On the sign of the real part of the Riemann zeta-function

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In fond memory of Alfred Jacobus (Alf) van der Poorten 1942–2010

Abstract We consider the distribution of $\arg\zeta(\sigma+it)$ on fixed lines $\sigma > \frac{1}{2}$, and in particular the density

$$d(\sigma) = \lim_{T\to+\infty} \frac{1}{2T} |\{t\in[-T,+T] : |\arg\zeta(\sigma+it)| > \pi/2\}|,$$

and the closely related density

$$d_-(\sigma) = \lim_{T\to+\infty} \frac{1}{2T} |\{t\in[-T,+T] : \Re\zeta(\sigma+it) < 0\}|.$$

Using classical results of Bohr and Jessen, we obtain an explicit expression for the characteristic function $\psi_\sigma(x)$ associated with $\arg\zeta(\sigma+it)$. We give explicit expressions for $d(\sigma)$ and $d_-(\sigma)$ in terms of $\psi_\sigma(x)$. Finally, we give a practical algorithm for evaluating these expressions to obtain accurate numerical values of $d(\sigma)$ and $d_-(\sigma)$.

1 Introduction

Several authors, including Edwards [9, pg. 121], Gram [11, pg. 304], Hutchinson [13, pg. 58], and Milioto [24, §2], have observed that the real part $\Re\zeta(s)$ of the Riemann zeta-function $\zeta(s)$ is "usually positive". This is plausible because the

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Dirichlet series $\zeta(s) = 1 + 2^{-s} + 3^{-s} + \cdots$ starts with a positive term, and the other terms n^{-s} may have positive or negative real part. In this paper our aim is to make precise the statement that $\Re\zeta(s)$ is "usually positive" for $\sigma := \Re(s) > \frac{1}{2}$.

Kalpokas and Steuding [17], assuming the Riemann hypothesis, have given a sense in which the statement is also true on the critical line $\sigma = \frac{1}{2}$. They showed that the mean value of the set of real values of $\zeta(\frac{1}{2} + it)$ exists and is equal to 1.

We do not assume the Riemann hypothesis, and our results do not appear to imply anything about the existence or non-existence of zeros of $\zeta(s)$ for $\sigma > \frac{1}{2}$.

Our results depend on the classical results of Bohr and Jessen [4, 5] concerning the value-distribution of $\zeta(s)$ in the half-plane $\sigma > \frac{1}{2}$. Since Bohr and Jessen there have been many further results on the value distribution of various classes of L-functions. See, for example, Joyner [16], Lamzouri [19, 20, 21], Laurinčikas [22], Steuding [27], and Voronin [31]. However, for our purposes the results of Bohr and Jessen are sufficient.

After defining our notation, we summarise the relevant results of Bohr and Jessen in §2. The densities $d(\sigma)$ and $d_-(\sigma)$, defined in §3, can be expressed in terms of the characteristic function $\psi_\sigma(x)$ of a certain random variable $\Im S$ associated with $\arg\zeta(\sigma + it)$. We consider ψ_σ and a related function $I(b,x)$ in §4–§7. In Theorem 1 we use the results of Bohr and Jessen to obtain an explicit expression for $\psi_\sigma(x)$. Theorem 2 relates $\log I(b,x)$ to certain polynomials $Q_n(x)$ which have non-negative integer coefficients with interesting congruence properties, and Theorem 3 gives an asymptotic expansion of $I(b,x)$ which shows a connection between $I(b,x)$ and the Bessel function J_0. Theorem 4 shows that $\psi_\sigma(x)$ decays rapidly as $x \to \infty$.

The explicit expression for ψ_σ is an infinite product over the primes, and converges rather slowly. In §8 we show how the convergence can be accelerated to give a practical algorithm for computing $\psi_\sigma(x)$ to high accuracy.

In §9 we show how $d(\sigma)$ and $d_-(\sigma)$ can be computed using $\psi_\sigma(x)$, and give the results of numerical computations in §10. Finally, in §11 we comment on how our results might be generalised.

Elliott [10] determined the characteristic function $\Psi_\sigma(x)$ of a limiting distribution associated with a certain sequence of L-functions. We note that Elliott's $\Psi_\sigma(x)$ is the same function as our $\psi_\sigma(x)$. For a possible explanation of this coincidence, using the concept of *analytic conductor*, we refer to [15, Ch. 5]. Here we merely note that Elliott's method of proof is quite different from our proof of Theorem 1, and applies only to sequences of L-functions $L(s,\chi)$ for which χ is a non-principal Dirichlet character.

Notation

$\mathbb{Z}$, $\mathbb{Q}$, $\mathbb{R}$, and $\mathbb{C}$ denote respectively the integers, rationals, reals and complex numbers. The real part of $z \in \mathbb{C}$ is denoted by $\Re z$, and the imaginary part by $\Im z$.

When considering $\zeta(s)$ we always have $\sigma := \Re s$. Unless otherwise specified, $\sigma > \frac{1}{2}$ is fixed.

Consider the open set G equal to $\mathbb{C}$ with cuts along $(-\infty+i\gamma,\beta+i\gamma]$ for each zero or pole $\beta+i\gamma$ of $\zeta(s)$ with $\beta\ge\frac12$. Since $\zeta(s)$ is holomorphic and does not vanish on G, we may define $\log\zeta(s)$ on G. We take the branch such that $\log\zeta(s)$ is real and positive on $(1,+\infty)$. On G we define $\arg\zeta(s)$ by

$$\log\zeta(s)=\log|\zeta(s)|+i\cdot\arg\zeta(s).$$

P is the set of primes, and $p\in P$ is a prime. When considering a fixed prime p we often use the abbreviations $b:=p^\sigma$ and $\beta:=\arcsin(1/b)$.

$|B|$ or $\lambda(B)$ denotes the Lebesgue measure of a set $B\subset\mathbb{C}$ (or $B\subset\mathbb{R}$). A set $B\subset\mathbb{C}$ is said to be *Jordan-measurable* if $\lambda(\partial B)=0$, where ∂B is the boundary of B.[1]

${}_2F_1(a,b;c;z)$ denotes the hypergeometric function of Gauss, see [1, 8].

2 Classical results of Bohr and Jessen

In [4, 5] Bohr and Jessen study several problems regarding the value distribution of the zeta function. In particular, for $\sigma>\frac12$ and a given subset $B\subset\mathbb{C}$, they consider the limit

$$\lim_{T\to\infty}\frac{1}{2T}|\{t\in\mathbb{R}:|t|<T,\log\zeta(\sigma+it)\in B\}|.$$

They prove that the limit exists when B is a rectangle with sides parallel to the real and imaginary axes.

Bohr and Jessen also characterize the limit. In modern terminology, they prove [5, Erster Hauptsatz, pg. 3] the existence of a probability measure $\mathbb{P}_\sigma$, absolutely continuous with respect to Lebesgue measure, such that for any rectangle B as above the limit is equal to $\mathbb{P}_\sigma(B)$.

Finally, they give a description of the measure $\mathbb{P}_\sigma$. To express it in modern language, consider the unit circle $\mathbb{T}=\{z\in\mathbb{C}:|z|=1\}$ with the usual probability measure μ (that is $\frac{1}{2\pi}\,d\theta$ if we identify $\mathbb{T}$ with the interval $[0,2\pi)$ in the usual way). Let P be the set of prime numbers. We may consider $\Omega:=\mathbb{T}^P$ as a probability space with the product measure $\mathbb{P}=\mu^P$. Each point of Ω is a sequence $\omega=(z_p)_{p\in P}$, with each $z_p\in\mathbb{T}$. Thus z_p may be considered as a random variable. The random variables z_p are independent and uniformly distributed on the unit circle.

