Two theorems on sums over zeros of the Riemann zeta function

Benjamin Durkan

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Abstract

This journal-style thesis presents two new results concerning discrete moments of derivatives of the Riemann zeta function.

In Chapter 2 we establish a generalisation of the Landau-Gonek Theorem, in particular proving asymptotics uniform in X and T for

$$S(X,T) = \sum_{T<\Im(\rho)\leq 2T} \chi(\rho) X^{\rho},$$

where $\rho = \beta + i\gamma$ are the non-trivial zeta zeros and χ is the factor from the functional equation $\zeta(s) = \chi(s)\zeta(1-s)$. This allows one to evaluate sums of approximate functional equations evaluated at the non-trivial zeta zeros, and as a consequence of this we are able to provide a new proof of the Generalised Shanks conjecture.

In Chapter 3 we consider sums of the form

$$I(\mu,\nu) = \sum_{0<\Im(\rho)\leq T} \zeta^{(\mu)}(\rho)\zeta^{(\nu)}(1-\rho).$$

These sums were first considered by Gonek in 1984, whereby a leading asymptotic was established. We extend this to a full asymptotic by establishing all of the lower order terms in the asymptotic expansion. As a corollary we recover a 2008 theorem due to Milinovich which provides a full asymptotic for $\sum_{0<\Im(\rho)\leq T} |\zeta'(\rho)|^2$, and we go further by establishing the full asymptotic for $\sum_{0<\Im(\rho)\leq T} |\zeta^{(\nu)}(\rho)|^2$ for all positive integers ν. Our theorem is entirely unconditional, but we provide sharper bounds on the assumption of the Riemann Hypothesis.

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Author's declaration

I declare that the work presented in this thesis, except where otherwise stated, is based on my own research carried out at the University of York and has not been submitted previously for any degree at this or any other university. Sources are acknowledged by explicit references.

Chapter 2 will be in an upcoming paper [10], 'Generalisations of the Landau-Gonek theorem and applications to zeta mean values', written jointly with Christopher Hughes and Andrew Pearce-Crump.

Chapter 3 will be in an upcoming paper [11], 'The discrete second moment of mixed derivatives of the Riemann zeta function', written jointly with Christopher Hughes and Andrew Pearce-Crump.

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Introduction

1.1 The Riemann zeta function

The central object of this thesis is the Riemann zeta function, defined for $\Re(s) > 1$ as

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s} \tag{1.1}$$

$$= \prod_{p \text{ prime}} \left(1 - \frac{1}{p^s}\right)^{-1}, \tag{1.2}$$

where the latter expression is referred to as the Euler product representation of $\zeta(s)$. This immediately shows us that $\zeta(s)$ is connected to the primes, a theme we shall see repeatedly in this thesis. Whilst (1.1) holds only in the region $\Re(s) > 1$, one may analytically continue $\zeta(s)$ to the entire complex plane, except for a simple pole at $s = 1$.

Riemann initially established this analytic continuation by proving the functional equation

$$\zeta(s) = \chi(s)\zeta(1-s), \tag{1.3}$$

where the χ-factor is defined by

$$\chi(s) = \pi^{s-1/2}\frac{\Gamma\left(\frac{1-s}{2}\right)}{\Gamma\left(\frac{s}{2}\right)}$$
$$= 2^s\pi^{s-1}\sin\left(\frac{\pi s}{2}\right)\Gamma(1-s).$$

Here, $\Gamma(s)$ is the Gamma function defined for $\Re(s) > 0$ by

$$\Gamma(s) = \int_0^\infty t^{s-1} e^{-t} dt.$$

There are a wide variety of proofs of (1.3) – see [66] for some examples.

The following diagram will be useful for our purposes as it contains much of the basic information about $\zeta(s)$.

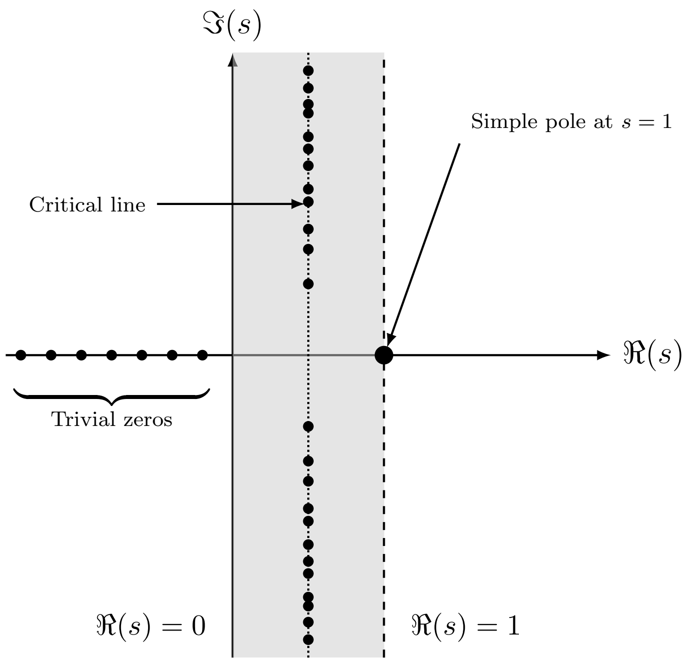


Figure 1.1: Basic properties of $\zeta(s)$

By virtue of (1.2) one may study $\zeta(s)$ in a straightforward manner whenever $\Re(s) > 1$ — perhaps most importantly it may easily be shown that $\zeta(s) \neq 0$ when $\Re(s) > 1$. Furthermore, using (1.3) allows us to consider $\zeta(s)$ in the region $\Re(s) < 0$ similarly (the functional equation allows us to 'flip' to $\Re(s) > 1$).

With more work, one can show that there are no zeros *on* the line $\Re(s) = 1$, a result which is in fact equivalent to the Prime Number Theorem (c.f. [66, Ch.3]). This shows that there is a relationship between the primes and the locations of the zeta zeros, an observation we will see repeatedly throughout this thesis.

It is the region in between, the *critical strip* whereby $0 \leq \Re(s) \leq 1$ which is most complicated. Denote by $N(T)$ the number of zeros of $\zeta(s)$ (counted with multiplicity) with $0 < \Im(s) \leq T$, i.e. the zeros contained within the critical strip with bounded height. The following theorem establishes an asymptotic for $N(T)$.

Theorem 1 (Riemann von-Mangoldt formula)**.** *As $T \to \infty$ we have*

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

Theorem 1 has as an immediate corollary that $\zeta(s)$ has infinitely many non-trivial zeros, since $N(T) \to \infty$ as $T \to \infty$, and furthermore that the zeros of $\zeta(s)$ get logarithmically denser as we get higher up the critical line.

