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On the zeros of Dirichlet L-functions

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Abstract

This paper [1], which was published online on 1 June 2011, has been retracted by agreement between the authors, the journal's Editor-in-Chief Derek Holt, the London Mathematical Society and Cambridge University Press. The retraction was agreed to prevent other authors from using incorrect mathematical results. (In this paper, we compute and verify the positivity of the Li coefficients for the Dirichlet L-functions using an arithmetic formula established in Omar and Mazhouda, *J. Number Theory* 125 (2007) no. 1, 50–58; J. Number Theory 130 (2010) no. 4, 1109–1114. Furthermore, we formulate a criterion for the partial Riemann hypothesis and we provide some numerical evidence for it using new formulas for the Li coefficients.)

1. *Introduction*

The Li criterion for the Riemann hypothesis (see [7]) is a necessary and sufficient condition that the sequence

$$\lambda_n = \sum_{\rho} \left[1 - \left(1 - \frac{1}{\rho} \right)^n \right]$$

is non-negative for all $n \in \mathbb{N}$ and where ρ runs over the non-trivial zeros of $\zeta(s)$. This criterion holds also for the Dirichlet L-functions and for a large class of Dirichlet series, the so-called Selberg class as given in [11]. More recently, Omar and Bouanani [10] extended the Li criterion for function fields and established an explicit and asymptotic formula for the Li coefficients.

Numerical computation of the first 100 of the Li coefficients λ_n which appear in this criterion was made by Maślanka in [9] and later by Coffey [3], who computed and verified the positivity of about 3300 of the Li coefficients λ_n. The main empirical observation made by Maślanka is that these coefficients can be separated into two parts, where one of them grows smoothly while the other is very small and oscillatory. This apparent smallness is quite unexpected. If it persisted until infinity then the Riemann hypothesis would be true. As we said above, this criterion was extended to a large class of Dirichlet series [11] and no calculation or verification of the positivity to date in the literature was made for other L-functions.

In this paper, we compute and verify the positivity of the Li coefficients for the Dirichlet L-functions using an arithmetic formula established in [11, 12]. Furthermore, we formulate a criterion for the partial Riemann hypothesis. Additional results are presented, including new formulas for the Li coefficients. Based on the numerical computations made below, we conjecture that these coefficients are increasing in n. Should this conjecture hold, the validity of the Riemann hypothesis would follow.

Next, we review the Li criterion for the case of the Dirichlet L-functions. Let χ be a primitive Dirichlet character of conductor q. The Dirichlet L-function attached to this character is defined by

$$L(s, \chi) = \sum_{n=1}^{\infty} \frac{\chi(n)}{n^s} \quad (\mathrm{Re}(s) > 1).$$

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For the trivial character $\chi = 1$, $L(s,\chi)$ is the Riemann zeta function. It is well known [4] that if $\chi \neq 1$ then $L(s,\chi)$ can be extended to an entire function in the whole complex plane and satisfies the functional equation

$$\xi(s,\chi) = \omega_\chi \xi(1-s,\overline{\chi}),$$

where

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

$$a = \begin{cases} 0 & \text{if } \chi(-1) = 1, \\ 1 & \text{if } \chi(-1) = -1, \end{cases} \quad \text{and} \quad \omega_\chi = \frac{\tau(\chi)}{\sqrt{q}\, i^a},$$

where $\tau(\chi)$ is the Gauss sum

$$\tau(\chi) = \sum_{m=1}^{q} \chi(m) e^{2\pi i m/q}.$$

The function $\xi(s,\chi)$ is an entire function of order one. The function $\xi(s,\chi)$ has a product representation

$$\xi(s,\chi) = \xi(0,\chi) \prod_\rho \left(1 - \frac{s}{\rho}\right), \tag{1}$$

where the product is over all the zeros of $\xi(s,\chi)$ in the order given by $|\mathrm{Im}(\rho)| < T$ for $T \to \infty$. If $N_\chi(T)$ counts the number of zeros of $L(s,\chi)$ in the rectangle $0 \leqslant \mathrm{Re}(s) \leqslant 1$, $0 < \mathrm{Im}(s) \leqslant T$ (according to multiplicities), one can show by standard contour integration the formula

$$N_\chi(T) = \frac{1}{2\pi} T \log T + c_1 T + O(\log T),$$

where

$$c_1 = \frac{1}{2\pi}(\log q - (\log(2\pi) + 1)).$$

We put

$$\lambda_\chi(n) = \sum_\rho \left[1 - \left(1 - \frac{1}{\rho}\right)^n\right],$$

where the sum over ρ is $\sum_\rho = \lim_{T \mapsto \infty} \sum_{|\mathrm{Im}(\rho)| \leqslant T}$.

Li's criterion says that $\lambda_\chi(n) > 0$ for all $n = 1, 2, \ldots$ if and only if all of the zeros of $\xi(s,\chi)$ are located on the critical line $\mathrm{Re}(s) = 1/2$.

The paper is organized as follows. In Section 2, we recall the arithmetic formula for the Li coefficients for the Dirichlet L-functions and we give an estimate for the error term of $\lambda_\chi(n)$. In Section 3, we show that $\lambda_\chi(n) \geqslant 0$ if every non-trivial zero of $L(s,\chi)$ with $|\mathrm{Im}(\rho)| < \sqrt{n}$ satisfies $\mathrm{Re}(\rho) = 1/2$ (that is the partial Riemann hypothesis) and we give an estimate for the difference $|\lambda_\chi(n) - \lambda_\chi(n,T)|$, where $\lambda_\chi(n,T)$ are the partial Li coefficients. In Section 4, we prove new formulas (integral and summation formulas) for the Li coefficients $\lambda_\chi(n)$. Finally, in Section 5, we report numerical computations of the Li coefficients using different formulas established in the previous sections unconditionally or under the Riemann hypothesis.

