\kappa_1)\, \overline{c_*(u\kappa_2)}\, u^{-2a}\, du + K_4 + O(\kappa_M/\tau)$$

and similarly the innermost sum of J_5 is

$$= \int_1^{\tau/\kappa_m} d_*(u\kappa_1)\, \overline{d_*(u\kappa_2)}\, u^{2a-2}\, du + K_5 + O(\kappa_m/\tau),$$

where K_4 and K_5 are bounded functions of T (for fixed m, R, and ϕ) which are independent of k_1 and k_2. The above error terms contribute an amount $\ll L^{-19}$ to J_4 and J_5. With our choice of mollifier coefficients $b(k)$ we will later show that

$$\sum_{k_1, k_2}\sum \frac{b(k_1)\, b(k_2)}{k_1^{\alpha} k_2^{\alpha}} k^{2\alpha - 2a} \ll L^{-1}$$

whenever $|\alpha - 1| \ll L^{-1}$. We assume this result for now, so that K_4 and K_5 contribute an amount $\ll L^{-1}$ to J_4 and J_5. We make the change of variable

$v=\tau^2/(u\kappa_1\kappa_2)$ in the integral term of J_5 with the result that the expressions for J_4 and J_5 combine to give

$$J/U=J_6+O(L^{-1}) \tag{12}$$

with

$$J_6=\sum_{k_1,k_2}\sum \frac{b(k_1)\,b(k_2)}{k_1^{2a}k_2^{2a}}\,k^{2a}\int_1^{\tau^2/(\kappa_1\kappa_2)} c_*(\kappa_1 v)\,\overline{c_*(\kappa_2 v)}\,v^{-2a}\,dv.$$

Notice that the asymmetry between κ_m and κ_M has disappeared. The combining of terms which led to (11) and (12) corresponds to the cancellation which Levinson [5, Sect. 10] found.

We now compute the integral in J_6. By repeated integration by parts we see that if P has N continuous derivatives then for $\alpha\neq 1$ and $0<A<B$,

$$\int_A^B P(\log v)\,v^\alpha dv=\sum_{n=0}^{N-1}(-1)^n\frac{P^{(n)}(\log v)}{(1+\alpha)^{n+1}}\,v^{1+\alpha}\Big|_A^B +\frac{(-1)^N}{(1+\alpha)^N}\int_A^B P^{(N)}(\log v)\,v^\alpha dv.$$

If P is a polynomial of degree $<N$ then the integral vanishes. Hence with $\phi_*(x)=\phi(x)(1-2x+\pi i/2L)^m$, so that $c_*(x)=\phi_*(L^{-1}\log x)$ and $d_*(x)=\phi_*(1-L^{-1}\log x)$, we have $J_6=J_7-J_8$, where

$$J_7=\frac{e^{2R}}{1-2a}\sum_{k_1,k_2}\sum\frac{b(k_1)\,b(k_2)}{k_1k_2}\,k^{2-2a}\sum_{n\geqslant 0}\frac{(-1)^n}{(2R)^n} \times\sum_{j=0}^{n}\binom{n}{j}\overline{\phi_*^{(j)}\left(1-\frac{\log k_1/k}{L}\right)}\,\phi_*^{(n-j)}\left(1-\frac{\log k_2/k}{L}\right)$$

and

$$J_8=\frac{1}{1-2a}\sum_{k_1,k_2}\sum\frac{b(k_1)\,b(k_2)}{k_1^{2a}k_2^{2a}}\,k^{2a}\sum_{n\geqslant 0}\frac{(-1)^n}{(2R)^n} \times\sum_{j=0}^{n}\binom{n}{j}\overline{\phi_*^{(j)}\left(\frac{\log(k_1/k)}{L}\right)}\,\phi_*^{(n-j)}\left(\frac{\log(k_2/k)}{L}\right). \tag{13}$$

Here we have used the fact that $\tau^{2-4a}=e^{2R}$. The sums over n are finite since ϕ_* is a polynomial.