Theorem 1 tells us about the number of non-trivial zeros within the critical strip, but it tells us nothing about *where* in the strip these zeros are located. The famous Riemann Hypothesis is the assertion that all of the non-trivial zeros lie on the line $\Re s = \frac{1}{2}$. Numerical computations have confirmed all zeros have $\Re(\rho) = \frac{1}{2}$ for $|\Im(\rho)| \leq 3 \times 10^{12}$ (see [61]), but this cannot rule out zeros off the critical line with $|\Im(\rho)|$ sufficiently large.

Unconditionally, little is known about the location of zeros within the critical strip. The best one can do with current technology is to prove a *zero-free region*, that is, pushing just to the left of the line $\Re(s) = 1$ and proving no zeros can exist in this narrow band. The classical zero-free result discovered in 1899 by de la Vallée Poussin [48], gives that there are no zeros ρ with

$$\Re(\rho) \geq 1 - \frac{C}{\log|\Im(\rho)|}$$

and $|\Im(\rho)| > 2$ for an absolute constant $C > 0$. Over the years the constant C has been incrementally improved numerous times. In 1899, de la Vallée Poussin showed that $C = \frac{1}{30.4679}$ was permissible, and the most recent advance in 2022 was by Mossinghoff, Trudgian & Yang [54] who established that $C = \frac{1}{5.558691}$ was permissible.

Asymptotically one can do slightly better; as shown by Vinogradov & Korobov, for sufficiently large $|\Im(\rho)|$ there are no zeros ρ with

$$\Re(\rho) \geq 1 - \frac{C(\varepsilon)}{(\log|\Im(\rho)|)^{2/3+\varepsilon}}.$$

Much work has been done to establish explicit zero-free regions in various ranges of $\Im(\rho)$, which we omit as this is rather disparate from the results of this thesis but we nonetheless encourage the reader to consult [12] for the current state of the art in this area.

In a slightly different direction, there have been some major advances in the study of critical zeros in recent decades. By use of mollifiers, Conrey [7] proved that at least 2/5 of the zeros lie on the critical line. Since then, there have been several incremental improvements to this; the strongest proportion to date is 5/12, due to Pratt, Robles, Zaharescu & Zeindler in 2018 [62].

For a detailed study of the Riemann zeta function, the reader is encouraged to consult [1, 40, 65, 53].

1.2 MOMENTS OF ZETA AND SUMS OVER ZEROS

A classical problem within analytic number theory is to study sums of the form $\sum_{0<\gamma\leq T} f(\rho)$, where f is a suitably chosen function and $\rho = \beta + i\gamma$ denotes zeros of $\zeta(s)$. Although sums over zeta zeros may appear unnatural, they underpin the explicit formulae which connect zeros to primes.

Indeed, one can obtain some interesting results depending on the choice of function f. If we consider the most straightforward case by setting $f(s) = 1$, then we recover $N(T)$ as defined previously.

With the choice $f(s) = \frac{X^s}{s}$ we recover the von Mangoldt explicit formula, which says that for any non-integer $X > 1$ we have

$$\sum_{n\leq X} \Lambda(n) = X - \sum_{|\Im(\rho)|\leq T} \frac{X^\rho}{\rho} + O\left(\frac{X(\log T)^3}{T}\right), \tag{1.4}$$

where $\Lambda(n)$ denotes the von Mangoldt function defined by

$$\Lambda(n) = \begin{cases} \log p & \text{if } n = p^k \text{ for a prime } p \text{ and integer } k \geq 1 \\ 0 & \text{otherwise} \end{cases}$$

The formula (1.4) can be found in, for example, [53, Theorem 12.5]. One may use this, in conjunction with the fact that no zeros ρ have $\Re(\rho) = 1$, to show that $\sum_{n\leq X} \Lambda(n) \sim X$ (since one can control the sum over zeros $\sum_{|\Im(\rho)|\leq T} \frac{X^\rho}{\rho} = o(X)$, the strength of this control depending on the proximity of zeta zeros ρ to the critical line). This is an equivalent formulation of the Prime Number Theorem. One can go even further; indeed, we have

$$\sum_{n\leq X}\Lambda(n) = X + E(X), \tag{1.5}$$

where (see [53, Chapter 6] for details)

$$E(X) \ll \begin{cases} X\exp(-C\sqrt{\log X}) & \text{using the classical zero-free region} \\ X\exp\left(-\frac{C(\log X)^{3/5}}{(\log\log X)^{1/5}}\right) & \text{using the Vinogradov-Korobov zero-free region} \\ X^{\frac{1}{2}+\varepsilon} & \text{under the Riemann Hypothesis} \end{cases}$$

One can do better under the assumption of the Riemann Hypothesis; indeed, von Koch [47] established that assuming the Riemann Hypothesis one has the power-saving bound $E(X) \ll X^{\frac{1}{2}}\log X$.

If one could prove a fixed-width zero-free region which states there are no zeros ρ with $\Re(\rho) \geq a$, then one could establish an error bound of the form $E(X) = O(X^{a+\varepsilon})$ (indeed this is where the error term under the Riemann Hypothesis comes from). Unfortunately such a result is not known. To see why the zero-free region has an impact on the error term in (1.5), observe that one may use Perron's formula to write

$$\sum_{n\leq X}\Lambda(n) = -\frac{1}{2\pi i}\int_{(c)}\frac{\zeta'}{\zeta}(s)\frac{X^s}{s}ds,$$

where (c) denotes the vertical line running from $c - i\infty$ to $c + i\infty$.

We may complete the contour with a rectangle (which introduces truncation errors), and to get the least possible error term we should like to pull the contour left as far as possible. The zero-free region tells us how far left we can shift the contour before encountering a zeta zero.

This highlights the powerful strength the study of zeta zeros has when considering problems relating to the distribution of primes. In particular, one sees that an improved zero-free region would yield a stronger error term in the Prime Number Theorem. The key is to be able to control sums $\sum_\rho \frac{X^\rho}{\rho}$, which under the Riemann Hypothesis exhibits square-root cancellation.

Perhaps as one might expect, establishing such cancellation is a significant problem, and the best one can do is to use the triangle inequality (which immediately loses information about cancellation) to write

$$\sum_{\Im(\rho)\le T} \frac{X^\rho}{\rho} \le \sum_{\Im(\rho)\le T} \frac{X^{\Re(\rho)}}{|\rho|} = O\left(\log^2 T \max_{|\Im(\rho)|\le T} X^{\Re(\rho)}\right). \tag{1.6}$$

Clearly the right-hand side of (1.6) is dominated by the term with maximal $|\rho|$.

We turn to a result due to Landau in [49], whereby we set $f(s) = X^s$ (this should be viewed as a converse to (1.4)).

Theorem 2 (Landau, 1911)**.** *Given fixed $X > 1$ we have*

$$\sum_{0<\gamma\le T} X^\rho = -\frac{T}{2\pi}\Lambda(X) + O(\log T)$$

as $T \to \infty$, where Λ is the von Mangoldt function.