2. *Li's coefficients*

Applying [11, Theorem 2.2] for the case of the Dirichlet L-functions, we get the following arithmetic formula.

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THEOREM 1. *Let χ be a primitive Dirichlet character of conductor $q > 1$. We have*

$$\lambda_\chi(n) = -\sum_{j=1}^{n} \binom{n}{j} \frac{(-1)^{j-1}}{(j-1)!} \sum_{k=1}^{+\infty} \frac{\Lambda(k)}{k} \chi(k)(\log k)^{j-1} + \frac{n}{2}\left(\log \frac{q}{\pi} - \gamma\right) + \tau_\chi(n), \tag{2}$$

where

$$\tau_\chi(n) = \begin{cases} \displaystyle\sum_{j=2}^{n} \binom{n}{j} (-1)^j \left(1 - \frac{1}{2^j}\right)\zeta(j) - \frac{n}{2}\sum_{l=1}^{+\infty} \frac{1}{l(2l-1)} & \text{if } \chi(-1) = 1, \\ \displaystyle\sum_{j=2}^{n} \binom{n}{j} (-1)^j 2^{-j} \zeta(j) & \text{if } \chi(-1) = -1. \end{cases}$$

Theorem 1 was also proved by Coffey in [3] and Li in [8]. The arithmetic formula above can be written as

$$\lambda_\chi(n) = \left[\log \frac{q}{\pi} + \psi\left(\frac{a+1}{2}\right)\right]\frac{n}{2} + \sum_{j=2}^{n} \binom{n}{j} \frac{1}{(j-1)!} 2^{-j} \psi^{(j-1)}\left(\frac{a+1}{2}\right) - \sum_{j=1}^{n} \binom{n}{j} \frac{(-1)^{j-1}}{(j-1)!} \sum_{k=1}^{+\infty} \frac{\Lambda(k)\chi(k)}{k} (\log k)^{j-1},$$

where $a = 0$ if $\chi(-1) = 1$ and 1 if $\chi(-1) = -1$, with $\psi(\frac{1}{2}) = -\gamma - 2\log 2$, $\psi(1) = -\gamma$ (γ is the Euler constant), $\psi^{(j-1)}(1) = (-1)^j (j-1)! \zeta(j)$ and $\psi^{(j-1)}(\frac{1}{2}) = (-1)^{j+1} j! (2^{j+1} - 1)\zeta(j+1)$. Here, $\psi = \Gamma'/\Gamma$ denotes the digamma function.

An asymptotic formula for the number $\lambda_\chi(n)$ was proved in [13, Theorem 3.1] using the arithmetic formula. Furthermore, it is equivalent to the Riemann hypothesis.

THEOREM 2. *We have*

$$\text{RH} \Leftrightarrow \lambda_\chi(n) = \tfrac{1}{2} n \log n + c_\chi n + O(\sqrt{n} \log n),$$

where

$$c_\chi = \tfrac{1}{2}(\gamma - 1) + \tfrac{1}{2}\log(q/\pi)$$

and γ is the Euler constant.

Here, we estimate the error term for $\lambda_\chi(n)$ using the arithmetic formula (2). We write (2) in the form

$$\lambda_\chi(n) = \tilde{\lambda}_\chi(n, M) + E_M,$$

where

$$\tilde{\lambda}_\chi(n, M) = \frac{n}{2}\left(\log \frac{q}{\pi} - \gamma\right) + \tau_\chi(n) - \sum_{j=1}^{n} \binom{n}{j} \frac{(-1)^{j-1}}{(j-1)!} \sum_{k \leqslant M} \frac{\Lambda(k)}{k} \chi(k)(\log k)^{j-1} \tag{3}$$

and

$$E_M = -\sum_{j=1}^{n} \binom{n}{j} \frac{(-1)^{j-1}}{(j-1)!} \sum_{k > M} \frac{\Lambda(k)}{k} \chi(k)(\log k)^{j-1} = -\sum_{k > M} \frac{\Lambda(k)}{k} \chi(k) L_{n-1}^1(\log k),$$

where L_{n-1}^1 is an associated Laguerre polynomial of degree $n - 1$.

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Next, for our computation in Section 5, we need to find M such that $|E_M| \leqslant 10^{-\nu}$. An estimate for the Laguerre polynomials is due to Koepf and Schmersau [6, Theorem 2]. Actually, they have shown that

$$|L_n^{\alpha}(x)| < e^{x/2}[(n+\alpha)/x]^{\alpha/2}$$

for $x \in [0, 4(n+\alpha)]$ when $n+\alpha > 0$ and α is an integer. Then we obtain

$$|E_M| \leqslant \sqrt{\frac{n}{\log M}} \sum_{m>M}^{+\infty} \frac{\Lambda(m)}{m} |\chi(m)| \leqslant \sqrt{\frac{n}{\log M}} \sum_{p^j>M}^{+\infty} \frac{\log p}{p^j} |\chi(p^j)|. \tag{4}$$

We have $|\chi(p^j)| < 1$. Therefore,

$$|E_M| \leqslant \sqrt{\frac{n}{\log M}} \sum_{p^j>M}^{+\infty} \frac{\log p}{p^j} \leqslant \begin{cases} \sqrt{\dfrac{n}{\log M}} \dfrac{\log M}{M} \leqslant \sqrt{n} \dfrac{\log M}{M} & \text{if } M+1 \text{ is prime,} \\ \sqrt{\dfrac{n}{\log M}} \dfrac{1}{M} \leqslant \dfrac{\sqrt{n}}{M} & \text{otherwise.} \end{cases} \tag{5}$$