Proposition 1. *Let $\sigma>\frac12$ and for each prime number q let z_q be the random variable defined on Ω such that $z_q(\omega)=z_q$ when $\omega=(z_p)_{p\in P}$. The sum of random variables*

$$S:=-\sum_{p\in P}\log(1-p^{-\sigma}z_p)=\sum_{p\in P}\sum_{k=1}^{\infty}\frac1k p^{-k\sigma}z_p^k$$

converges almost everywhere, so S is a well defined random variable.

[1] A bounded set B is Jordan-measurable if and only if for each $\varepsilon>0$ we can find two finite unions of rectangles with sides parallel to the real and imaginary axes, say S and T, such that $S\subseteq B\subset T$ and $\lambda(T\smallsetminus S)<\varepsilon$ (see for example Halmos [12]).

Proof. The random variables $Y_p := -\log(1 - p^{-\sigma} z_p)$ are independent. The mean value of each Y_p is zero since

$$\mathbb{E}(Y_p) = \frac{1}{2\pi}\int_0^{2\pi}\sum_{k=1}^{\infty}\frac{1}{k}p^{-k\sigma}e^{ik\theta}\,d\theta = 0.$$

It can be shown in a similar way that $E(|Y_p|^2) \sim p^{-2\sigma}$. Thus $\sum_p E(|Y_p|^2)$ converges. A classical result of probability theory [12, Thm. B, Ch. IX] proves the convergence almost everywhere of the series for S. □

The measure $\mathbb{P}_\sigma$ of Bohr and Jessen is the distribution of the random variable S. For each Borel set $B \subset \mathbb{C}$, we have

$$\mathbb{P}_\sigma(B) = \mathbb{P}\{\omega \in \Omega : S(\omega) \in B\}.$$

The main result of Bohr and Jessen is that, for each rectangle R with sides parallel to the axes,

$$\mathbb{P}_\sigma(R) = \lim_{T\to\infty}\frac{1}{2T}|\{t \in \mathbb{R} : |t| < T, \log\zeta(\sigma+it) \in R\}| \tag{1}$$

and the limit exists. It is easy to deduce that (1) is also true for each Jordan-measurable subset $R \subset \mathbb{C}$, and for sets R of the form $\mathbb{R}\times B$, where B is a Jordan-measurable subset of $\mathbb{R}$.

3 Some quantities related to the argument of the zeta function

Define a measure μ_σ on the Borel sets of $\mathbb{R}$ by $\mu_\sigma(B) := \mathbb{P}_\sigma(\mathbb{R}\times B)$. If we take a Jordan subset $B \subset \mathbb{R}$, the main result of Bohr and Jessen implies that

$$\mu_\sigma(B) = \lim_{T\to\infty}\frac{1}{2T}|\{t \in \mathbb{R} : |t| < T, \arg\zeta(\sigma+it) \in B\}|.$$

The measure μ_σ is the distribution function of the random variable $\Im S$. In fact

$$\mu_\sigma(B) = \mathbb{P}_\sigma(\mathbb{R}\times B) = \mathbb{P}\{\omega \in \Omega : S(\omega) \in \mathbb{R}\times B\} = \mathbb{P}\{\omega \in \Omega : \Im S(\omega) \in B\}.$$

We are interested in the functions $d(\sigma)$, $d_+(\sigma)$, and $d_-(\sigma)$ defined by

$$d(\sigma) := \lim_{T\to\infty}\frac{1}{2T}|\{t \in \mathbb{R} : |t| < T, |\arg\zeta(\sigma+it)| > \pi/2\}|,$$

$$d_+(\sigma) := \lim_{T\to\infty}\frac{1}{2T}|\{t \in \mathbb{R} : |t| < T, \Re\zeta(\sigma+it) > 0\}|,$$

$$d_-(\sigma) := \lim_{T\to\infty}\frac{1}{2T}|\{t \in \mathbb{R} : |t| < T, \Re\zeta(\sigma+it) < 0\}|.$$

Informally, $d_+(\sigma)$ is the probability that $\Re\zeta(\sigma+it)$ is positive; $d_-(\sigma)$ is the probability that $\Re\zeta(\sigma+it)$ is negative. We show in §10 that $d(\sigma)$ is usually a good approximation to $d_-(\sigma)$. Observe that $d(\sigma) = 1-\mu_\sigma([-\pi/2,\pi/2])$, $d_+(\sigma)+d_-(\sigma) = 1$, and $d_+(\sigma) = \sum_{k\in\mathbb{Z}} \mu_\sigma(2k\pi-\pi/2, 2k\pi+\pi/2)$.

4 The characteristic function ψ_σ

Recall that the *characteristic function* $\psi(x)$ of a random variable Y is defined by the Fourier transform $\psi(x) := \mathrm{E}[\exp(ixY)]$. We omit a factor 2π in the exponent to agree with the statistical literature.

Proposition 2. *The characteristic function of the random variable $\Im S$ is given by*

$$\psi_\sigma(x) = \prod_p I(p^\sigma, x), \tag{2}$$

where, writing $b := p^\sigma$, $I(b,x)$ is defined by

$$I(b,x) := \frac{1}{2\pi}\int_0^{2\pi} \exp\left(-ix \arg(1-b^{-1}e^{i\theta})\right)\, d\theta. \tag{3}$$

Proof. By definition

$$\psi_\sigma(x) = \int_\Omega \exp\left(ix\Im S(\omega)\right)\, d\omega = \int_\Omega \prod_p \exp\left(-ix\arg(1-p^{-\sigma}z_p)\right)\, d\omega.$$

By independence the integral of the product is the product of the integrals, so

$$\psi_\sigma(x) = \prod_p \int_\Omega \exp\left(-ix\arg(1-p^{-\sigma}z_p)\right)\, d\omega.$$

Each random variable z_p is distributed as $e^{i\theta}$ on the unit circle, so

$$\psi_\sigma(x) = \prod_p \frac{1}{2\pi}\int_0^{2\pi} \exp\left(-ix\arg(1-p^{-\sigma}e^{i\theta})\right)\, d\theta = \prod_p I(p^\sigma, x). \qquad \square$$

5 The function $I(b,x)$

In this section we study the function $I(b,x)$ defined by (3). It is easy to see from (3) that $I(b,x)$ is an even function of x. Hence, from (2), the same is true for $\psi_\sigma(x)$.