6. The Mollifier

It is clear from (13) that we need to estimate the sums

$$S_{N_1,N_2}(\alpha)=\sum_{k_1,k_2}\sum\frac{b(k_1)\,b(k_2)}{k_1^{\alpha}k_2^{\alpha}}k^{2\alpha-2a}\left(L^{-1}\log\frac{k_1}{k}\right)^{N_1}\left(L^{-1}\log\frac{k_2}{k}\right)^{N_2} \quad (14)$$

for N_1 and N_2 non-negative integers. Evidently J_7 involves the sums $S_{N_1,N_2}(1)$ and J_8 the sums $S_{N_1,N_2}(2a)$. We apply the Möbius inversion formula to the part of $S_{N_1,N_2}(\alpha)$ which involves $k=\gcd(k_1,k_2)$. Thus

$$k^{\gamma}\left(\log\frac{k_1}{k}\right)^{N_2}\left(\log\frac{k_2}{k}\right)^{N_2}$$
$$=\sum_{j|k}j^{\gamma}\sum_{n_1=0}^{N_1}\sum_{n_2=0}^{N_2}\binom{N_1}{n_1}\binom{N_2}{n_2}\left(\log\frac{k_1}{j}\right)^{n_1}\left(\log\frac{k_2}{j}\right)^{n_2}g_j(N,\gamma),$$

where $\gamma=2\alpha-2a$, $N=N_1-n_1+N_2-n_2$, and

$$g_j(N,\gamma)=\sum_{d|j}\mu(d)\,d^{-\gamma}(\log d)^N.$$

We substitute this into (14) and interchange the summation on k_1 and k_2 with that on j. Hence

$$L^{N_1+N_2}S_{N_1,N_2}(\alpha)=\sum_{n_1=0}^{N_1}\sum_{n_2=0}^{N_2}\binom{N_1}{n_1}\binom{N_2}{n_2}\sum_{j\leqslant y}j^{\gamma}g_j(N,\gamma)\,T_j(n_1,\alpha)\,T_j(n_2,\alpha),$$

where

$$T_j(i,\alpha)=\sum_{\substack{k\leqslant y\\ k\equiv 0 \bmod j}}b(k)\,k^{-\alpha}\left(\log\frac{k}{j}\right)^{i}.$$

Let $k=nj$ and $x=y/j$. Then

$$T_j(i,\alpha)=(-1)^i j^{-\alpha}\frac{d^i}{d\alpha^i}\left(\sum_{n\leqslant x}b(nj)\,n^{-\alpha}\right). \quad (15)$$

For the coefficients $b(k)$ of the mollifier we take

$$b(k)=\frac{\mu(k)}{k^{1/2-a}}\,\hbar\left(\frac{\log y/k}{\log y}\right),$$

where $\hbar$ is a polynomial which satisfies $\hbar(1)=1$, so that $b(1)=1$, and $\hbar(0)=0$. We substitute this into (15) and see that

$$T_j(i,\alpha)=(-1)^i\mu(j)\,j^{-\beta}\,G_j^{(i)}(\beta),$$

where $\beta = \alpha - a + \frac{1}{2}$ and

$$G_j(\beta) = \sum_{\substack{n \leqslant x \\ (n,j)=1}} \mu(n)\, n^{-\beta}\, h\left(\frac{\log x/n}{\log y}\right).$$

Hence

$$L^{N_2+N_2} S_{N_1,N_2}(\alpha) = \sum_{n_1=0}^{N_1} \sum_{n_2=0}^{N_2} \binom{N_1}{n_1}\binom{N_2}{n_2}(-1)^{n_1+n_2}$$
$$\times \sum_{j \leqslant y} \frac{u^2(j)}{j} G_j^{(n_1)}(\beta)\, G_j^{(n_2)}(\beta)\, g_j(N, \gamma). \tag{16}$$