Let M be such that $|E_M| \leqslant 10^{-\nu}$. Then

$$\begin{cases} \sqrt{n} \dfrac{\log M}{M} \leqslant 10^{-\nu} & \text{if } M+1 \text{ is prime,} \\ \dfrac{\sqrt{n}}{M} \leqslant 10^{-\nu} & \text{otherwise.} \end{cases}$$

Using the theory of the Lambert W function, we choose

$$M = \begin{cases} -\sqrt{n}\, W_{-1}\left(-\dfrac{10^{-\nu}}{\sqrt{n}} \right) & \text{if } M+1 \text{ is prime,} \\ \sqrt{n} 10^{\nu} & \text{otherwise,} \end{cases} \tag{6}$$

where W_{-1} denotes the branch satisfying $W(x) \leqslant -1$ and $W(x)$ is the Lambert W function, which is defined to be the multivalued inverse of the function $w \longmapsto we^w$.

3. *Partial Li criterion*

In the following proposition, we propose a partial Li criterion which relates the partial Riemann hypothesis to the positivity of the Li coefficients up to a certain order.

PROPOSITION 1. *If every non-trivial zero ρ of $L(s, \chi)$ with $|\mathrm{Im}(\rho)| < T^2$ satisfies $\mathrm{Re}(\rho) = 1/2$, then $\lambda_\chi(n) \geqslant 0$ for all $n \leqslant T$.*

Proof. We have

$$\lambda_\chi(n) = \sum_\rho \left[1 - \left(1 - \frac{1}{\rho} \right)^n \right].$$

Note that there are $O(\log u)$ zeros in $[u, u+1]$. Then

$$\begin{aligned} \lambda_\chi(n) &= \sum_\rho \left[1 - \mathrm{Re}\left(1 - \frac{1}{\rho} \right)^n \right] \\ &= \sum_{\rho;|\mathrm{Im}(\rho)|<T^2} \left[1 - \mathrm{Re}\left(1 - \frac{1}{\rho} \right)^n \right] + \sum_{\rho;T^2<|\mathrm{Im}(\rho)|<T^2(\log T)^2} \left[1 - \mathrm{Re}\left(1 - \frac{1}{\rho} \right)^n \right] \\ &\quad + \sum_{\rho;|\mathrm{Im}(\rho)|>T^2(\log T)^2} \left[1 - \mathrm{Re}\left(1 - \frac{1}{\rho} \right)^n \right]. \end{aligned} \tag{7}$$

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Let $\rho = \beta + i\gamma$; then we obtain

$$1 - \left(1 - \frac{1}{\rho}\right)^n = 1 - \left(\frac{1 + (\beta - 1)/i\gamma}{1 + \beta/i\gamma}\right)^n, \quad \frac{1 + (\beta - 1)/i\gamma}{1 + \beta/i\gamma} = \left(1 - \frac{\beta}{\gamma^2}\right) + \frac{i}{\gamma} + O\left(\frac{1}{\gamma^3}\right)$$

and

$$\mathrm{Re}\left(\frac{1 + (\beta - 1)/i\gamma}{1 + \beta/i\gamma}\right)^n = \left(1 - \frac{\beta}{\gamma^2}\right)^n + O\left(\frac{1}{\gamma^4}\right).$$

Therefore,

$$\begin{aligned} \sum_{|\gamma| > T^2 \log T} \left[1 - \mathrm{Re}\left(1 - \frac{1}{\rho}\right)^n\right] &= \sum_{|\gamma| > T^2 \log T} \left[1 - \left(1 - \frac{\beta}{\gamma^2}\right)^n + O\left(\frac{1}{\gamma^4}\right)\right] \\ &= \sum_{|\gamma| > T^2 \log T} \frac{n\beta}{\gamma^2} + O\left(\frac{1}{\gamma^4}\right) \\ &= O(1). \end{aligned} \tag{8}$$

And,

$$\begin{aligned} \sum_{T^2 < |\gamma| < T^2 (\log T)^2} \left[1 - \mathrm{Re}\left(1 - \frac{1}{\rho}\right)^n\right] &= \sum_{T^2 < |\gamma| < T^2 (\log T)^2} \left[1 - \left(1 - \frac{\beta}{\gamma^2}\right)^n + O\left(\frac{1}{\gamma^4}\right)\right] \\ &= \sum_{T^2 < |\gamma| < T^2 (\log T)^2} \frac{n\beta}{\gamma^2} + O\left(\frac{1}{\gamma^4}\right) \\ &= O((\log T)^3). \end{aligned} \tag{9}$$

Indeed, since $n \leqslant T$, we obtain

$$\begin{aligned} \sum_{T^2 < |\gamma| < T^2 (\log T)^2} \frac{n\beta}{\gamma^2} &\ll (\log T) \left[\sum_{j = T^2}^{T^2 (\log T)^2} \frac{n}{j}\right] \\ &\ll T \log T \left[\sum_{j = T^2}^{T^2 (\log T)^2} \frac{1}{j}\right] \\ &\ll T \log T \left[\frac{(\log T)^2}{T}\right] \\ &\ll (\log T)^3. \end{aligned}$$

Finally, it suffices to prove that, under the Riemann hypothesis, there exists a positive constant c_0 such that

$$\sum_{|\mathrm{Im}(\rho)| < T^2} \left[1 - \mathrm{Re}\left(1 - \frac{1}{\rho}\right)^n\right] \geqslant c_0 T \log T. \tag{10}$$

Thus,

$$\begin{aligned} \sum_{|\gamma| < T^2} \left[1 - \mathrm{Re}\left(1 - \frac{1}{\rho}\right)^n\right] &\geqslant \sum_{|\gamma| < T^2} \frac{n^2}{2\gamma^2} \\ &\geqslant \frac{T^2}{2} \sum_{|\gamma| < T} \frac{1}{\gamma^2} \\ &\geqslant \frac{1}{2} N_\chi(T). \end{aligned} \tag{11}$$

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Recall that

$$N_\chi(T) = \frac{1}{2\pi} T \log T + c_1 T + O(\log T).$$

Then (10) is proved. □

REMARK.