Proposition 3. *Let* $b>1$ *and* $\beta=\arcsin(b^{-1})$. *Then*

$$\begin{aligned} I(b,x) &= \frac{1}{\pi}\int_0^\pi \cos\Bigl(x\arctan\frac{\sin t}{b-\cos t}\Bigr)\,dt \\ &= \frac{2b}{\pi}\int_0^\beta \frac{\cos(xt)\cos t}{\sqrt{1-b^2\sin^2 t}}\,dt = \frac{2}{\pi}\int_0^1 \cos\Bigl(x\arcsin\frac{t}{b}\Bigr)\frac{dt}{\sqrt{1-t^2}}\,. \end{aligned}$$

Proof. By elementary trigonometry we find

$$\arg(1-b^{-1}e^{it}) = -\arctan\frac{\sin t}{b-\cos t}. \tag{4}$$

Substituting in (3) gives

$$I(b,x) = \frac{1}{2\pi}\int_0^{2\pi}\exp\Bigl(ix\arctan\frac{\sin t}{b-\cos t}\Bigr)\,dt = \frac{1}{\pi}\int_0^\pi \cos\Bigl(x\arctan\frac{\sin t}{b-\cos t}\Bigr)\,dt.$$

To obtain the second representation, note that $\arctan(\sin t/(b-\cos t))$ is increasing on the interval $[0,\gamma]$ and decreasing on $[\gamma,\pi]$, where $\gamma=\arccos b^{-1}$. We split the integral on $[0,\pi]$ into integrals on $[0,\gamma]$ and $[\gamma,\pi]$. In each of the resulting integrals we change variables, putting $u:=\arctan(\sin t/(b-\cos t))$. Then

$$t = \arccos\Bigl(b\sin^2 u \pm \cos u\sqrt{1-b^2\sin^2 u}\,)\Bigr)\,,$$

where the sign is "$+$" on the first interval and "$-$" on the second interval. After some simplification, the second representation follows. The third representation follows by the change of variables $t\mapsto\arcsin(t/b)$. □

Lemma 1. *For* $|t|<1$ *and all* $x\in\mathbb{C}$,

$$\cos(2x\arcsin t) = {}_2F_1(-x,x;\tfrac12;t^2) = 1+\sum_{n=1}^\infty \frac{(2t)^{2n}}{(2n)!}\prod_{j=0}^{n-1}(j^2-x^2). \tag{5}$$

Proof. In [1, eqn. 15.1.17] (also [8, eqn. 15.4.12]) we find the identity

$$\cos(2az) = {}_2F_1(-a,a;\tfrac12;\sin^2 z).$$

Replacing a by x and z by $\arcsin t$, we get the first half of (5). The second half follows from the definition of the hypergeometric function. □

Remark 1. An independent proof uses the fact that $f(t):=\cos(2x\arcsin t)$ satisfies the differential equation $(1-t^2)f''(t)-tf'(t)+4x^2f(t)=0$, where primes denote differentiation with respect to t.

Remark 2. When $x\in\mathbb{Z}$, the series (5) reduces to a polynomial.

Proposition 4. *For $b > 1$ we have*

$$I(b,2x) = {}_2F_1(-x,x;1;b^{-2}) = 1 + \sum_{n=1}^{\infty} \frac{1}{b^{2n} n!^2} \prod_{j=0}^{n-1} (j^2 - x^2).$$

Proof. From Proposition 3, we have

$$I(b,2x) = \frac{2}{\pi} \int_0^1 \cos\left(2x \arcsin \frac{t}{b}\right) \frac{dt}{\sqrt{1-t^2}}\,.$$

The expression of $I(b,2x)$ as a sum follows from Lemma 1, using a well-known integral for the Beta function $B(n+\frac{1}{2},\frac{1}{2})$:

$$\frac{2}{\pi} \int_0^1 \frac{t^{2n}\,dt}{\sqrt{1-t^2}} = \frac{1}{\pi} B\left(n+\tfrac{1}{2},\tfrac{1}{2}\right) = \frac{(2n)!}{n!^2 2^{2n}}\,.$$

The identification of $I(b,2x)$ as ${}_2F_1(-x,x;1;b^{-2})$ then follows from the definition of the hypergeometric function ${}_2F_1$. □

Corollary 1. *If $x \in \mathbb{Z}$, $b^2 \in \mathbb{Q}$ and $b > 1$, then $I(b,2x) \in \mathbb{Q}$.*

Proof. Since $I(b,2x)$ is even, we can assume that $x \geq 0$. Applying Euler's transformation [1, (15.3.4)] to the hypergeometric representation of Proposition 4, we obtain $I(b,2x) = (1-b^{-2})^x\,{}_2F_1(-x,1-x;1;1/(1-b^2))$, but the series for ${}_2F_1(-x,1-x;1;z)$ terminates, so is rational for $z \in \mathbb{Q}$. □

We can now prove our first main result, which gives an explicit expression for the characteristic function ψ_σ defined in §2–§4.

Theorem 1. *For $\sigma > \frac{1}{2}$, the characteristic function ψ_σ of Proposition 2 is the entire function given by the convergent infinite product*

$$\psi_\sigma(2x) = \prod_p \left(1 + \sum_{n=1}^{\infty} \frac{1}{n!^2} \prod_{j=0}^{n-1} (j^2 - x^2) \cdot \frac{1}{p^{2n\sigma}}\right). \tag{6}$$

Proof. The identity (6) follows from Proposition 2 and Proposition 4. Since $\sum p^{-2\sigma}$ converges, the infinite product (6) converges for all $x \in \mathbb{C}$. □

6 The function $\log I(b,x)$

The explicit formula for ψ_σ given by Theorem 1 is not suitable for numerical computation because the infinite product over primes converges too slowly. In §8 we show how this difficulty can be overcome. First we need to consider the function $\log I(b,x)$.

Theorem 2. *Suppose that $b > \max(1,|x|)$. There exist even polynomials $Q_n(x)$ of degree $2n$ with $Q_n(0) = 0$ and nonnegative integer coefficients $q_{n,k}$ such that*

$$\log I(b,2x) = -\sum_{n=1}^{\infty} \frac{Q_n(x)}{n!^2}\frac{1}{b^{2n}} = -\sum_{n=1}^{\infty}\sum_{k=1}^{n} \frac{q_{n,k}}{n!^2}\frac{x^{2k}}{b^{2n}}\,. \tag{7}$$

The polynomials $Q_n(x)$ are determined by the recurrence

$$Q_1(x) = x^2, \quad Q_{n+1}(x) = (n!)^2x^2 + \sum_{j=0}^{n-1}\binom{n}{j}\binom{n}{j+1}Q_{j+1}(x)Q_{n-j}(x)\,. \tag{8}$$

Also, the polynomials $Q_n(x)$ satisfy

$$|Q_n(x)| \le n!(n-1)!\max(1,|x|)^{2n}. \tag{9}$$

Proof. By Proposition 4 there exist even polynomials P_n with $P_n(0) = 0$, such that

$$I(b,2x) = 1 + \sum_{n=1}^{\infty}\frac{P_n(x)}{n!^2}\frac{1}{b^{2n}}\,.$$

It follows that

$$\log I(b,2x) = \sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k}\Big(\sum_{n=1}^{\infty}\frac{P_n(x)}{n!^2}\frac{1}{b^{2n}}\Big)^k.$$

It is clear that expanding the powers gives a series of the desired form (7).

To prove the recurrence for the Q_n, we temporarily consider x as fixed and define $f(y) := I(y^{-1/2},2x)$. Then, by (7),

$$\log f(y) = -\sum_{n=1}^{\infty}\frac{Q_n}{n!^2}y^n\,. \tag{10}$$

By Proposition 4 we have $f(y) = {}_2F_1(x,-x;1;y)$, so $f(y)$ satisfies the hypergeometric differential equation

$$y(1-y)f'' + (1-y)f' + x^2 f = 0,$$

where primes denote differentiation with respect to y. Define $g(y) := f'(y)/f(y)$. Then it may be verified [2] that $g(y)$ satisfies the Riccati equation

$$y(g'+g^2) + g + \frac{x^2}{1-y} = 0. \tag{11}$$

Let $g(y) = \sum_{n=0}^{\infty} g_n y^n$, where the g_n are polynomials in x, e.g. $g_0 = -x^2$. Equating coefficients in (11), we get the recurrence

[2] Usually a Riccati equation is reduced to a second-order linear differential equation, see for example Ince [14, §2.15]. We apply the standard argument in the reverse direction.

$$g_n = -\left(\frac{1}{n+1}\right)\left(x^2 + \sum_{j=0}^{n-1} g_j g_{n-1-j}\right), \text{ for } n \geq 0. \tag{12}$$

Now, from (10) and the definitions of f and g, we have

$$g(y) = \frac{f'(y)}{f(y)} = \frac{d}{dy}\log f(y) = -\frac{d}{dy}\sum_{n=1}^{\infty}\frac{Q_n(x)}{n!^2}y^n,$$

so we see that

$$g_n = -\frac{Q_{n+1}}{n!(n+1)!}\,. \tag{13}$$

Substituting (13) in (12) and simplifying, we obtain the recurrence (8).