Denote the inner sum over j by $V_{N,n_1,n_2}(\alpha)$. We shall show that only those S_{N_1,N_2} with $\max\{N_1, N_2\} \leqslant 1$ are significant and for these only the V_{N,n_1,n_2} with $N=0$ (i.e., $n_1 = N_1, n_2 = N_2$) contribute significantly. First of all, $g_j(0, \gamma) = F(j, \gamma)$. Then by Cauchy's theorem,

$$g_j(N, \gamma) \ll F_1(j, 1 - 2\delta) \log^N L.$$

Next, by Lemma 11 and partial summation,

$$\sum_{j \leqslant y} \frac{\mu^2(j)}{j^{1-\varepsilon}} F_1^3(j, 1 - 2\delta) \ll \min\left\{\frac{y^\varepsilon}{\varepsilon}, \log y\right\}$$

for $\varepsilon \geqslant 0$. From Lemma 10 and these estimates it follows that

$$V_{N,n_1,n_2}(\alpha) \ll L^{n_1+n_2-1}(\log L)^{N+4}$$
$$\ll L^{N_1+N_2-2}(\log L)^5$$

if $N > 0$, and

$$V_{0,n_1,n_2}(\alpha) \ll L^{n_1+n_2-2}\log^5 L = L^{N_1+N_2-2}\log^5 L$$

if $\max\{n_1, n_2\} \geqslant 2$. Thus by (16) and the above,

$$S_{N_1,N_2}(\alpha) \ll L^{-2}\log^5 L \tag{17}$$

if $\max\{N_1, N_2\} \geqslant 2$, and $S_{0,0}(\alpha) = V_{0,0,0}(\alpha)$, $S_{0,1}(\alpha) = S_{1,0}(\alpha) = -V_{0,1,0}(\alpha)L^{-1} + O(L^{-2}\log^5 L)$, and $S_{1,1}(\alpha) = V_{0,1,1}(\alpha)L^{-2} + O(L^{-2}\log^5 L)$. Also by Lemma 10,

$$V_{0,0,0}(\alpha) = \sum_{j \leqslant y} \frac{\mu^2(j)}{j} \frac{F(j,\gamma)}{F^2(j,\beta)}\left[(\beta - 1)\, h\left(\frac{\log y/j}{\log y}\right)\right.$$
$$\left. + \frac{1}{\log y} h'\left(\frac{\log y/j}{\log y}\right)\right]^2 + O(L^{-2}\log^5 L).$$

It follows from Lemma 11 that

$$\sum_{j\leqslant y}\frac{\mu^2(j)}{j}\frac{F(j,y)}{F(j,\beta)^2}\left(\frac{\log y/j}{\log y}\right)^d = C_0\frac{\log y}{d+1}+O(1),$$

where it is easily seen that the constant C_0 is

$$=1+O\left(\frac{1}{|\frac{1}{2}-a|}\right)=1+O(L^{-1}).$$

Hence

$$V_{0,0,0}(\alpha)=(\beta-1)^2(\log y)\,P_1+2(\beta-1)\,P_2+\frac{1}{\log y}P_3+O(L^{-2}\log^5 L),$$

where

$$P_1=\int_0^1 h(t)^2\,dt,\ P_2=\int_0^1 h(t)\,h'(t)\,dt=\frac{1}{2},$$

and

$$P_3=\int_0^1 h'(t)^2\,dt.$$

Similarly, $V_{0,1,0}(\alpha)=(\beta-1)P_1\log y+P_2+O(L^{-1}\log^5 L)$ and $V_{0,1,1}(\alpha)=(\log y)\,P_1+O(\log^5 L)$. Therefore, since $\log y=L/2+O(1)$,

$$S_{0,0}(\alpha)=L^{-1}((\beta-1)^2L^2P_1/2+2(\beta-1)\,LP_2+2P_3)+O(L^{-2}\log^5 L),$$
$$S_{0,1}(\alpha)=S_{1,0}(\alpha)=-L^{-1}((\beta-1)\,LP_1/2+P_2)+O(L^{-2}\log^5 L),$$