- Recall that the 10^{13} first zeros of the Riemann zeta function lie on the line $\mathrm{Re}(s) = 1/2$ (see [5]). Then, from Proposition 1, the first 10^6 Li coefficients $\lambda_\zeta(n)$ are non-negative.
- In Section 5, we will use the first 10^4 critical zeros of the Dirichlet L-functions to compute the first Li coefficients $\lambda_\chi(n)$. Then, from Proposition 1 above, we affirm that the first 100 Li coefficients are non-negative.

Conversely. From the work of Brown [2], the first observation is that the first 'non-trivial' inequality $\lambda_\chi(2) \geqslant 0$ is sufficient to establish the non-existence of a Siegel zero for $\xi(s,\chi)$ (see [2, Corollary 1]).

Let $r > 1$ be a real number. By the invariance of the zeros ρ of $\xi(s,\chi)$ under the map $\rho \longmapsto 1 - \overline{\rho}$,

$$\forall \rho, \quad \left| \frac{\rho}{\rho - 1} \right| \leqslant r \Leftrightarrow \forall \rho, \rho \in D_r,$$

where D_r is the closed region bounded by the lines $\{z \in \mathbb{C} : \mathrm{Re}(z) = 0, 1\}$ and the arcs of two circles. The second observation (see [2, Theorem 3]) is that, for large $N \in \mathbb{N}$, the inequalities $\lambda_\chi(1) \geqslant 0, \ldots, \lambda_\chi(n) \geqslant 0$ imply the existence of a certain zero-free region for $\xi(s,\chi)$, that is, there exist constants N, μ, ν depending only on q such that if $\lambda_\chi(1) \geqslant 0, \ldots, \lambda_\chi(n) \geqslant 0$ hold, and $n \geqslant N$, then the zeros of $\xi(s,\chi)$ belong to D_r, where $r = \sqrt{1 + T^{-2}}$ and $T = (n/\mu \log^2(\nu n))^{1/3}$.

Let us define the partial Li coefficients by

$$\lambda_\chi(n,T) = \sum_{\rho; |\mathrm{Im}\,\rho| \leqslant T} 1 - \left(1 - \frac{1}{\rho}\right)^n$$

with a parameter T. An estimate for the error term $|\lambda_\chi(n) - \lambda_\chi(n,T)|$ is stated in the following proposition.

PROPOSITION 2. *We have*

$$|\lambda_\chi(n) - \lambda_\chi(n,T)| \leqslant \frac{3n^2}{2T^2} \left[\frac{1}{2\pi} T \log T + \left(\frac{1}{\pi} + \log\left(\frac{q}{2\pi e} \right) \right) T + \frac{1}{2} \right]. \tag{12}$$

Proof. Note that $\rho = \beta + i\gamma$, where β, $\gamma \in \mathbb{R}$ and $0 \leqslant \beta \leqslant 1$. We have

$$\lambda_\chi(n) - \lambda_\chi(n,T) = \frac{1}{2} \mathrm{Re} \left[\sum_{|\gamma| > T} \left(2 - \left(\frac{\rho - 1}{\rho} \right)^n - \left(\frac{\rho}{\rho - 1} \right)^n \right) \right].$$

Using a binomial expansion of the inner term in the sum in the right-hand side, we obtain

$$\mathrm{Re}\left[2 - \left(\frac{\rho - 1}{\rho} \right)^n - \left(\frac{\rho}{\rho - 1} \right)^n \right] = \mathrm{Re}\left[n \left(\frac{1}{\rho} + \frac{1}{1 - \rho} \right) - \frac{n(n-1)}{2} \left(\frac{1}{\rho^2} + \frac{1}{(1 - \rho)^2} \right) \right] + \mathrm{Re}\left[\sum_{k=3}^{n} \binom{n}{k} (-1)^{k-1} (\rho^{-k} + (1 - \rho)^{-k}) \right]. \tag{13}$$

We have

$$\frac{1}{1 + \gamma^2} \leqslant \mathrm{Re}\left(\frac{1}{\rho} + \frac{1}{1 - \rho} \right) \leqslant \frac{1}{\gamma^2}$$

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and

$$\frac{1}{1+\gamma^2} - \frac{2}{\gamma^4} \leqslant \mathrm{Re}\left(\frac{1}{\rho^2} + \frac{1}{(1-\rho)^2}\right) \leqslant \frac{2}{\gamma^2}.$$

Suppose now that $|\gamma| \geqslant T \geqslant n$; then $(n-3)/|\gamma| \ldots (n-k)/|\gamma| \leqslant 1$ for all $n \geqslant k \geqslant 3$. Then

$$\sum_{k=3}^{n} \binom{n}{k} \frac{1}{|\gamma|^k} \leqslant 2\frac{n^3}{|\gamma|^3} \sum_{k=3}^{\infty} \frac{1}{k!} = (2e-5)\frac{n^3}{|\gamma|^3} \leqslant \frac{n^3}{2|\gamma|^3}.$$