From the recurrence (8) it is clear that $Q_n(x)$ is an even polynomial of degree $2n$, such that $Q_n(0) = 0$. Writing $Q_n(x) = \sum_{k=1}^{n} q_{n,k} x^{2k}$, we see from the recurrence (8) that the coefficients $q_{n,k}$ are nonnegative integers.

In view of (13), the inequality (9) is equivalent to $|g_n(x)| \leq \max(1,|x|)^{2n+2}$, which may be proved by induction on n, using the recurrence (12).

Finally, in view of (9), the series in (7) converge for $b > \max(1,|x|)$. □

Corollary 2. *If $b > 1$, then $I(b,2x)$ is nonzero in the disk $|x| < b$.*

Proof. This follows from the convergence of the series for $\log I(b,2x)$. □

Proposition 5. *The numbers $q_{n,k}$ are determined by $q_{n,1} = (n-1)!^2$ for $n \geq 1$, and*

$$q_{n+1,k} = \sum_{j=0}^{n-1}\binom{n}{j}\binom{n}{j+1}\sum_{r=\mu}^{\nu} q_{j+1,r}\, q_{n-j,k-r} \tag{14}$$

for $2 \leq k \leq n+1$, where $\mu = \max(1, k-n+j)$ and $\nu = \min(j+1, k-1)$. Also, $q_{n,k}$ is a positive integer for each $n \geq 1$ and $1 \leq k \leq n$.

Proof. The recurrence is obtained by equating coefficients of x^{2k} in (8). Positivity of the $q_{n,k}$ for $1 \leq k \leq n$ follows. □

Remark 3. We may consider the sum over r in (14) to be over all $r \in \mathbb{Z}$ if we define $q_{n,k} = 0$ for $k < 1$ and $k > n$. The given values μ and ν correspond to the nonzero terms of the resulting sum.

Corollary 3. *We have $\sum_{k=1}^{n} q_{n,k} = n!\,(n-1)!$.*

Proof. This is easily obtained if we substitute $x = 1$ in the recurrence (8). □

Corollary 4. *We have*

$$q_{n,n} = 2^{2n} n!(n-1)! \sum_{k=1}^{\infty} \frac{1}{j_{0,k}^{2n}} \tag{15}$$

where $(j_{0,k})$ is the sequence of positive zeros of the Bessel function $J_0(z)$.

Table 1 The coefficients $q_{n,k}$.

$n \diagdown k$	1	2	3	4	5	6	7
1	1						
2	1	1					
3	4	4	4				
4	36	33	42	33			
5	576	480	648	720	456		
6	14400	10960	14900	18780	17900	9460	
7	518400	362880	487200	648240	730800	606480	274800

Proof. Define $q_n := q_{n,n}$. With $k = n+1$, the recurrence (14) gives, for $n \geq 1$,

$$q_{n+1} = \sum_{j=0}^{n-1} \binom{n}{j} \binom{n}{j+1} q_{j+1} q_{n-j} = \sum_{j=1}^{n} \binom{n}{j} \binom{n}{j-1} q_j q_{n-j+1}.$$

This recurrence appears in Carlitz [7, eqn. (4)], where it is shown that the solution satisfies (15). $\square$

Remark 4. The sequence (q_n) is A002190 in Sloane's on-line encyclopedia of integer sequences (OEIS), where the generating function $-\log(J_0(2\sqrt{x}))$ is given. The numbers q_n enjoy remarkable congruence properties. In fact, (15) is analogous to Euler's identity $|B_{2n}| = 2(2n)! \sum_{k=1}^{\infty} (2\pi k)^{-2n}$, and the numbers q_n are analogous to Bernoulli numbers. We refer to Carlitz [7] for further discussion.

Remark 5. There are other recurrences giving the polynomials Q_n and the numbers $q_{n,k}$. We omit discussion of them here due to space limitations.

7 Bounds and asymptotic expansions

Since $I(b,x)$ is an even function of x, there is no loss of generality in assuming that $x \geq 0$ when giving bounds or asymptotic results for $I(b,x)$. This simplifies the statement of the results. Similarly remarks apply to $\psi_\sigma(x)$, which is also an even function.

Consider the first representation of $I(b,x)$ in Proposition 3. If b is large, then

$$\arctan\left(\frac{\sin\theta}{b-\cos\theta}\right) = \frac{\sin\theta}{b} + \mathcal{O}\left(b^{-2}\right).$$

However, it is well-known [32, §2.2] that the Bessel function $J_0(x)$ has an integral representation

$$J_0(x) = \frac{1}{\pi}\int_0^\pi \cos(x\sin\theta)\, d\theta\,. \tag{16}$$

Thus, we expect $I(b,x)$ to be approximated in some sense by $J_0(x/b)$. A more detailed analysis confirms this (see Proposition 7 and Corollary 9). The connection with Bessel functions makes Corollary 4 less surprising than it first appears.

Proposition 6. *For all $b > 1$ and $x \in \mathbb{R}$, we have $|I(b,x)| \le 1$.*

Proof. This follows from the final integral in Proposition 3. □

Lemma 2. *For $t \in [0,1]$ and $c_1 = \pi/2 - 1 < 0.5708$, we have*

$$0 \le \arcsin(t) - t \le c_1 t^3.$$

Proof. Let $f(t) = (\arcsin(t) - t)/t^3$. We see from the Taylor series that $f(t)$ is non-negative and increasing in $[0,1]$. Thus $\sup_{t\in[0,1]} f(t) = f(1) = \pi/2 - 1$. □

Lemma 3. *Suppose $b > 1$, $t \in [0,1]$, and c_1 as in Lemma 2. Then*

$$0 \le b\arcsin(t/b) - t \le c_1 t^3/b^2.$$

Proof. Replace t by t/b in Lemma 2, and multiply both sides of the resulting inequality by b. □

Proposition 7. *Suppose $b > 1$, $x > 0$, and $c_2 = (2 - 4/\pi)/3 < 0.2423$. Then*

$$|I(b,x) - J_0(x/b)| \le c_2 x/b^3.$$

Proof. From the last integral of Proposition 3, we have

$$I(b,bx) = \frac{2}{\pi}\int_0^1 \cos\left(bx\arcsin\frac{t}{b}\right)\frac{dt}{\sqrt{1-t^2}}\,.$$

Also, from the integral representation (16) for J_0, we see that

$$J_0(x) = \frac{2}{\pi}\int_0^1 \cos(xt)\frac{dt}{\sqrt{1-t^2}}\,.$$

Thus, by subtraction,

$$I(b,bx) - J_0(x) = \frac{2}{\pi}\int_0^1 f(b,x,t)\frac{dt}{\sqrt{1-t^2}}\,, \tag{17}$$

where $f(b,x,t) = \cos(bx\arcsin(t/b)) - \cos(xt)$. Using $|\cos x - \cos y)| \le |x-y|$, we have

$$|f(b,x,t)| \le |bx\arcsin(t/b) - xt|.$$

Thus, from Lemma 3,

$$|f(b,x,t)| \le c_1 t^3 x/b^2.$$

Taking norms in (17) gives

$$|I(b,bx)-J_0(x)| \le \frac{2c_1 x}{\pi b^2}\int_0^1 \frac{t^3\,dt}{\sqrt{1-t^2}}\,. \tag{18}$$