Clearly it is the prime powers which give the main contribution to the sum (since Λ is supported only on prime powers); the way we interpret this is that the zeros ρ can 'sense' when X is a prime power. This highlights the arithmetic nature of the sum. Note, however, that Theorem 2 is not uniform in X; the error term does not account for different ranges of X in relation to T since it assumes X fixed. In 1985 Gonek [23] was able to make Theorem 2 uniform in both X and T, as follows.

Theorem 3 (Gonek, 1985)**.** *Uniformly for $X, T > 1$ we have*

$$\begin{aligned}\sum_{0<\gamma\le T} X^\rho = -\frac{T}{2\pi}\Lambda(X) &+ O(X\log(2XT)\log\log(3X)) \\ &+ O\left(\log X \min\left(T, \frac{X}{\langle X\rangle}\right)\right) + O\left(\log T \min\left(T, \frac{1}{\log X}\right)\right),\end{aligned}$$

where $\langle X\rangle$ is the distance from X to the closest prime power (different from X).

It is clear that Theorem 2 follows from Theorem 3, and further that if X is an integer no larger than T, we have

$$\sum_{0<\gamma\le T} X^\rho = -\frac{T}{2\pi}\Lambda(X) + O\left(X\log(2XT)\log\log(3X)\right),$$

that is, the latter two error terms in Theorem 3 are absorbed into the first error term.

We also have the following corollary of Theorem 3.

Corollary 4. *If $X \in \mathbb{N}$ is such that $X \leq T$, then*

$$\sum_{0<\gamma\leq T} \frac{1}{X^\rho} = -\frac{T}{2\pi}\frac{\Lambda(X)}{X} + O(\log(2XT)\log\log(3X)). \tag{1.7}$$

with the constant implicit in the big-O term absolute.

We observe that the functional equation (1.3) implies that if ρ is a zeta zero, so too is $1-\overline{\rho}$ (in fact they have the same imaginary part), which gives $\sum_{0<\gamma\leq T} \frac{1}{X^\rho} = \sum_{0<\gamma\leq T} X^{\overline{\rho-1}}$. This is enough to deduce Corollary 4.

The reader will notice the repeated presence of the von Mangoldt function in these explicit formulae. This is not a coincidence, and we shall explain briefly why this is the case now. When we are evaluating sums over the zeta zeros, our strategy consists of converting our sum into a contour integral; we are tacitly using the following well-known result, which says that for a closed contour $\mathcal{R}$ containing no poles of $f(s)$ we have

$$\sum_{0<\gamma\leq T} f(\rho) = \frac{1}{2\pi i}\oint_{\mathcal{R}} \frac{\zeta'}{\zeta}(s)f(s)ds. \tag{1.8}$$

This is a straightforward variant of the argument principle, which one may recover by setting $f(s) = 1$ in (1.8). We shall make repeated use of (1.8) throughout this thesis without further reference.

Now, for $\Re(s) > 1$ we have

$$\frac{\zeta'}{\zeta}(s) = -\sum_{n=1}^{\infty} \frac{\Lambda(n)}{n^s},$$

and so we choose a rectangular contour $\mathcal{R}$ which has one vertical edge just to the right of $\Re(s) = 1$ since this permits us to obtain sums involving $\Lambda(n)$. If we choose the left-hand vertical segment to lie to the left of $\Re(s) = 0$, an application of (1.3) will result in an integral involving $\frac{\zeta'}{\zeta}(s)$ and also $\chi(1-s)$, which can be dealt with via stationary phase techniques. Our truncation height will depend on the context – in Chapter 2 (where our theorem is for a sum over zeros with $T < \gamma < 2T$) we choose $\mathcal{R}$ to be the positively oriented rectangular contour with vertices at $c+iT, c+2iT, 1-c+2iT, 1-c+iT$ (where $c = 1+\frac{1}{\log T}$), and in Chapter 3 (where our theorem is for a sum with $1 < \gamma < T$) we choose $\mathcal{R}$ to have vertices $c+i, c+iT, 1-c+iT, 1-c+i$ instead.

The starting point in both Theorems 2 and 3 is to apply (1.8) with $f(\rho) := X^\rho$. The strength of (1.8) is clear; it converts a seemingly intractable sum into a contour integral which can be attacked via tools from complex analysis. Since this thesis is dedicated to understanding sums over zeros, (1.8) will be used repeatedly.

We introduce the more classical discrete moments by putting them in context of the study of simple zeros of $\zeta(s)$, that is, the zeta zeros which occur with multiplicity one. The simple zeros conjecture asserts that every non-trivial zeta zero is simple; whilst this has resisted proof so far, it is widely believed, and we shall now discuss some of the progress on the problem.

Denote by $N^*(T)$ the number of simple zeros of $\zeta(s)$ with imaginary part at most T. By a straightforward argument we can show that $N^*(T) \gg T$ as follows. Following Conrey, Ghosh & Gonek [7], we use Cauchy-Schwarz to write

$$\left|\sum_{0<\gamma\le T} \zeta'(\rho)\right|^2 \le N^*(T) \sum_{0<\gamma\le T} |\zeta'(\rho)|^2. \tag{1.9}$$

It is clear that (1.9) counts only the simple zeros, since if a zero ρ had multiplicity larger than 1 then $\zeta'(\rho)$ would vanish. If we can understand the moments on the left and right hand sides, we can understand the count of simple zeros, since

$$N^*(T) \ge \frac{\left|\sum_{0<\gamma\le T} \zeta'(\rho)\right|^2}{\sum_{0<\gamma\le T} |\zeta'(\rho)|^2}. \tag{1.10}$$

This places in context the importance of the types of discrete moment we study in this thesis. It is important to note that our application of Cauchy-Schwarz in (1.9) suffers from the so-called 'loss of logarithm problem' –the count $N^*(T) \gg T$ is not best possible, and by using a considerably more involved argument involving mollifiers, Conrey, Ghosh & Gonek [9] established a positive proportion result $N^*(T) \gg T\log T$. We do not study mollified moments in this thesis.

There are two types of moment we shall study in this thesis, both of which are to be viewed as different types of average of zeta and its derivatives. We firstly consider sums of the form $\sum_{0<\gamma\le T} \zeta^{(\nu)}(\rho)$, which allows us to average the higher derivatives of zeta (and since we don't take absolute values, this sum includes information about oscillation of $\zeta^{(\nu)}(\rho)$).

Secondly, we consider the more classical family of discrete moments $\sum_{0<\gamma\leq T}\left|\zeta^{(\nu)}(\rho)\right|^{2k}$; since we have absolute values here, these moments are especially useful when considering extreme values of $\zeta^{(\nu)}(\rho)$ since the dominant contribution to these moments occurs when $\zeta^{(\nu)}(\rho)$ is unusually large. In Chapter 3 we specialise to the case $k=1$, but we discuss the state of the art for $k\in\mathbb{N}$.