Therefore,

$$\begin{aligned} \mathrm{Re}\left[2 - \left(\frac{\rho-1}{\rho}\right)^n - \left(\frac{\rho}{\rho-1}\right)^n\right] &\leqslant \frac{n}{\gamma^2} + \frac{n^2-n}{\gamma^2} + \sum_{k=3}^{n} \binom{n}{k} \frac{2}{|\gamma|^k} \\ &\leqslant \frac{n}{\gamma^2} + \frac{n^3}{2|\gamma|^3} \\ &\leqslant \frac{3n^2}{2|\gamma|^2}. \end{aligned} \tag{14}$$

Then

$$|\lambda_\chi(n) - \lambda_\chi(n,T)| \leqslant \frac{3}{4} n^2 \sum_{|\gamma|>T} \frac{1}{\gamma^2}.$$

We have

$$\frac{1}{2} \sum_{|\gamma|>T} \frac{1}{\gamma^2} \leqslant \int_T^\infty -\frac{d}{dt}[t^{-2}]_{t=x}(N_\chi(x) - N_\chi(T))\,dx = \int_T^\infty x^{-2}\,dN_\chi(x). \tag{15}$$

Furthermore,

$$\begin{aligned} \int_T^\infty x^{-2}\,dN_\chi(x) &= \int_T^\infty x^{-2}\left[\frac{1}{2\pi}\log x + \frac{1}{2\pi} + \log\left(\frac{q}{2\pi e}\right) + \frac{1}{x}\right]dx \\ &= T^{-2}\left[\frac{1}{2\pi}\log T + \frac{1}{2\pi}T\log T + \frac{1}{2\pi}T + \log\left(\frac{q}{2\pi e}\right)T + \frac{1}{2}\right]. \end{aligned}$$

Finally, we get

$$|\lambda_\chi(n) - \lambda_\chi(n,T)| \leqslant \frac{3}{2}\frac{n^2}{T^2}\left[\frac{1}{2\pi}T\log T + \left(\frac{1}{\pi} + \log\left(\frac{q}{2\pi e}\right)\right)T + \frac{1}{2}\right]$$

and Proposition 2 follows. □

For our computations at the end of this paper, we need to find T_0 such that $|\lambda_\chi(n) - \lambda_\chi(n,T)| \leqslant 10^{-k}$. To do so, it suffices to find T_0 such that

$$\frac{3n^2}{4\pi}\frac{\log T}{T} \leqslant \frac{10^{-k}}{3} \Leftrightarrow \frac{\log T}{T} \leqslant \frac{4\pi 10^{-k}}{9n^2}.$$

Using the theory of the Lambert W function, we get

$$T_0 = -\frac{9n^2}{4\pi} W_{-1}\left(-\frac{4\pi}{9n^2}10^{-k}\right),$$

where W_{-1} denotes the branch satisfying $W(x) \leqslant -1$ and $W(x)$ is the Lambert W function, which is defined to be the multivalued inverse of the function $w \longmapsto we^w$.

4. *New formulas for the Li coefficients*

In this section, we give new formulas for the Li coefficients under the Riemann hypothesis (integral and summation formulas) which will be used to compute and verify the positivity of the Li coefficients $\lambda_\chi(n)$ under the Riemann hypothesis.

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From (1), we have

$$\log\xi\left(\frac{z}{z-1},\chi\right)=\log\xi\left(\frac{1}{1-z},\chi\right)=\log\xi(0,\chi)+\sum_{n=1}^{\infty}\lambda_\chi(n)\frac{z^n}{n}. \tag{16}$$

The number $\lambda_\chi(n)$ does not depend on the choice of the logarithm. Rewrite (16) at the point $z=-1$. Note that the region of convergence for this is an open disk of radius 2 centered at $z=-1$ and it encloses in particular the entirety of the closed unit disk, except for the point $z=1$ that is a pole of $\xi(1/(1-z),\chi)$.

Assume that the Riemann hypothesis holds. Then we have

$$\begin{aligned}\log\xi\left(\frac{1}{1-z},\chi\right)&=\log\xi(0,\chi)+\sum_{n=1}^{\infty}\lambda_\chi(n)\frac{z^n}{n}\\&=C_\chi(0)+\sum_{n=1}^{\infty}C_\chi(n)(z+1)^n.\end{aligned} \tag{17}$$

Expanding $(z+1)^n$, we obtain

$$\lambda_\chi(n)=n\sum_{j=1}^{\infty}\binom{j}{n}C_\chi(j). \tag{18}$$

We have

$$N_\chi(T)=\frac{1}{\pi}\mathrm{Im}\left(\log\xi_\chi\left(\frac{1}{2}+iT\right)\right)=\sum_{n=1}^{\infty}\frac{C_\chi(n)}{\pi}\left(\mathrm{Im}\left(\frac{2\gamma+i}{2\gamma-i}+1\right)\right)^n, \tag{19}$$

where we have used the substitution $\frac{1}{2}+i\gamma=1/(1-z)$ or $z=(2\gamma+i)/(2\gamma-i)$. Then, since

$$\left(\mathrm{Im}\left(\frac{2\gamma+i}{2\gamma-i}+1\right)\right)^n=\frac{(4\gamma)^n}{(4\gamma^2+1)^{n/2}}\sin\left(n\tan^{-1}\frac{1}{2\gamma}\right)=2^n\cos^n\theta\sin(n\theta),$$
$$\cos\theta:=\frac{2\gamma}{\sqrt{4\gamma^2+1}},$$

we get

$$\pi N_\chi(\gamma)=\sum_{n=1}^{\infty}C_\chi(n)2^n\cos^n\theta\sin(n\theta).$$

Using the identity

$$\int_0^{\pi/2}\cos^n\theta\sin(n\theta)\sin(2m\theta)\,d\theta=\frac{\pi}{2^{n+2}}\binom{n}{m},\quad m,n\in\mathbb{N},$$

we deduce that

$$\int_0^{\pi/2}\pi N_\chi(\gamma)\sin(2m\theta)\,d\theta=\sum_{n=1}^{\infty}C_\chi(n)\frac{\pi}{4}\binom{n}{m}.$$