and

$$S_{1,1}(\alpha)=L^{-1}P_1/2+O(L^{-2}\log^5 L).$$

Now we substitute these estimates for S_{N_1,N_2} into (13) and (14). We expand the polynomials $\phi_*^{(j)}(x)$ around $x=1$ in the case of J_7 and around $x=0$ for J_8. By (17) only the terms which involve $\log k_1/k$ or $\log k_2/k$ to a power smaller than the second are significant. Hence

$$\begin{aligned}J_7=\frac{e^{2R}}{1-2a}\sum_{n\geqslant 0}\frac{(-1)^n}{(2R)^n}\sum_{j=0}^{n}\binom{n}{j}&[\phi_*^{(j)}(1)\,\phi_*^{(n-j)}(1)\,S_{0,0}(1)\\&-(\phi_*^{(j+1)}(1)\,\phi_*^{(n-j)}(1)+\phi_*^{(j)}(1)\,\phi_*^{(n-j+1)}(1))\,S_{0,1}(1)\\&+\phi_*^{(j+1)}(1)\,\phi_*^{(n-j+1)}(1)\,S_{1,1}(1)]+O(L^{-1}\log^5 L)\end{aligned}$$

and

$$J_8 = \frac{1}{1-2a} \sum_{n \geqslant 0} \frac{(-1)^n}{(2R)^n} \sum_{j=0}^{n} \binom{n}{j} [\phi_*^{(j)}(0)\, \phi_*^{(n-j)}(0)\, S_{0,0}(2a)$$
$$+ (\phi_*^{(j+1)}(0)\, \phi_*^{(n-j)}(0) + \phi_*^{(j)}(0)\, \phi_*^{(n-j+1)}(0))\, S_{0,1}(2a)$$
$$+ \phi_*^{(j+1)}(0)\, \phi_*^{(n-j+1)}(0)\, S_{1,1}(2a)] + O(L^{-1} \log^5 L).$$

We can remove the $\pi i/2L$ term which appears in the definition of ϕ_*. Let $\phi_m(x) = \phi(x)(1-2x)^m$. Then

$$|\phi_*^{(j)}(x) - \phi_m^{(j)}(x)| \ll L^{-1}$$

for $0 \leqslant x \leqslant 1$. Thus, every ϕ_* which appears in the above expressions for J_7 and J_8 can be replaced by ϕ_m with a total error which is $\ll L^{-1}$.

Our expressions for J_7 and J_8 can be simplified considerably. We observe that $(\beta - 1) = \frac{1}{2} - a$ when $\alpha = 1$ and $\beta - 1 = a - \frac{1}{2}$ when $\alpha = 2a$ so that $(\beta - 1)\, L = \pm R$. Hence

$$J_7 = \frac{e^{2R}}{2R} \sum_{n \geqslant 0} \frac{(-1)^n}{(2R)^n} \left[\left(R^2 \frac{P_1}{2} + 2P_2 R + 2P_3\right) \Psi_1^{(n)}(1) \right.$$
$$\left. + \left(R \frac{P_1}{2} + P_2\right) 2\Psi_2^{(n)}(1) + \frac{P_1}{2} \Psi_3^{(n)}(1) \right] + O(L^{-1} \log^5 L),$$

and

$$J_8 = \frac{1}{2R} \sum_{n \geqslant 0} \frac{(-1)^n}{(2R)^n} \left[\left(R^2 \frac{P_1}{2} - 2P_2 R + 2P_3\right) \Psi_1^{(n)}(0) \right.$$
$$\left. - \left(P_2 - \frac{P_1}{2} R\right) \Psi_2^{(n)}(0) + \frac{P_1}{2} \Psi_3^{(n)}(0) \right] + O(L^{-1} \log^5 L),$$

where $\Psi_1(x) = \phi_m(x)^2$, $\Psi_2(x) = \phi_m(x)\, \phi_m'(x)$, and $\Psi_3(x) = \phi_m'(x)^2$. If $\Psi(x)$ is a polynomial, then by integrating by parts repeatedly we see that

$$\int_0^1 e^{2Rx}\, \Psi(x)\, dx = \frac{1}{2R} \sum_{n \geqslant 0} \frac{(-1)^n}{(2R)^n} (e^{2R} \Psi^{(n)}(1) - \Psi^{(n)}(0)).$$