1.2.1 SHANKS-TYPE MOMENTS

In 1961, Shanks conjectured (based on numerical evidence from Haselgrove [29]) that, when averaged over the non-trivial zeta zeros $\rho=\frac{1}{2}+i\gamma$, the derivative $\zeta'(\rho)$ is real and positive. This is *prima facie* an unusual conjecture – indeed, $\zeta'(s)$ is a complex valued function and the zeros ρ are also complex, yet Shanks' assertion is that the imaginary parts cancel out on average. It turns out that this conjecture is true, and much can be said quantitatively. The following summarises the progress which has been made over the past century on this problem.

Table 1.1: Progress on Shanks' conjecture

Authors	Result
Shanks (1961)	Formulated conjecture
Conrey, Ghosh & Gonek [9] (1985)	Leading asymptotic
Fujii [16] (1994, 2012)	Full asymptotic
Kaptan, Karabulut & Yildirim [42] (2011)	Leading asymptotic for higher derivatives
Hughes & Pearce-Crump [37] (2022)	Full asymptotic for higher derivatives
Hughes, Martin & Pearce-Crump [36] (2024)	Heuristic for leading order
Pearce-Crump [59] (2024)	Sharpened error term
Durkan, Hughes, Pearce-Crump [10] (2025)	New proof of full asymptotic

We now give more details on the results contained in Table 1.1. In 1985 Conrey, Ghosh & Gonek [9] established, starting with (1.8), that

$$\sum_{0<\gamma\leq T}\zeta'(\rho)=\frac{T}{4\pi}\log^2 T+O(T\log T). \tag{1.11}$$

The truth of Shanks' conjecture follows as an immediate corollary of (1.11). Whilst the error term is clearly subdominant to the main term, it is only so by a factor of a logarithm. In obtaining the lower order terms, one can better understand the true behaviour of the function. This is what Fujii [16] then did unconditionally (but with a considerably smaller error term on the assumption of the Riemann Hypothesis) –

where C_0 and C_1 are the Laurent coefficients given by

$$\zeta(s) = \frac{1}{s-1} + C_0 + C_1(s-1) + \cdots ,$$

Fujii showed that

$$\sum_{0<\gamma\le T} \zeta'(\rho) = \frac{T}{4\pi}\log^2\left(\frac{T}{2\pi}\right) + (-1+C_0)\frac{T}{2\pi}\log\left(\frac{T}{2\pi}\right) + (1-C_0-C_0^2+3C_1)\frac{T}{2\pi} + E(T), \tag{1.12}$$

where $E(T)$ is an error term given by

$$E(T) \ll \begin{cases} T\exp(-C\sqrt{\log T}) & \text{for a positive constant } C\text{, unconditionally} \\ \sqrt{T}(\log T)^{\frac{7}{2}} & \text{conditional on the Riemann Hypothesis.} \end{cases}$$

Following this, in 2011 Kaptan, Karabulut & Yildirim [42] established an analogue of (1.11) for the higher derivatives, proving the following:

$$\sum_{0<\gamma\le T} \zeta^{(\nu)}(\rho) = \frac{(-1)^{\nu+1}}{\nu+1}\frac{T}{2\pi}\left(\log\frac{T}{2\pi}\right)^{\nu+1} + O(T(\log T)^{\nu}) . \tag{1.13}$$

This alternating sign phenomenon shows that for odd ν, $\zeta^{(\nu)}(\rho)$ is real and positive in the mean, whereas for even ν, $\zeta^{(\nu)}(\rho)$ is real and negative in the mean. This is known as the Generalised Shanks conjecture in the literature.

Subsequently in 2022, Hughes & Pearce-Crump [37] established the full asymptotic for the sum in (1.13), with a power saving error term (in the case $\nu = 1$ they established that under the Riemann Hypothesis, $E(T) \ll \sqrt{T}(\log T)^{\frac{13}{4}}$). In his thesis, Pearce-Crump [59] provided a sharpening on the error term given in [37] by establishing that under the Riemann Hypothesis, one has $E(T) \ll T^{\frac{1}{2}}(\log T)^{\nu+\frac{9}{4}}$. The full asymptotic of (1.12), and the leading asymptotic of (1.13), will both follow from our main result of Chapter 2.

The proof of our result in Chapter 2 builds on 2024 work of Hughes, Martin & Pearce-Crump [36], where the authors gave a heuristic which recovers the leading term of (1.13), based on summing the approximate functional equation for $\zeta^{(\nu)}(s)$ over the zeta zeros, with the entire weight placed on the first term of the approximate functional equation. Whilst their heuristic does give the correct leading term, the error terms dominate. However, in Chapter 2 we consider the entire approximate functional equation, and in doing so we recover (1.12) and (1.13), with a sufficiently small error term.

1.2.2 The classical discrete moments

We now turn to the type of moment on the right-hand side of (1.9). Clearly since the absolute value is within the sum, these moments $\sum_{0<\gamma\leq T}\left|\zeta^{(\nu)}(\rho)\right|^{2k}$ are all real and non-negative. These moments have been studied extensively in the literature, and we shall give an overview of what is known so far, before explaining precisely what we do in this thesis which extends on that.

The following table outlines the progress that has been made on this problem, which we shall elaborate on.

Table 1.2: Progress on discrete moments $\sum_{0<\gamma\leq T}|\zeta^{(\nu)}(\rho)|^{2k}$

Authors	Result
Gonek (1984)	Leading asymptotic for $\sum_{0<\gamma\leq T}\zeta^{(\mu)}(\rho)\zeta^{(\nu)}(1-\rho)$
Ng (2004)	Upper and lower bounds for fourth moment of $\lvert\zeta'(\rho)\rvert$
Milinovich (2008)	Full asymptotic for second moment of $\lvert\zeta'(\rho)\rvert$
Milinovich (2010)	Near-sharp upper bound for $2k$th moment of $\lvert\zeta'(\rho)\rvert$
Milinovich & Ng (2014)	Sharp lower bound for $2k$th moment of $\lvert\zeta'(\rho)\rvert$
Kirila (2020)	Sharp upper bound for $2k$th moment of $\left\lvert\zeta^{(\nu)}(\rho)\right\rvert$
Benli, Elma & Ng (2023)	Sharp lower bound for $2k$th moment of $\left\lvert\zeta^{(\nu)}(\rho)\right\rvert$

We start by discussing the case $\nu = 1$. It was conjectured independently by Gonek [24] and Hejhal [32] that for each real k,

$$\sum_{0<\gamma\leq T}|\zeta'(\rho)|^{2k} \asymp T(\log T)^{(k+1)^2}.$$

Following the conjecture of Gonek & Hejhal, Hughes, Keating & O'Connell [35] provided an independent and stronger conjecture for the first derivative case, based on models arising from Random Matrix Theory. In particular, they conjectured the following.