Hence,

$$\sum_{n=1}^{\infty}C_\chi(n)\binom{n}{m}=4\int_0^{\pi/2}N_\chi(\gamma)U_{m-1}(\cos(2\theta))\sin(2\theta)\,d\theta,$$

where U_{m-1} are the Chebyschev polynomials of the second kind. Using

$$U_{m-1}(\cos\theta):=\frac{\sin(m\theta)}{\sin(\theta)},\quad\cos(2\theta)=\cos^2\theta-\sin^2\theta=\frac{4\gamma^2-1}{4\gamma^2+1},$$
$$\sin(2\theta)\,d\theta=-2\cos\theta\,d(\cos\theta)$$

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and that as γ proceeds from 0 to ∞, θ subtends an angle from $\pi/2$ to 0, we obtain

$$\sum_{n=1}^{\infty} C_\chi(n)\binom{n}{m} = 8\int_0^\infty N_\chi(\gamma)U_{m-1}\left(\frac{4\gamma^2-1}{4\gamma^2+1}\right) \times \frac{2\gamma}{\sqrt{4\gamma^2+1}} \times \frac{2}{(4\gamma^2+1)^{3/2}}\,d\gamma.$$

Therefore, from (18) we get for all $n \in \mathbb{N}$ the following proposition.

PROPOSITION 3. *Under the Riemann hypothesis, we have*

$$\lambda_\chi(n) = 32n\int_0^\infty \frac{\gamma}{(4\gamma^2+1)^2}N_\chi(\gamma)U_{n-1}\left(\frac{4\gamma^2-1}{4\gamma^2+1}\right)d\gamma. \tag{20}$$

Next, we give another formula for the Li coefficients. Recall that the function $N_\chi(T)$ is a real step function, increasing by unity each time a new critical zero is counted:

$$N_\chi(T) = \sum_{\rho,\mathrm{Im}(\rho)>0} \phi(T-\mathrm{Im}(\rho)) = \sum_{k=1}^{\infty} \alpha_k \phi(T-\gamma_k), \tag{21}$$

where $\rho_j = \beta_k + i\gamma_k, \gamma_k > 0$ and $\phi(x-a) = 1$ if $x \geqslant a$ and 0 if $x < a$. The zeros are ordered so that $\gamma_{k+1} > \gamma_k$ and the α_k count the number of zeros with imaginary part γ_k including the multiplicities. Simplification of the integral formula (20) is stated in the following proposition.

PROPOSITION 4. *Under the Riemann hypothesis, we have*

$$\lambda_\chi(n) = 2\sum_{k=1}^{\infty}\alpha_k\left(1 - T_n\left(\frac{4\gamma_k^2-1}{4\gamma_k^2+1}\right)\right), \quad n \in \mathbb{N}.$$

Proof. By (21), the formula (20) can be written as follows:

$$\begin{aligned}
\lambda_\chi(n) &= 32n\sum_{k=1}^{\infty}\alpha_k\int_0^\infty \phi(\gamma-\gamma_k)\frac{\gamma}{(4\gamma^2+1)^2}U_{n-1}\left(\frac{4\gamma^2-1}{4\gamma^2+1}\right)d\gamma \\
&= 2n\sum_{k=1}^{\infty}\alpha_k\int_{\gamma_k}^\infty \frac{16\gamma}{(4\gamma^2+1)^2}U_{n-1}\left(\frac{4\gamma^2-1}{4\gamma^2+1}\right)d\gamma \\
&= 2n\sum_{k=1}^{\infty}\alpha_k\left[\frac{1}{n}T_n(y)\right]_{(4\gamma_k^2-1)/(4\gamma_k^2+1)}^{1} \\
&= 2\sum_{k=1}^{\infty}\alpha_k\left(1 - T_n\left(\frac{4\gamma_k^2-1}{4\gamma_k^2+1}\right)\right),
\end{aligned}$$

using the following relation between the Chebyshev polynomials of the second kind and the first kind:

$$\int U_n(x)\,dx = \frac{1}{n+1}T_{n+1}(x). \qquad \square$$

This is a remarkable summation expression for the Li coefficients. We numerically evaluate some of the first terms by the right-hand-side expression and find them to be indeed close to the required values of the Li coefficients. This is reassuring, and the results are presented in the tables below.

Under the Riemann hypothesis, from the above arguments used in the proof of Propositions 3 and 4, one can derive the following formula:

$$\lambda_\chi(n,T) = 2\sum_{k=1}^{N}\alpha_k\left(1 - T_n\left(\frac{4\gamma_k^2-1}{4\gamma_k^2+1}\right)\right),$$

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where $N = [N_\chi(T)]$ with $[x] = x - \{x\}$ and $\{x\}$ denotes the fractional part of x (the last formula will be denoted $\lambda_\chi(n, N)$). Therefore, the latter formula allows one to estimate the error term $|\lambda_\chi(n) - \lambda_\chi(n, N)|$ in Proposition 4 by evaluating directly the partial Li coefficients as in Proposition 2.