The integral in (18) is easily seen to have the value $2/3$. Thus, replacing x by x/b in (18) completes the proof. □

Corollary 5. *If $b>1$, $x>0$, c_2 as in Proposition 7, and $c_3=\sqrt{2/\pi}<0.7979$, then*

$$|I(b,x)| \le c_2 x/b^3 + c_3 (b/x)^{1/2}. \tag{19}$$

Proof. It is known [1, 9.2.28–9.2.31] that $|J_0(x)| \le \sqrt{2/(\pi x)}$ for real, positive x. Thus, the result follows from Proposition 7. □

Remark 6. The crossover point in Corollary 5 is for $b \approx x^{3/7}$: the first term in (19) dominates if $b \ll x^{3/7}$; the second term dominates if $b \gg x^{3/7}$.

Corollary 6. *If $x>1$ and $b \ge x^{1/2}$, then*

$$|I(b,x)| \le c_3 (b/x)^{1/2}(1+c_5 b^{-1/2}),$$

where c_2, c_3 are as above, and $c_5 = c_2/c_3 < 0.3037$.

Proof. From Corollary 5 we have

$$|I(b,x)| \le c_3 (b/x)^{1/2}(1+c_5 x^{3/2}/b^{7/2}).$$

The condition $b \ge x^{1/2}$ implies that $x^{3/2}/b^{7/2} \le b^{-1/2}$. □

For the remainder of this section we write $\beta := \arcsin(1/b)$.

Proposition 8. *For $b>1$ and real positive x, we have*

$$I(b,x) = -\Re\left(\frac{2ie^{ix\beta}}{\pi}\int_0^\infty e^{-xu}\frac{\sqrt{b^2-1}\cosh u - i\sinh u}{\sqrt{1-(\cosh u + i\sqrt{b^2-1}\sinh u)^2}}\,du\right). \tag{20}$$

Proof. From the second integral in Proposition 3 we get $I(b,x)=\Re J(b,x)$, where

$$J(b,x) = \frac{2b}{\pi}\int_0^\beta e^{ixt}\frac{\cos t}{\sqrt{1-b^2\sin^2 t}}\,dt\,.$$

The function $1-b^2\sin^2 t$ has zeros at $t=\pm\beta+k\pi$ with $k\in\mathbb{Z}$ and only at these points. Also, $\beta=\arcsin(1/b)\in(0,\pi/2)$. Hence, if Ω denotes the complex plane $\mathbb{C}$ with two cuts along the half-lines $(-\infty,-\beta]$ and $[\beta,+\infty)$, then the function $(\cos t)/\sqrt{1-b^2\sin^2 t}$ is analytic on Ω. We consider the branch that is real and positive in the interval $(0,\beta)$. We apply Cauchy's Theorem to the half strip $\Im t>0$, $0<\Re t<\beta$, obtaining

$$J(b,x)=\frac{i}{\pi}\int_0^\infty e^{-xu}\frac{2b\cosh u}{\sqrt{1+b^2\sinh^2 u}}\,du\;-\;\frac{ie^{ix\beta}}{\pi}\int_0^\infty e^{-xu}\frac{2b\cos(\beta+iu)}{\sqrt{1-b^2\sin^2(\beta+iu)}}\,du.$$

The first integral does not contribute to the real part. Taking the real part of the second integral and simplifying gives (20). □

In the following theorem we give an asymptotic expansion of $I(b,x)$.

Theorem 3. *For $b>1$ fixed and real $x\to+\infty$, there is an asymptotic expansion of $I(b,x)$. If $\beta=\arcsin(1/b)$, the first three terms are given by*

$$\begin{aligned}I(b,x)=\;&\frac{2}{\sqrt{2\pi}}\frac{(b^2-1)^{1/4}}{x^{1/2}}\cos(x\beta-\pi/4)\\&+\frac{(b^2+2)}{4\sqrt{2\pi}}\frac{(b^2-1)^{-1/4}}{x^{3/2}}\sin(x\beta-\pi/4)\\&-\frac{(9b^4-28b^2+4)}{64\sqrt{2\pi}}\frac{(b^2-1)^{-3/4}}{x^{5/2}}\cos(x\beta-\pi/4)+\mathcal{O}\left(\frac{1}{x^{7/2}}\right).\end{aligned}$$

Proof. We apply the Laplace method and Watson's Lemma [25, Ch. 3, pg. 71] to the representation (20). □

Corollary 7. *For fixed $b>1$, the function $I(b,x)$ has infinitely many real zeros.*

Proof. This is immediate from the first term of the asymptotic expansion above. The zeros are near the points $\pm\left(\frac{3\pi}{4}+k\pi\right)/\beta$ for $k\in\mathbb{Z}_{\geq 0}$. □

Corollary 8. *For fixed $\sigma>\frac{1}{2}$, the function $\psi_\sigma(x)$ has infinitely many real zeros.*

Proof. This is immediate from Proposition 2 and Corollary 7. □

Corollary 9. *If $b>1$ and $\beta=\arcsin(1/b)$, then for real $x\to+\infty$ we have*

$$I(b,x)=\beta^{1/2}(b^2-1)^{1/4}J_0(\beta x)+\mathcal{O}(x^{-3/2}).$$

Proof. The Bessel function $J_0(x)$ has an asymptotic expansion which gives

$$J_0(x)=\left(\frac{2}{\pi x}\right)^{1/2}\left(\cos(x-\pi/4)+\frac{1}{8x}\sin(x-\pi/4)+\mathcal{O}\left(\frac{1}{x^2}\right)\right).$$

Therefore, from Theorem 3, the difference $I(b,x)-\beta^{1/2}(b^2-1)^{1/4}J_0(\beta x)$ is of the order indicated. □

Now we give a bound on the function $I(b,x)$ which is sharper than Corollary 5 in the region $x\gg b^{7/3}$.

Proposition 9. *For $b\geq\sqrt{2}$ and real $x\geq 5$, we have*

$$|I(b,x)|\leq 1.1512\sqrt{b/x}. \tag{21}$$

Proof. We consider the representation (20). Take $A := \sqrt{b^2-1}$ so the condition $b \ge \sqrt{2}$ implies that $A \ge 1$. It can be shown that, for $A \ge 1$ and real $u > 0$, the inequality

$$\Big|\frac{A\cosh u - i\sinh u}{\sqrt{1-(\cosh u + iA\sinh u)^2}}\Big| \le \frac{c_4\sqrt{A}}{\min(u^{1/2},1)}$$

holds. Here, the optimal constant is $c_4 = \sqrt{\coth(2)} < 1.0185$, attained at $A = u = 1$. (We omit details of the proof, which is elementary but tedious.) Hence, from (20),

$$\begin{aligned}|I(b,x)| &\le \frac{2c_4}{\pi}(b^2-1)^{1/4}\Big\{\int_0^1 u^{-1/2}e^{-xu}\,du + \int_1^\infty e^{-xu}\,du\Big\}\\ &< \frac{2c_4\sqrt{b}}{\pi}\left(\sqrt{\pi/x} + e^{-x}/x\right).\end{aligned}$$

For $x \ge 5$ we have $(2c_4/\pi)(\sqrt{\pi/x}+e^{-x}/x) \le 1.1512/\sqrt{x}$. □

Remark 7. The constant 1.1512 in (21) can be reduced if we do not ask for uniformity in b. From Theorem 3, we have

$$|I(b,x)| \le c_3(1-b^{-2})^{1/4}(b/x)^{1/2} + \mathcal{O}\left(x^{-3/2}\right) \text{ as } x \to +\infty,$$

so the constant can be reduced to $c_3 = (2/\pi)^{1/2} < 0.7979$ for all $x \ge x_0(b)$.