Conjecture 1. *For $\Re(k) \geq -3/2$ and bounded,*

$$\sum_{0<\gamma\leq T}|\zeta'(\rho)|^{2k} \sim \frac{G^2(k+2)}{G(2k+3)}a(k)T\left(\log\frac{T}{2\pi}\right)^{(k+1)^2}, \tag{1.14}$$

where

$$a(k) = \prod_p\left(1-\frac{1}{p}\right)^{k^2}\sum_{m=0}^{\infty}\left(\frac{\Gamma(m+k)}{m!\Gamma(k)}\right)^2 p^{-m}$$

and G is the Barnes G-function defined by

$$G(z) = (2\pi)^{z/2} \exp\left(-\frac{1}{2}(z^2 + \gamma_0 z + z)\right) \prod_{n\geq 1} \left(1 + \frac{z}{n}\right)^n e^{-z+\frac{z^2}{2n}}$$

with γ_0 denoting the Euler-Mascheroni constant.

Remark 1. *The reader may ask whether Conjecture 1 extends to higher derivatives. The models which led to the formulation of Conjecture 1 rely on a product representation for the characteristic polynomial for $\zeta'(s)$, an analogue of which does not exist for higher derivatives.*

Although this conjecture is deep, rigorously not much is known from a number theoretic standpoint. The case $k = 1$ was handled by Gonek in [26] who proved the following very general theorem (which agrees with Conjecture 1 for $k = 1$).

Theorem 5 ([26], Theorem 1)**.** *As $T \to \infty$, for α real with $|\alpha| \leq \frac{1}{2}\log\left(\frac{T}{2\pi}\right)$ and $\mu, \nu \in \mathbb{N}$, we have*

$$\begin{aligned}&\sum_{0<\gamma\leq T} \zeta^{(\mu)}\left(\rho + i\frac{\alpha}{\log\left(\frac{T}{2\pi}\right)}\right) \zeta^{(\nu)}\left(1 - \rho - i\frac{\alpha}{\log\left(\frac{T}{2\pi}\right)}\right)\\ &= \frac{(-1)^{\mu+\nu}T}{2\pi} \log^{\mu+\nu+2}\left(\frac{T}{2\pi}\right)\left(\frac{1}{\mu+\nu+1} - H(\mu,\nu,2\pi\alpha) - H(\mu,\nu,-2\pi\alpha)\right)\\ &+ O(T(\log T)^{\mu+\nu+1}),\end{aligned}$$

where

$$H(\mu,\nu,2\pi\alpha) = \mu! \sum_{\ell=0}^{\infty} \frac{(2\pi\alpha i)^\ell}{(\ell+\mu+1)!(\ell+\mu+\nu+2)}.$$

Theorem 5 is unconditional. However, if we assume the Riemann Hypothesis we may use $\overline{\zeta(1-\rho)} = \zeta(\rho)$, so by setting $\alpha = 0$ and $\mu = \nu$ in Theorem 5 we obtain a leading asymptotic for $\sum_{0<\gamma\leq T} \left|\zeta^{(\nu)}\left(\frac{1}{2} + i\gamma\right)\right|^2$. In particular, as pointed out by Gonek,

$$\sum_{0<\gamma\leq T} \left|\zeta^{(\nu)}\left(\frac{1}{2} + i\gamma\right)\right|^2 = \frac{\nu^2}{(2\nu+1)(\nu+1)^2} \frac{T}{2\pi}\left(\log\frac{T}{2\pi}\right)^{2\nu+2} + O\left(T(\log T)^{2\nu+1}\right). \tag{1.15}$$

In 2007, Conrey & Snaith [6] conjectured the full asymptotic for (1.15) in the special case $\nu = 1$.

Then in 2008, in his thesis Milinovich [50] extended (1.15) to a full asymptotic in the special case $\nu = 1$ and established the coefficients of the resulting degree four polynomial and giving an error term demonstrating square-root cancellation.

Theorem 6 ([50], Theorem 1.3.1)**.** *Assume the Riemann Hypothesis. Then*

$$\sum_{0<\gamma\leq T} \left|\zeta'\left(\frac{1}{2}+i\gamma\right)\right|^2 = \frac{T}{2\pi}\sum_{j=0}^{4} A_j \left(\log\frac{T}{2\pi}\right)^j + O\left(T^{1/2+\varepsilon}\right),$$

where

$$A_4 = \frac{1}{12}$$
$$A_3 = \frac{2\gamma_0 - 1}{3}$$
$$A_2 = 1 - 2\gamma_0 + \gamma_0^2 - 2\gamma_1$$
$$A_1 = -(2 - 4\gamma_0 + 2\gamma_0^2 + 2\gamma_0^3 + 10\gamma_0\gamma_1 - 4\gamma_1 + \gamma_2)$$
$$A_0 = \frac{6 + 6\gamma_0(5\gamma_1 + 4\gamma_2 - 2) + 6\gamma_0^2(\gamma_0 + \gamma_0^2 + 6\gamma_1 + 1) - 12\gamma_1 + 42\gamma_1^2 + 3\gamma_2 + 10\gamma_3}{3},$$

where the γ_n are the Stieltjes constants given by expanding $\zeta(s)$ around $s = 1$,

$$\zeta(s) = \frac{1}{s-1} + \gamma_0 - \gamma_1(s-1) + \frac{\gamma_2}{2!}(s-1)^2 + \cdots + (-1)^n\frac{\gamma_n}{n!}(s-1)^n + \cdots$$

Currently, only bounds of the conjectured order of magnitude are available for $k \geq 2$.

Ng proved in [57] that under the assumption of the Riemann Hypothesis,

$$\sum_{0<\gamma\leq T} \left|\zeta'\left(\frac{1}{2}+i\gamma\right)\right|^4 \asymp T(\log T)^9,$$

and went even further by establishing numerical upper and lower bounds. The upper bound was sharpened slightly in [19, Theorem 1]. Much work has been done in the intervening years, which we outline now. For the higher moments of the first derivative Milinovich & Ng [52] established sharp lower bounds of the form

$$\sum_{0<\gamma\leq T} \left|\zeta'\left(\frac{1}{2}+i\gamma\right)\right|^{2k} \gg T(\log T)^{(k+1)^2},$$

conditional on the Generalised Riemann Hypothesis. In the reverse direction Milinovich [51] proved under the assumption of the Riemann Hypothesis that

$$\sum_{0<\gamma\leq T}\left|\zeta'\left(\frac{1}{2}+i\gamma\right)\right|^{2k} \ll T(\log T)^{(k+1)^2+\varepsilon}$$

for arbitrary $\varepsilon > 0$, which is exceptionally close to the conjectured upper bound. In 2020, Kirila [46] was able to strengthen the bound by removing the ε (by use of an adaptation of an argument of Harper [28]) and as a consequence proved that

$$\sum_{0<\gamma\leq T}\left|\zeta'\left(\frac{1}{2}+i\gamma\right)\right|^{2k} \asymp T(\log T)^{(k+1)^2},$$

under the Riemann Hypothesis.

In fact, Kirila's methods went even further and extended to higher derivatives.