5. *Numerical computations*

In this section, we compute and verify the positivity of the values of $\lambda_\chi(n)$ unconditionally or under the Riemann hypothesis. We first compute unconditionally (without assuming the Riemann hypothesis) $\tilde{\lambda}_\chi(n, M)$ by using (3) and computing prime numbers up to M (see Section 2). We also compute under the Riemann hypothesis

$$\lambda_\chi(n, N) = 2\sum_{k=1}^{N} \alpha_k \left(1 - T_n\left(\frac{4\gamma_k^2 - 1}{4\gamma_k^2 + 1}\right)\right) \quad \text{with } N = 10^4. \tag{22}$$

Furthermore, we carried out the calculations for several examples of characters. Some illustrative examples are cited below. We restricted the tables below for $n \leqslant 40$. However, one can find the other values of $n > 40$ represented in Figures 1–4

REMARK. In fact, by the summation formula (22), we could compute more coefficients $\lambda_\chi(n)$ in a less time consuming way than by the arithmetic formula (3), where computation of the first 50 coefficients lasted more than a week.

Based on the tables below, we conjecture the following result.

CONJECTURE. The coefficients $\lambda_\chi(n)$ are positive and increasing in n.

This conjecture was partially numerically verified for the case of the Riemann zeta function (see [**3**, Appendix D] and [**9**]) and by the authors in a work in progress for the Hecke L-functions [**14**].

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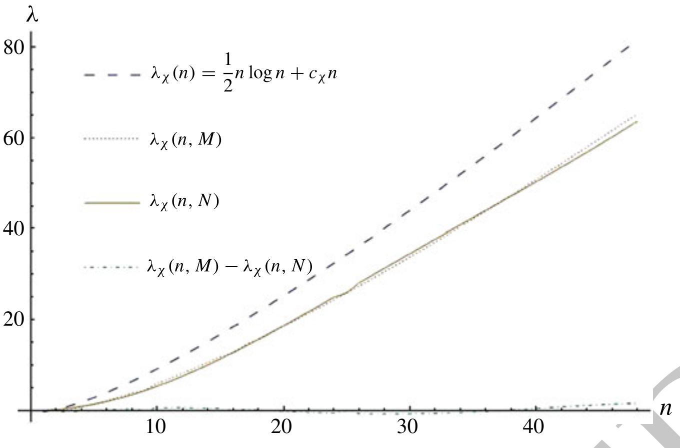

FIGURE 1. *Case of* $\chi \pmod 3$.

$\chi \pmod 3$					
n	$\tilde{\lambda}_\chi(n, M)$	$\lambda_\chi(n, N)$	n	$\tilde{\lambda}_\chi(n, M)$	$\lambda_\chi(n, N)$
1	0.05316	0.056442	19	17.18050	17.16170
2	0.22763	0.22542	20	18.58480	18.69100
3	0.14844	0.50592	21	20.01400	20.24310
4	0.89344	0.89624	22	21.46700	21.81300
5	1.35725	1.39404	23	22.94280	23.39600
6	2.12951	1.99635	24	24.44030	24.98820
7	2.98573	2.69962	25	25.95870	26.58590
8	3.91334	3.49978	26	27.49700	28.18600
9	4.40970	4.39225	27	29.05460	29.78580
10	5.94841	5.37202	28	30.63070	31.38330
11	7.04344	6.43371	29	32.22460	32.97700
12	8.18382	7.57163	30	33.83580	34.56580
13	9.36580	8.77987	31	35.46370	36.14940
14	10.58620	10.05230	32	37.10770	37.72780
15	11.84230	11.38280	33	38.76730	39.3014
16	12.81150	12.76510	34	40.44210	40.87120
17	14.45250	14.19300	35	42.13150	42.43870
18	15.80260	15.66050	36	43.83530	44.00550

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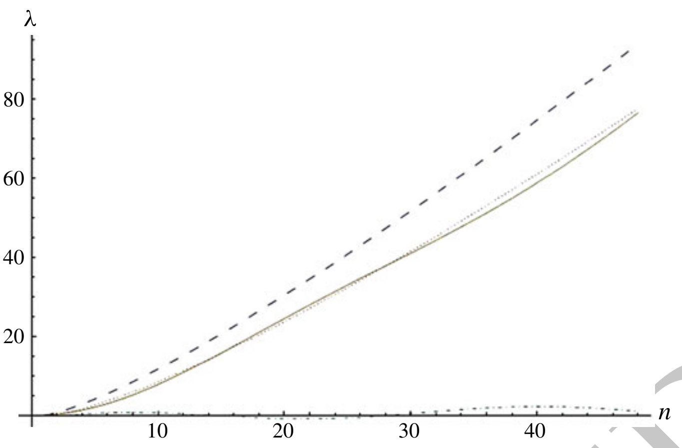

FIGURE 2. *Case of* χ (mod 5).