Hence

$$J_7 - J_8 = \left(\frac{P_1}{2} R^2 + 2P_3\right) \int_0^1 e^{2Rx}\, \Psi_1(x)\, dx + P_1 R \int_0^1 e^{2Rx}\, \Psi_2(x)\, dx$$
$$+ \frac{P_1}{2} \int_0^1 e^{2Rx}\, \Psi_3(x)\, dx + W + O(L^{-1} \log^5 L),$$

where

$$W=\frac{P_2}{R}\sum_{n\geqslant 0}\frac{(-1)^n}{(2R)^n}\,[e^{2R}(R\Psi_1^{(n)}(1)+\Psi_2^{(n)}(1)) + (R\Psi_1^{(n)}(0)+\Psi_2^{(n)}(0))].$$

Since $\Psi_2(x)=\frac{1}{2}\Psi_1'(x)$, it follows that

$$\begin{aligned}\sum_{n\geqslant 0}\frac{(-1)^n}{(2R)^n}(R\Psi_1^{(n)}(x)+\Psi_2^{(n)}(x)) &= \frac{1}{2}\left(-\sum_{n\geqslant 0}\frac{(-1)^{n-1}}{(2R)^{n-1}}\Psi_1^{(n)}(x)+\sum_{n\geqslant 0}\frac{(-1)^n}{(2R)^n}\Psi_1^{(n+1)}(x)\right)\\ &= R\Psi_1(x).\end{aligned}$$

Hence $W=P_2(e^{2R}\Psi_1(1)+\Psi_1(0))=\frac{1}{2}(e^{2R}\Psi_1(1)+\Psi_1(0))$, since $P_2=\int_0^1 h(t)\,h'(t)\,dt=\frac{1}{2}(h(1)^2-h(0)^2)=\frac{1}{2}$. Let $\Phi=\int_0^1 e^{2Rx}\Psi_1(x)\,dx=\int_0^1 e^{2Rx}\,\phi_m(x)^2\,dx$ and let $\Phi'=\int_0^1 e^{2Rx}\Psi_3(x)\,dx=\int_0^1 e^{2Rx}\phi_m'(x)^2dx$. Then

$$\begin{aligned}\int_0^1 e^{2Rx}\Psi_2(x)\,dx &= \frac{1}{2}\int_0^1 e^{2Rx}(2\phi_m(x)\,\phi_m'(x))\,dx\\ &= \frac{1}{2}(e^{2R}\phi_m(1)^2-\phi_m(0)^2)-R\Phi.\end{aligned}$$

Recall that $\phi_m(0)=\phi(0)=1$ and $\phi_m(1)^2=\phi(1)^2$. Hence

$$J_7-J_8=\tfrac{1}{2}[(e^{2R}\phi(1)^2+1)+RP(e^{2R}\phi(1)^2-1)+P\Phi'+(4P'-R^2P)\,\Phi] + O(L^{-1}\log^5 L),$$

where we have written P for P_1 and P' for P_3. It follows from (5), (12), and (13) that

$$\alpha_m\geqslant 1-\inf\frac{\log F_m(R)}{R},$$

where

$$F_m(R)=\tfrac{1}{2}[(e^{2R}\phi(1)^2+1)+RP(e^{2R}\phi(1)^2-1)+P\Phi'+(4P'-R^2P)\,\Phi],$$

and the inf is over all $R>0$, all real polynomials h with $h(0)=0$ and $h(1)=1$, and all real polynomials ϕ satisfying $\phi(0)=1$ and $\phi'(x)=\phi'(1-x)$. It is clear that the inf will be the same if we require only that $\not{h}$ and ϕ be continuously differentiable on $[0, 1]$ and satisfy the same boundary conditions and functional equation, and that $R \geqslant 0$. We choose

$$\not{h}(x) = \frac{\sinh \Lambda x}{\sinh \Lambda},$$

where $\Lambda^2 = [\Phi' + R(e^{2R}\phi(1)^2 - 1) - R^2\Phi]/(4\Phi)$. Then $\not{h}(0) = 0$, $\not{h}(1) = 1$, and

$$F_m(R) = \tfrac{1}{2}(e^{2R}\phi(1)^2 + 1) + 2(P\Lambda^2 + P')\,\Phi.$$

It is easily verified that with this choice of $\not{h}$,

$$P\Lambda^2 + P' = \Lambda \coth \Lambda$$

from which the Theorem follows. (The choice of $\not{h}$ was made following a suggestion by K. Foster to use the calculus of variations.)