Theorem 7 (Kirila)**.** *Under the Riemann Hypothesis, for $k \geq \frac{1}{2}$ and $\nu \in \mathbb{N}$ we have*

$$\sum_{0<\gamma\leq T}\left|\zeta^{(\nu)}\left(\frac{1}{2}+i\gamma\right)\right|^{2k} \ll_{k,\nu} T(\log T)^{k(k+2\nu)+1}.$$

In 2023 work of Benli, Elma & Ng [3, Cor. 1.3], under the Riemann Hypothesis a lower bound of the same magnitude was obtained (with the restriction that $k, \nu \in \mathbb{N}$)

$$\sum_{0<\gamma\leq T}\left|\zeta^{(\nu)}\left(\frac{1}{2}+i\gamma\right)\right|^{2k} \gg_{k,\nu} T(\log T)^{k(k+2\nu)+1}. \tag{1.16}$$

Note also that (1.16) removes the assumption of the Generalised Riemann Hypothesis of [52] in the case $\nu = 1$ and replaces it with the weaker assumption of the Riemann Hypothesis.

Combining this with Theorem 7 allows us to deduce that, on the assumption of the Riemann Hypothesis,

$$\sum_{0<\gamma\leq T}\left|\zeta^{(\nu)}\left(\frac{1}{2}+i\gamma\right)\right|^{2k} \asymp_{k,\nu} T(\log T)^{k(k+2\nu)+1}.$$

— 2 —

Generalisations of the Landau-Gonek Theorem and applications to zeta mean values

Abstract

The Landau–Gonek Theorem evaluates X^ρ summed over the non-trivial zeros of the Riemann zeta function. Their result shows great sensitivity to the arithmetic nature of X. We prove a related result concerning the sum of $\chi(\rho)X^\rho$ over the zeros of zeta, where $\chi(s)$ is the term arising in the functional equation for the zeta function. Again, this result depends deeply on whether X is an integer or not. We show the result splits into three cases, depending on whether X is smaller than T, about the same size as T, or bigger than T. The reason this result is useful is that it easily permits the calculation of discrete moments of the Riemann zeta function via the approximate functional equation. As an application of this result, we provide an alternative proof of Shanks' conjecture.

2.1 Introduction

Since Riemann's 1859 memoir [63], the link between primes and the non-trivial zeros of the Riemann zeta function $\zeta(s)$ has been a central topic within analytic number theory. A common theme is to consider sums of the form

$$\sum_{0<\gamma\leq T} f(\rho) \tag{2.1}$$

for a function $f(s)$, where $\rho = \beta + i\gamma$ is a non-trivial zero of the Riemann zeta function $\zeta(s)$.

Landau [49] established the following result for $f(s) = X^s$, a variation on a sum that occurs naturally when studying the Prime Number Theorem.

Theorem 8 (Landau, 1911)**.** *Given fixed $X > 1$ we have*

$$\sum_{0<\gamma\leq T} X^\rho = -\frac{T}{2\pi}\Lambda(X) + O(\log T),$$

as $T \to \infty$, where $\Lambda(n)$ is the von Mangoldt function.

This result tells us that the main term in the sum under consideration only appears when X is a prime or a prime power, since $\Lambda(n)$ is only supported when n equals a prime power. Such a sum, relating the non-trivial zeros to the primes, is referred to as an explicit formula. Gonek [22, 23] made Landau's Theorem uniform in both X and T.

Theorem 9 (Gonek, 1985)**.** *Uniformly for $X, T > 1$ we have*

$$\sum_{0<\gamma\leq T} X^\rho = -\frac{T}{2\pi}\Lambda(X) + O(X\log(2XT)\log\log(3X))$$
$$+ O\left(\log X \min\left(T, \frac{X}{\langle X\rangle}\right)\right) + O\left(\log(2T)\min\left(T, \frac{1}{\log X}\right)\right),$$

where $\langle X\rangle$ is the distance from X to the closest prime power (different from X).

When we restrict X to be an integer, Gonek also notes that the last two error terms are subsumed by the first two error terms. He also highlights the highly different behaviour between the case when X is an integer and when X is an arbitrary real number.

Gonek's result was further generalised by Fujii [13, 14] who found lower order terms in the expansion.

So far, we have been restricted to the case that $X > 1$. Gonek noted that we can also consider the case $0 < X < 1$ by noting that the functional equation for the zeta function, given by

$$\zeta(s) = \chi(s)\zeta(1-s) \tag{2.2}$$

implies that if ρ is a zeta zero, so too is $1 - \overline{\rho}$ (in fact they have the same imaginary part). Then $\sum_{0<\gamma\leq T} X^{-\rho} = \sum_{0<\gamma\leq T} X^{\overline{\rho-1}}$. Using this observation leads to the following corollary.

Corollary 10 (Gonek, 1993). *Uniformly for $X > 1$ and $T > 1$, we have*

$$\sum_{0<\gamma\leq T} X^{-\rho} = -\frac{T}{2\pi}\frac{\Lambda(X)}{X} + O(\log(2XT)\log\log(3X)) + O\left(\log X \min\left(\frac{T}{X}, \frac{1}{\langle X\rangle}\right)\right) + O\left(\log(2T)\min\left(\frac{T}{X}, \frac{1}{X\log X}\right)\right), \tag{2.3}$$

where $\langle X\rangle$ is the distance from X to the closest prime power (different from X).

Again, when we restrict X to be an integer, Gonek also notes that the last two error terms are subsumed by the first two error terms.

Another natural function to consider in (2.1) is $f(s) = \zeta'(s)$. Indeed, it was a conjecture by Shanks [64] (based on numerical evidence from Haselgrove [29]) that, when summed over the non-trivial zeta zeros, $\zeta'(\rho)$ is real and positive in the mean. This is a surprising conjecture, since both $\zeta'(s)$ and the non-trivial zeros are complex. This conjecture was first proved by Conrey, Ghosh and Gonek [5] where they showed that

$$\sum_{0<\gamma\leq T} \zeta'(\rho) = \frac{T}{4\pi}\left(\log\frac{T}{2\pi}\right)^2 + O(T\log T),$$

from which Shanks' conjecture follows immediately. Trudgian [67] also gave an alternative proof of this result.

This has been refined considerably since then. Fujii [16, 15] established the full asymptotic, and in 2022 Hughes and Pearce-Crump [37] sharpened the error term under the Riemann Hypothesis (RH).

Theorem 11 (Fujii, 1994).

$$\sum_{0<\gamma\leq T} \zeta'(\rho) = \frac{T}{4\pi}\left(\log\frac{T}{2\pi}\right)^2 + (\gamma_0 - 1)\frac{T}{2\pi}\log\left(\frac{T}{2\pi}\right) + (1-\gamma_0-\gamma_0^2-3\gamma_1)\frac{T}{2\pi} + \mathcal{E}(T)$$

where

$$\mathcal{E}(T) = \begin{cases} O\left(T\exp(-C\sqrt{\log T})\right) & \textit{unconditionally, for some } C > 0 \\ O(T^{1/2}(\log T)^{13/4}) & \textit{under RH, due to Hughes–Pearce-Crump, 2022} \end{cases}$$

Here γ_0 and γ_1 are the Stieltjes constants given by the following coefficients of the Laurent expansion of $\zeta(s)$ around $s = 1$

$$\zeta(s) = \frac{1}{s-1} + \gamma_0 - \gamma_1(s-1) + \frac{\gamma_2}{2}(s-1)^2 + \ldots. \tag{2.4}$$

One can similarly deal with the higher derivatives with $f(s) = \zeta^{(\nu)}(s)$ in (2.1). In 2011, Kaptan, Karabulut and Yıldırım [42] established the leading-order asymptotic for this function.