χ (mod 5)					
n	$\tilde{\lambda}_\chi(n, M)$	$\lambda_\chi(n, N)$	n	$\tilde{\lambda}_\chi(n, M)$	$\lambda_\chi(n, N)$
1	0.13183	0.08562	21	25.37770	26.21450
2	0.29872	0.34152	22	27.08610	27.92160
3	0.91468	0.76482	23	28.81730	29.60960
4	1.58476	1.35081	24	30.57020	31.27780
5	2.63432	2.09300	25	32.34400	32.92720
6	3.66199	2.98332	26	34.13770	34.56020
7	4.77362	4.01225	27	35.95070	36.18030
8	5.95664	5.16902	28	37.78220	37.79200
9	7.06010	6.44188	29	39.63160	39.40090
10	8.50254	7.81828	30	41.49820	41.01320
11	9.85298	9.28519	31	43.38150	42.63540
12	11.24880	10.82930	32	45.28090	44.2746
13	12.68620	12.43740	33	47.19590	45.93760
14	14.16200	14.09650	34	49.12610	47.63100
15	15.67350	15.79410	35	51.07100	49.36130
16	17.68370	17.51860	36	53.03020	51.13410
17	14.45250	19.25930	37	55.00320	52.95430
18	20.40000	21.00670	38	56.98980	54.82600
19	22.03340	22.75260	39	58.98950	56.75210
20	23.69300	24.49030	40	61.00210	58.73450

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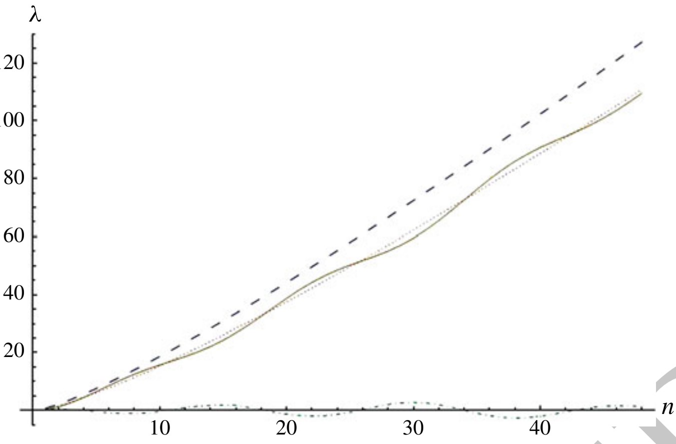

FIGURE 3. *Case of* χ (mod 20).

χ (mod 20)					
n	$\tilde{\lambda}_\chi(n, M)$	$\lambda_\chi(n, N)$	n	$\tilde{\lambda}_\chi(n, M)$	$\lambda_\chi(n, N)$
1	0.695021	0.319128	21	39.93370	41.70260
2	1.68502	1.24419	22	42.33530	44.31350
3	2.99412	2.68343	23	44.75970	46.59570
4	4.48123	4.50032	24	47.20580	48.55720
5	6.10005	6.53527	25	49.67270	50.26430
6	7.82087	8.63067	26	52.15960	51.83150
7	9.62565	10.65500	27	54.66570	53.403100
8	11.50180	12.52230	28	57.19040	55.12930
9	13.32220	14.20280	29	59.73290	57.14130
10	15.43400	15.72450	30	62.29260	59.52940
11	17.47760	17.16450	31	64.86910	62.32740
12	19.56650	18.63130	32	67.46160	65.50710
13	21.69710	20.24300	33	70.06980	68.98220
14	23.86610	22.10320	34	72.69310	72.62260
15	26.07070	24.28030	35	75.33110	76.27560
16	28.54690	26.79300	36	77.98350	79.79060
17	30.57800	29.60520	37	80.64970	83.04340
18	32.87670	32.63050	38	83.32940	85.95580
19	35.20320	35.74610	39	86.02230	88.50750
20	37.55600	38.81360	40	88.72800	90.73760

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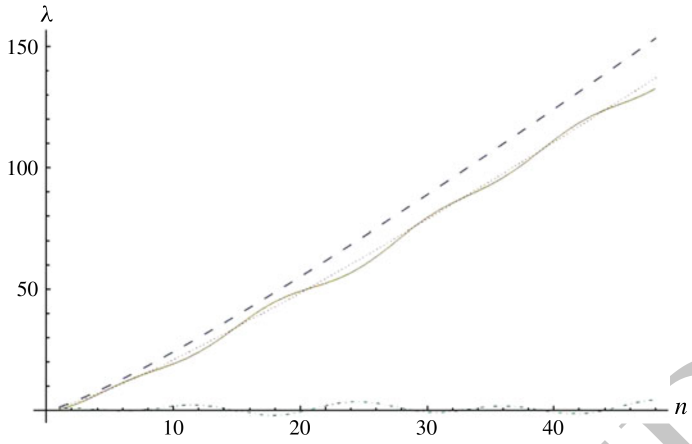

FIGURE 4. *Case of* $\chi \pmod{60}$.

$\chi \pmod{60}$					
n	$\tilde{\lambda}_\chi(n, M)$	$\lambda_\chi(n, N)$	n	$\tilde{\lambda}_\chi(n, M)$	$\lambda_\chi(n, N)$
1	1.12226	0.48626	21	51.46920	50.88960
2	2.78363	1.86950	22	54.42010	52.52830
3	4.64204	3.94169	23	57.39370	54.44350
4	6.83662	6.41363	24	60.38910	56.86290
5	8.84658	8.98530	25	63.40530	59.89590
6	11.11670	11.41720	26	66.44150	63.50750
7	13.47080	13.58380	27	69.49700	67.53000
8	15.89630	15.49640	28	72.57090	71.70750
9	18.06830	17.28820	29	75.6628	75.7637
10	20.92710	19.16770	30	78.77180	79.47310
11	23.52000	21.35250	31	81.89750	82.71770
12	26.15820	24.00100	32	85.03940	85.51520
13	28.83810	27.16160	33	88.19690	88.00960
14	31.55630	30.75170	34	91.36950	90.42920
15	34.31030	34.57380	35	94.55690	93.02160
16	37.56690	38.36300	36	97.75850	95.98430
17	39.91620	41.85530	37	100.97400	99.40850
18	42.76420	44.85610	38	104.20300	103.25300
19	45.64000	47.29300	39	107.44500	107.35200
20	48.54210	49.23760	40	110.70000	111.46000

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