7. Proof of Corollary

To establish the numerical results of the Corollary we make appropriate choices of ϕ and R for the various values of m. It will be convenient to let

$$\phi(x) = \beta_0 + \sum_{i \geqslant 1} \beta_i (1 - 2x)^{2i-1},$$

where $\sum \beta_i = 1$. Then it is clear that $\phi(0) = 1$ and $\phi'(x) = \phi'(1 - x)$. We choose R and ϕ for $0 \leqslant m \leqslant 5$ as listed here.

m	0	1	2	3	4	5
R	1.475231	1.209994	1.302341	1.539005	1.905703	2.007073
β_0	0.488490	0.497750	0.500933	0.500345	0.500089	0.500096
β_1	0.669654	0.996201	1.262516	1.403534	1.402774	1.060701
β_2	−0.252488	−1.274186	−1.977039	−2.290576	−2.189703	−0.896136
β_3	0.124709	1.242630	1.890841	2.117707	1.924119	0.335339
β_4	−0.030365	−0.462395	−0.677251	−0.731010	−0.637279	—
$1 - \frac{\log F_m(R)}{R}$	0.36581	0.81378	0.95844	0.98731	0.99484	0.99702

The values in the last row are truncations of the actual values. These choices of R and ϕ were found using a conjugate gradient algorithm for minimizing a function of several variables.

To prove the second assertion in the Corollary we take $R = 1$ and

$\phi(x) = 1 - x$ so that $\phi(1) = 0$. If $f \in C^2[0, 1]$ and $M = \max_{0 \leqslant x \leqslant 1} |f(x)|$, then by integrating by parts twice,

$$\int_0^1 f(x)(1-2x)^n \, dx$$
$$= \frac{(-1)^n f(1) + f(0)}{2(n+1)} + \frac{(-1)^{n+1} f'(1) + f'(0)}{4(n+1)(n+2)} + O\left(\frac{M}{n^3}\right).$$

Hence with obvious choices of f and n we obtain

$$\Phi = \int_0^1 e^{2x}(1-x)^2(1-2x)^{2m} dx = \frac{1}{2(2m+1)} + O\left(\frac{1}{m^3}\right)$$
$$= \frac{1}{4m} - \frac{1}{8m^2} + O\left(\frac{1}{m^3}\right),$$

and

$$\Phi' = \int_0^1 e^{2x}(2m+1-(2m+2)\,x)^2(1-2x)^{2m-2} \, dx$$
$$= \frac{e^2 + (2m+1)^2}{2(2m-1)} + \frac{-2e^2(2m+3) - 2(2m+1)}{4(2m-1)(2m)} + O\left(\frac{1}{m}\right)$$
$$= m + \frac{3}{2} + O\left(\frac{1}{m}\right).$$

Therefore,

$$\Lambda^2 = (\Phi' - 1 - \Phi)/(4\Phi) \gg m^2$$

so that $\coth \Lambda = 1 + O(e^{-2m})$, and

$$F_m(1) = \tfrac{1}{2} + 2\Phi\Lambda \coth \Lambda = \tfrac{1}{2} + \sqrt{\Phi(\Phi' - 1 - \Phi)}(1 + O(e^{-2m}))$$
$$= \tfrac{1}{2} + \sqrt{1/4(1 + O(m^{-2}))}(1 + O(e^{-2m})) = 1 + O(m^{-2}).$$

Hence $\log F_m \ll m^{-2}$ and we have verified the Corollary.

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