Theorem 12 (Kaptan–Karabulut–Yıldırım, 2011)**.** *We have*

$$\sum_{0<\gamma\leq T} \zeta^{(\nu)}(\rho) = \frac{(-1)^{\nu+1}}{\nu+1}\frac{T}{2\pi}\left(\log\frac{T}{2\pi}\right)^{\nu+1} + O(T(\log T)^{\nu}). \tag{2.5}$$

In words, this result says that $\zeta^{(\nu)}(s)$ is real and positive/negative in the mean depending on whether ν is odd/even, a result the second two authors of this paper have coined the generalised Shanks' conjecture.

Hughes and Pearce-Crump [37] subsequently established the full asymptotic with all lower order terms made explicit, and with power-savings on the error term.

In 2023, Hughes, Martin, and Pearce-Crump [33] devised a simple heuristic which gives the correct main term for this sum, but with an error term that dominates the main term. The starting point of their heuristic is to use the approximate formula

$$\zeta^{(\nu)}(\sigma+it) = (-1)^{\nu}\sum_{m\leq t}\frac{(\log m)^{\nu}}{m^{\sigma+it}} + O(t^{-\sigma}(\log t)^{\nu}), \tag{2.6}$$

valid for $\sigma > 0$ and t large. Then, upon swapping the order of summation and summing over the zeta zeros using Corollary 10, one recovers immediately the correct leading term of Theorem 12. However, they showed the error terms dominate, so the argument is heuristic, not rigorous. This heuristic may be viewed as taking the approximate functional equation for the derivatives of the zeta function (see Section 2.6) and placing the entire weight on the first piece, and then summing over the zeta zeros. The aim of this paper is to develop a result allowing us to use both pieces of the approximate functional equation, making the heuristic rigorous.

Finally, a combination of some of the functions considered above was considered by Fujii [15] where he considered $f(s) = \zeta'(s)X^s$, and by Pearce-Crump [58] where he considered $f(s) = \zeta^{(\nu)}(s)X^s$. In both of these instances, the behaviour of such sums changing depending on whether X is an integer or a general real number is observed. In both cases the asymptotics are more complicated than those written out above — we refer the reader to their papers for the full results.

2.2 RESULTS

In this paper we prove Theorem 16, where we establish uniform asymptotics for (2.1) with $f(s) = \chi(s)X^s$, where $\chi(s)$ is the factor from the functional equation (2.2) for zeta.

Let

$$S(X,T) = \sum_{T<\gamma\leq 2T} \chi(\rho)X^{\rho}.$$

We prove an asymptotic for the sum $S(X,T)$ which is uniform in both X and T. Theorem 13 may be viewed as an oscillatory analogue of Theorem 9.

Theorem 13. *Uniformly for $X \geq 1$ and $T > 1$ we have*

$$S(X,T) = \begin{cases} -X \displaystyle\sum_{\frac{T}{2\pi X}<n\leq\frac{T}{\pi X}} \Lambda(n)e^{2\pi Xni} + E(X,T) & \text{if } X \leq \frac{T}{2\pi} \\ X(\log X)e^{2\pi Xi} + E(X,T) & \text{if } \frac{T}{2\pi} < X \leq \frac{T}{\pi} \\ -X \displaystyle\sum_{\frac{\pi X}{T}\leq n<\frac{2\pi X}{T}} \frac{\Lambda(n)}{n}e^{\frac{2\pi Xi}{n}} + E(X,T) & \text{if } X > \frac{T}{\pi} \end{cases}$$

where

$$E(X,T) = O\left(T^{1/2}(\log T)^2\right) + O\left(\frac{X^{1+1/\log T}(\log T)^2}{T^{1/2}}\right) + O\left(\frac{T^{3/2}\log T}{|T-2\pi X| + T^{1/2}}\right) + O\left(\frac{T^{3/2}\log T}{|T-\pi X| + T^{1/2}}\right). \quad (2.7)$$

Remark. *Note that the last two error terms are the same size as the main terms at the jumps, when $X = \frac{T}{2\pi}$ and $X = \frac{T}{\pi}$. Also note that the two sums over n become empty at precisely those jumps.*

We illustrate the theorem in Figure 2.1 by plotting $S(X,T)$ in the complex plane for all T above the first zeta zero and below $300,000$ and $X = 2000$. It is a discrete set consisting of 1,466,163 points, and is beautifully intricate. The points in blue are for $T < \pi X$, those in red are for $\pi X < T \leq 2\pi X$ (red), and those in green are for $T > 2\pi X$, clearing showing that $S(X,T)$ has three distinct parts, all captured by our theorem.

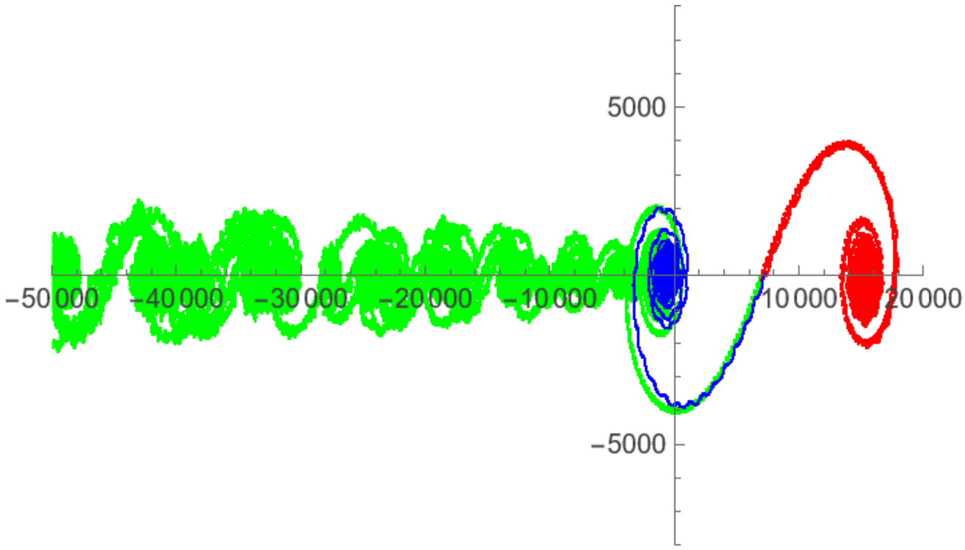


Figure 2.1: The complex values of $S(X,T)$, plotted for $T < 300,000$ with $X = 2000$. Note that the $\Re$- and $\Im$-axes have very different scalings

Our Theorem immediately recovers and sharpens the error term in a theorem due to Pearce-Crump [59, 60] where he considered $X = 1$. This result was previously known with a worse error term in [8, 44], so the results in this paper carries on the progression of improving the error term in this special case. We state this result as follows.