The following conjecture is consistent with our analytic results, for example Corollary 5 and Theorem 3, and with extensive numerical evidence.

Conjecture 1. For all $b > 1$ and $x > 0$, we have $|I(b,x)| < \sqrt{\dfrac{2b}{\pi x}}\,.$

To conclude this section, we give a bound on $\psi_\sigma(x)$.

Theorem 4. *Let $\sigma > \frac{1}{2}$ be fixed. Then $|\psi_\sigma(x)| \le 1$ for all $x \in \mathbb{R}$. Also, there exists a positive constant $c \ge 0.47$ and $x_0(\sigma)$ such that*

$$|\psi_\sigma(x)| \le \exp\left(-\frac{c\,x^{1/\sigma}}{\log(x^{1/\sigma})}\right) \text{ for all real } x \ge x_0(\sigma).$$

Proof. The first inequality is immediate from the definition of $\psi_\sigma(x)$ as the characteristic function of a random variable.

To prove the last inequality, it is convenient to write $y := x^{1/\sigma}$. Let $\mathscr{P}(y)$ be the set of primes p in the interval $(y^{1/2}, y]$. We can assume that $\psi_\sigma(x) \ne 0$, because otherwise the inequality is trivial. From Proposition 6 and Corollary 6, we have

$$|\psi_\sigma(x)| \le \prod_{p\in\mathscr{P}(y)} |I(p^\sigma,x)| \le \prod_{p\in\mathscr{P}(y)} \left(c_3(p/y)^{\sigma/2}(1+c_5p^{-\sigma/2})\right),$$

which implies

$$-\log|\psi_\sigma(x)| \geq \sum_{p\in\mathscr{P}(y)} \left(-\log(c_3) + \tfrac{\sigma}{2}(\log y - \log p)\right) + \mathcal{O}(y^{1-\sigma/2})\,.$$

Using $\log(c_3) < -0.22$ and $\sigma > 1/2$ gives

$$-\log|\psi_\sigma(x)| \geq (\pi(y) - \pi(y^{1/2}))(\tfrac{\sigma}{2}\log y + 0.22) - \tfrac{\sigma}{2}\sum_{p\in\mathscr{P}(y)} \log p + \mathcal{O}(y^{3/4}), \quad (22)$$

where, as usual, $\pi(y)$ denotes the number of primes in the interval $[1,y]$.

From standard results on the distribution of primes [28], we have

$$\pi(y) = \frac{y}{\log y} + \frac{y}{\log^2 y} + \mathcal{O}\left(\frac{y}{\log^3 y}\right) \text{ and } \sum_{p\in\mathscr{P}(y)} \log p = y + \mathcal{O}\left(\frac{y}{\log^2 y}\right).$$

Substituting in (22), we see that the leading terms of order y cancel, leaving

$$-\log|\psi_\sigma(x)| \geq (\tfrac{\sigma}{2} + 0.22)\frac{y}{\log y} + \mathcal{O}\left(\frac{y}{\log^2 y}\right).$$

Since $\frac{\sigma}{2} + 0.22 > 0.47$, the Theorem follows, provided y is sufficiently large. □

Remark 8. We find numerically that, for $\sigma \in (0.5, 1.1)$, we can take $c = 1$ and $x_0 = 5$ in Theorem 4.

8 An algorithm for computing $\psi_\sigma(x)$

There is a well-known technique, going back at least to Wrench [33], for accurately computing certain sums/products over primes. The idea is to express what we want to compute in terms of the *prime zeta function*

$$P(s) := \sum_p p^{-s} \quad (\Re(s) > 1).$$

The prime zeta function can be computed from $\log\zeta(s)$ using Möbius inversion:

$$P(s) = \sum_{r=1}^{\infty} \frac{\mu(r)}{r} \log\zeta(rs)\,. \quad (23)$$

In fact, (23) gives the analytic continuation of $P(s)$ in the half-plane $\Re s > 0$ (see Titchmarsh [29, §9.5]), but we only need to compute $P(s)$ for real $s > 1$.

To illustrate the technique, temporarily ignore questions of convergence. From Theorem 2, we have

$$\log I(p^\sigma, x) = -\sum_{n=1}^{\infty} \frac{Q_n(x/2)}{n!^2} p^{-2n\sigma}.$$

Thus, taking logarithms in (2),

$$\log \psi_\sigma(x) = -\sum_p \sum_{n=1}^{\infty} \frac{Q_n(x/2)}{n!^2} p^{-2n\sigma} = -\sum_{n=1}^{\infty} \frac{Q_n(x/2)}{n!^2} P(2n\sigma). \tag{24}$$

Unfortunately, this approach fails, because $\psi_\sigma(x)$ has (infinitely many) real zeros – see Corollary 8. In fact, the series (24) converges for $|x| < |x_1(\sigma)|$, where $x_1(\sigma)$ is the zero of $\psi_\sigma(x)$ closest to the origin, and diverges for $|x| > |x_1(\sigma)|$.

Fortunately, a simple modification of the approach avoids this difficulty. Instead of considering a product over all primes, we consider the product over sufficiently large primes, say $p > p_0(x,\sigma)$. Corollary 2 guarantees that $I(p^\sigma, x)$ has no zeros in the disk $|x| < 2p^\sigma$. Thus, to evaluate $\psi_\sigma(x)$ for given σ and x, we should choose $2p_0^\sigma > |x|$, that is $p_0 > |x/2|^{1/\sigma}$. In practice, to ensure rapid convergence, we might choose p_0 somewhat larger, say $p_0 \approx |4x|^{1/\sigma}$.

For the primes $p \le p_0$, we avoid logarithms and compute $I(p^\sigma, x)$ directly from the hypergeometric series of Proposition 4.

To summarize, the algorithm for computing $\psi_\sigma(x)$ with absolute error $\mathcal{O}(\varepsilon)$, for $x \in \mathbb{R}$, is as follows.

Algorithm for the characteristic function $\psi_\sigma(x)$

1. $p_0 \leftarrow \lceil |4x|^{1/\sigma} \rceil$.
2. $A \leftarrow \displaystyle\prod_{p \le p_0} \left(1 + \sum_{n=1}^{N} \frac{1}{p^{2n\sigma} n!^2} \prod_{j=0}^{n-1} (j^2 - (x/2)^2)\right)$, where N is sufficiently large that the error in truncating the sum is $\mathcal{O}(\varepsilon)$. [Here A is the product over primes $\le p_0$.]
3. $B \leftarrow \exp\left(-\displaystyle\sum_{n=1}^{N'} \frac{Q_n(x/2)}{n!^2} \left\{P(2n\sigma) - \sum_{p \le p_0} p^{-2n\sigma}\right\}\right)$, where N' is sufficiently large that the error in truncating the sum is $\mathcal{O}(\varepsilon)$, and $Q_n(x/2)$ is evaluated using the recurrence (8). [Here B is the product over primes $> p_0$.]
4. return $A \times B$.

Remarks on the algorithm for $\psi_\sigma(x)$

1. At step 3, $P(2n\sigma)$ can be evaluated using equation (23); time can be saved by precomputing the required values $\zeta(rs)$.
2. It is assumed that the computation is performed in floating-point arithmetic with sufficiently high precision and exponent range [6, Ch. 3]. For efficiency the precision should be varied dynamically as required, for example, to compensate for cancellation when summing the hypergeometric series at step 2, or when computing the term $\{P(2n\sigma) - \sum_{p \le p_0} p^{-2n\sigma}\}$ at step 3.
3. At step 3 an alternative is to evaluate $Q_n(x/2)$ using a table of coefficients $q_{n,k}$; these can be computed in advance using the recurrence of Proposition 5. This saves time (especially if many evaluations of $\psi_\sigma(x)$ at different points x are required, as is the case when evaluating $d(\sigma)$), at the expense of space and the requirement to estimate N' in advance.
4. The algorithm runs in polynomial time, in the sense that the number of bit-operations required to compute $\psi_\sigma(x)$ with absolute error $O(\varepsilon)$ is bounded by a polynomial (depending on σ and x) in $\log(1/\varepsilon)$.

9 Evaluation of $d(\sigma)$ and $d_-(\sigma)$

In this section we show how the densities $d(\sigma)$ and $d_-(\sigma)$ of §3 can be expressed in terms of the characteristic function ψ_σ.

Proposition 10. *For $\sigma > 1$, the support of the measure μ_σ of §3 is contained in the compact interval $[-L(\sigma), L(\sigma)]$, where*

$$L(\sigma) := \sum_p \arcsin(p^{-\sigma}).$$

Proof. Recall that μ_σ is the distribution of the random variable $\Im S$ considered in §2. From (4), $\Im S$ is equal to the sum of terms $-\arctan((\sin t)/(p^\sigma - \cos t))$ whose values are contained in the interval $[-\arcsin p^{-\sigma}, \arcsin p^{-\sigma}]$. Therefore the range of $\Im S$ is contained in the interval $[-L(\sigma), L(\sigma)]$. □

Remark 9. It may be shown that the support of μ_σ is exactly the interval $[L(\sigma), L(\sigma)]$.

Remark 10. As in van de Lune [23], we define σ_0 to be the (unique) real root in $(1, +\infty)$ of the equation $L(\sigma) = \pi/2$, and σ_1 to be the real root in $(1, +\infty)$ of $L(\sigma) = 3\pi/2$. These constants are relevant in §10.

Proposition 11. *For* $\sigma > \frac{1}{2}$,

$$d(\sigma) = 1 - \frac{2}{\pi}\int_0^\infty \psi_\sigma(x)\sin\Big(\frac{\pi x}{2}\Big)\,\frac{dx}{x}\,. \tag{25}$$

Proof. Recall from §3 that $1-d(\sigma) = \mu_\sigma([-\pi/2,\pi/2])$. Since ψ_σ is the characteristic function associated to the distribution μ_σ, a standard result[3] in probability theory gives

$$1-d(\sigma) = \frac{1}{2\pi}\lim_{X\to\infty}\int_{-X}^{X}\frac{\exp(ix\pi/2)-\exp(-ix\pi/2)}{ix}\psi_\sigma(x)\,dx\,.$$

Since $\psi_\sigma(x)$ is an even function, we obtain (25). □

To evaluate $d(\sigma)$ numerically from (25), we have to perform a numerical integration. The following theorem shows that the integral may be replaced by a rapidly-converging sum if $\sigma > 1$.

Theorem 5. *Let* $\sigma > 1$ *and* $\ell > \max(\pi/2, L(\sigma))$. *Then we have*

$$d(\sigma) = 1 - \frac{\pi}{2\ell} - \frac{2}{\pi}\sum_{n=1}^{\infty}\frac{1}{n}\psi_\sigma\Big(\frac{\pi n}{\ell}\Big)\sin\Big(\frac{n\pi^2}{2\ell}\Big)\,. \tag{26}$$

Proof. Consider the function $\widetilde{\rho}(x)$ equal to $\rho_\sigma(x)$ in the interval $[-\ell,\ell]$. Now extend $\widetilde{\rho}(x)$ to the real line $\mathbb{R}$, making it periodic with period 2ℓ. Thus

$$\widetilde{\rho}(x) = \sum_{n\in\mathbb{Z}} f_n \exp\left(\frac{\pi i n x}{\ell}\right), \quad \text{where} \quad f_n = \frac{1}{2\ell}\int_{-\ell}^{\ell}\widetilde{\rho}(x)\exp\left(-\frac{\pi i n x}{\ell}\right)dx.$$

Now $\widetilde{\rho}(x) = \rho_\sigma(x)$ for $|x|\le\ell$ and $\rho_\sigma(x) = 0$ for $|x|>\ell$. Therefore

$$f_n = \frac{1}{2\ell}\int_{-\ell}^{\ell}\rho_\sigma(x)\exp\left(-\frac{\pi i n x}{\ell}\right)dx = \frac{1}{2\ell}\int_{\mathbb{R}}\rho_\sigma(x)\exp\left(-\frac{\pi i n x}{\ell}\right)dx = \frac{1}{2\ell}\psi_\sigma\left(\frac{\pi n}{\ell}\right).$$

Since $\psi_\sigma(x)$ is an even function,

$$\widetilde{\rho}(x) = \frac{1}{2\ell}\sum_{n\in\mathbb{Z}}\psi_\sigma\Big(\frac{\pi n}{\ell}\Big)\exp\left(\frac{\pi i n x}{\ell}\right) = \frac{1}{2\ell} + \frac{1}{\ell}\sum_{n=1}^{\infty}\psi_\sigma\Big(\frac{\pi n}{\ell}\Big)\cos\frac{\pi n x}{\ell}\,\cdot \tag{27}$$

Now $d(\sigma) = 1-\mu_\sigma([-\pi/2,\pi/2]) = 1-\int_{-\pi/2}^{\pi/2}\rho_\sigma(t)\,dt$. Since $\pi/2\le\ell$, we may replace $\rho_\sigma(t)$ by $\widetilde{\rho}(t)$ in the integral. Hence, multiplying the equality (27) by the characteristic function of $[-\pi/2,\pi/2]$ and integrating, we get (26). □

[3] Attributed to Paul Lévy.

Remark 11. The sum in (26) can be seen as a numerical quadrature to approximate the integral in (25), taking a Riemann sum with stepsize $h = \pi/\ell$. However, we emphasise that (26) is *exact* under the conditions stated in Theorem 5. This is a consequence of the measure μ_σ having finite support when $\sigma > 1$. If $\sigma \in (\frac{1}{2}, 1]$ then μ_σ no longer has finite support and (26) only gives an approximation; however, this approximation converges rapidly to the exact result as $\ell \to \infty$, because μ_σ is well-approximated by measures with finite support.

Remark 12. If we take $m := 4\ell/\pi$ in the Theorem 5, we get the slightly simpler form

$$d(\sigma) = 1 - \frac{2}{m} - \frac{2}{\pi}\sum_{n=1}^{\infty}\frac{1}{n}\psi_\sigma\left(\frac{4n}{m}\right)\sin\left(\frac{2\pi n}{m}\right) \tag{28}$$

for $m > \max(2, M(\sigma))$, where $M(\sigma) = 4L(\sigma)/\pi$. A good choice if $L(\sigma) < \pi$ is $m = 4$; then only the odd terms in the sum (28) contribute.

Computation of $d_-(\sigma)$

Recall that $d_-(\sigma)$ is the probability that $\Re\zeta(\sigma + it) < 0$. Let $a_k = a_k(\sigma)$ be the probability that $|\arg\zeta(\sigma + it)| > (2k+1)\pi/2$, that is

$$a_k := 1 - \mu_\sigma([-(k+\tfrac{1}{2})\pi, (k+\tfrac{1}{2})\pi]).$$

Then

$$d_-(\sigma) = \sum_{k=0}^{\infty}(a_{2k} - a_{2k+1}) = \sum_{k=0}^{\infty}(-1)^k a_k\,. \tag{29}$$

We have seen that, for $\sigma > 1$ and $m > \max(2, 4L(\sigma)/\pi)$, eqn. (28) gives $a_0 = d(\sigma)$. Similarly, under the same conditions we have

$$a_k = 1 - \frac{4k+2}{m} - \frac{2}{\pi}\sum_{n=1}^{\infty}\frac{1}{n}\psi_\sigma\left(\frac{4n}{m}\right)\sin\left(\frac{(4k+2)\pi n}{m}\right). \tag{30}$$

Using (29) and (30) in conjuction with an algorithm for the computation of ψ_σ, we can compute $d_-(\sigma)$ and also, of course, $d_+(\sigma) = 1 - d_-(\sigma)$. If $\sigma \in (\frac{1}{2}, 1]$ then we can take the limit of (30) as $m \to \infty$, or use an analogue of Proposition 11, to evaluate the constants a_k.

Table 2 $d(\sigma)$ for various $\sigma \in (0.5, 1.165]$

σ	$d(\sigma)$
$0.5+10^{-11}$	0.6533592249148917497
$0.5+10^{-5}$	0.4962734204446697434
0.6	$7.9202919267432753125 \times 10^{-2}$
0.7	$2.5228782796068962969 \times 10^{-2}$
0.8	$5.1401888600187247641 \times 10^{-3}$
0.9	$3.1401743610642112427 \times 10^{-4}$
1.0	$3.7886623606688718671 \times 10^{-7}$
1.1	$6.3088749952505014038 \times 10^{-22}$
1.15	$1.3815328080907034247 \times 10^{-103}$
1.16	$1.1172074815779368125 \times 10^{-194}$
1.165	$1.2798207752318534603 \times 10^{-283}$

10 Numerical results

In [3] we described a computation of the first fifty intervals ($t > 0$) on which $\Re\zeta(1+it)$ takes negative values. The first such interval occurs for $t \approx 682112.9$, and has length ≈ 0.05. From the lengths of the first fifty intervals we estimated that $d_-(1) \approx 3.85 \times 10^{-7}$. We also mentioned a Monte Carlo computation which gave $d_-(1) \approx 3.80 \times 10^{-7}$. The correct value is $3.7886\ldots \times 10^{-7}$. The difficulty of improving the accuracy of these computations or of extending them to other values of σ was one motivation for the analytic approach of the present paper.

The algorithm of §8 was implemented independently by two of us, using in one case Mathematica and in the other Magma. The Mathematica implementation precomputes a table of coefficients $q_{n,k}$; the Magma implementation uses the recurrence for the polynomials Q_n directly. The results obtained by both implementations are in agreement, and also agree (up to the expected statistical error) with results obtained by the Monte Carlo method in the region $0.6 \le \sigma \le 1.1$ where the latter method is feasible.

Table 2 gives some computed values of $d(\sigma)$ for $\sigma \in (0.5, 1.165]$. From van de Lune [23] we know that $d(\sigma) = d_-(\sigma) = 0$ for $\sigma \ge \sigma_0 \approx 1.19234$. Table 2 shows that $d(\sigma)$ is very small for σ close to σ_0. For example, $d(\sigma) < 10^{-100}$ for $\sigma \ge 1.15$. The small size of $d(\sigma)$ makes the computation difficult for $\sigma \ge 1.15$. We need to compute $\psi_\sigma(4n/m)$ to more than 100 decimal places to compensate for cancellation in the sum (28), in order to get any significant figures in $d(\sigma)$.

Selberg [26] (see also [16, 18, 30]) showed that, for $t \sim \mathrm{unif}(T, 2T)$,

$$\frac{\log\zeta(1/2+it)}{\sqrt{\frac{1}{2}\log\log T}} \xrightarrow{d} X + iY \tag{31}$$

as $T \to \infty$, with $X, Y \sim N(0,1)$. This implies that $d(1/2) = 1$, but gives no indication of the speed of convergence of $d(\sigma)$ as $\sigma \downarrow \frac{1}{2}$. Table 2 shows that convergence is very slow – for $\sigma - \frac{1}{2} \ge 10^{-11}$ we have $d(\sigma) < \frac{2}{3}$.

Table 3 The difference $d(\sigma) - d_-(\sigma)$

σ	$d(\sigma) - d_-(\sigma)$
$0.5 + 10^{-11}$	0.1547533823
0.6	$8.073328981 \times 10^{-11}$
0.7	$2.676004882 \times 10^{-32}$
0.8	$7.655052120 \times 10^{-210}$

It appears from numerical computations that $\Re\zeta(1/2+it)$ is "usually positive" for those values of t for which computation is feasible. This is illustrated by several of the Figures in [2]. Because the function $\sqrt{\log\log T}$ grows so slowly, the region that is feasible for computation may not show the typical behaviour of $\zeta(\sigma+it)$ for large t on or close to the critical line $\sigma = \frac{1}{2}$.

Table 3 gives the difference $d(\sigma) - d_-(\sigma)$. For $\sigma > 0.8$, there is no appreciable difference between $d(\sigma)$ and $d_-(\sigma)$. This is because the probability that $|\arg\zeta(\sigma+it)| > 3\pi/2$ is very small in this region. Indeed, $d(\sigma) = d_-(\sigma)$ for all $\sigma \geq \sigma_1 \approx 1.0068$, where σ_1 is the positive real root of $L(\sigma) = 3\pi/2$.

There is an appreciable difference between $d(\sigma)$ and $d_-(\sigma)$ very close to the critical line. For example, $d_-(0.5+10^{-11}) \approx 0.4986058426$, but $d(0.5+10^{-11}) \approx 0.6533592249$. Our numerical results suggest that $\lim_{\sigma\downarrow 1/2} d_-(\sigma) = 1/2$.

It is plausible that $d_-(\frac{1}{2}) = d_+(\frac{1}{2}) = \frac{1}{2}$, but Selberg's result (31) does not seem to be strong enough to imply this.

11 Conclusion

We have shown a precise sense in which $\Re\zeta(s)$ is "usually positive" in the half-plane $\sigma = \Re(s) > \frac{1}{2}$, given an explicit expression for the characteristic function ψ_σ, and given a feasible algorithm for the accurate computation of ψ_σ, and consequently for the computation of the densities $d(\sigma)$ and $d_-(\sigma)$.

Our results could be generalised to cover Dirichlet L-functions because the character $\chi(p)$ in the Euler product

$$L(s,\chi) = \prod_p (1-\chi(p)p^{-s})^{-1}$$

can be absorbed into the random variable z_p whenever $|\chi(p)| = 1$. Thus, it would only be necessary to omit, from sums/products over primes, all primes p for which $\chi(p)$ is zero, i.e. the finite number of primes that divide the modulus of the L-function. This would, of course, change the numerical results. Nevertheless, we expect $\Re L(s,\chi)$ to be "usually positive" for $\Re(s) > \frac{1}{2}$.

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