Corollary 14. *We have*

$$\sum_{0<\gamma\leq T} \chi(\rho) = -\frac{T}{2\pi} + \begin{cases} O\left(Te^{-a\sqrt{\log T}}\right) & \textit{unconditionally} \\ O(T^{1/2}(\log T)^2) & \textit{under RH} \end{cases}$$

for some $a > 0$.

Proof of Corollary 14. Setting $X = 1$ in Theorem 13 and summing over dyadic intervals we have

$$\begin{aligned}\sum_{0<\gamma\le T}\chi(\rho) &= \sum_{k=1}^{\lfloor \frac{\log(T/(2\pi))}{\log 2}\rfloor} S(1,\frac{1}{2^k}T)\\ &= -\sum_{n\le \frac{T}{2\pi}}\Lambda(n) + O\left(T^{1/2}(\log T)^2\right)\\ &= -\frac{T}{2\pi} + \begin{cases} O\left(Te^{-a\sqrt{\log T}}\right) & \text{unconditionally}\\ O(T^{1/2}(\log T)^2) & \text{under RH}\end{cases}\end{aligned}$$

The truncation of the dyadic sum is chosen so that both $2^{-k}T$ is larger than the lowest zero for all k and also so that we only ever require the first case in Theorem 13. Since X is an integer in this corollary, $e^{2\pi iXn} = 1$ for all n. We remark that the error term being conditional/unconditional arises solely from our evaluation of the sum of the von Mangoldt function. □

Theorem 13 permits other positive integers, not just $X = 1$, to be summed over all zeros up to height T, with a similar result.

Corollary 15. *Let $X \in \mathbb{N}$ be such that $X = o(T)$ be an integer. Then*

$$\sum_{0<\gamma\le T}\chi(\rho)X^{\rho} = -\frac{T}{2\pi} + O(X\log X) + \begin{cases} O\left(Te^{-a\sqrt{\log T}}\right) & \textit{unconditionally}\\ O(T^{1/2}(\log T)^2) & \textit{under RH}\end{cases}$$

for some $a > 0$.

Proof of Corollary 15. There are three regions when performing the dyadic summation, corresponding to the three cases in Theorem 13. For k such that $\frac{1}{2^k}T \ge 2\pi X$, we have a contribution from the first case in that theorem, and the n-sums combine to yield

$$-X\sum_{n\le \frac{T}{2\pi X}}\Lambda(n) = -\frac{T}{2\pi} + \begin{cases} O\left(Te^{-a\sqrt{\log T}}\right) & \text{unconditionally}\\ O(T^{1/2}(\log T)^2) & \text{under RH}\end{cases}$$

There is exactly one value of k such that $X \in \left(\frac{1}{2\pi}2^{-k}T, \frac{1}{\pi}2^{-k}T\right]$, and that will cause the middle case of the theorem to contribute $X\log X$.

And finally, the k such that $\frac{1}{2^k}T < 2\pi X$ will yield contributions from the third case, where the n-sums combine to yield

$$-X \sum_{n<X} \frac{\Lambda(n)}{n} e^{2\pi i X/n} \ll X \sum_{n<X} \frac{\Lambda(n)}{n} = O(X \log X)$$

where, as before, we choose to stop at the dyadic interval when k is the largest integer such that $2^{-k}T > 2\pi$.

When summed over all the dyadic intervals, the errors contribute

$$\sum_{k=1}^{\lfloor \frac{\log T/(4\pi)}{\log 2} \rfloor} E(X, 2^{-k}T) = O(T(\log T)^2) + O(X \log X)$$

where the last two terms for $E(X, 2^{-k}T)$ in (2.7) potentially dominate for only one k, when $2^{-k}T \approx 2\pi X$, say, when it yields $O(X \log X)$.

Unfortunately for T so small, that error term now dominates the main term contributions from the second and third cases of the theorem. In order to not lose these interesting subsidiary main terms, in the main theorem we evaluate the sum of zeros between T and $2T$, rather than over all zeros up to T. □

As two further corollaries, we will use Theorem 13 to deduce new proofs for Theorems 11 and 12 in Sections 2.5 and 2.6, respectively. Briefly, we follow the idea of Hughes, Martin and Pearce-Crump [33], but rather than use the approximate formula (2.6), we use the full approximate functional equation (2.14) for the derivative of zeta. Our result enables us to control how much weight is put into each part of the approximate functional equation, and this, when combined with Theorem 13, turns their heuristic into a full proof.

After we placed an early version of this paper on the ArXiV, we were approached by Seth Hardy [27] who informed us he had discovered similar results to us, completely independently, and he shared with us his unpublished preprint.

2.3 Overview of paper

In Section 2.4, we prove a key result using the method of stationary phase. Specifically, we calculate the integral

$$J(\sigma, r, T) = \int_T^{2T} \chi(\sigma + it) r^{it} dt$$

which will enable us to evaluate $S(X,T)$.

We then prove the main result of this paper, Theorem 13. To do this, we begin by using Cauchy's Theorem to write

$$S(X,T) = \sum_{T<\gamma\leq 2T} \chi(\rho)X^{\rho} = \frac{1}{2\pi i}\int_{\mathcal{R}} \frac{\zeta'}{\zeta}(s)\chi(s)X^{s}\, ds,$$

where $\mathcal{R}$ is a suitable contour containing all the required non-trivial zeros of the zeta function. We will show that the contribution from the horizontal sides of this integral can be absorbed into an error term, while the vertical segments both contribute to the main terms. For the right-hand side of the contour, we can expand the zeta functions as their Dirichlet series and then apply the result in our lemma concerning $J(\sigma,r,T)$. We apply a standard trick using the functional equation for the zeta function to map the left-hand side of the contour onto the right-hand side. We then follow a similar method to that used on the original right-hand side.

In Section 2.5 we demonstrate the utility of Theorem 13 by applying it to derive the full unconditional asymptotic in Theorem 11, which gives a new proof of Shanks' conjecture.

In Section 2.6 we outline how one can use Theorem 13 to obtain the asymptotic that proves the generalised Shanks' conjecture. We obtain the leading-order result, given by Theorem 12. This section, together with the calculations in the previous section, completes our proof of showing that the heuristic in [33] can be made rigorous by using the approximate functional equation.

2.4 Proof of Theorem 13

We start this section by proving the following lemma used to prove Theorem 13.

Let

$$J(\sigma,r,T) = \int_{T}^{2T} \chi(\sigma+it)r^{it}dt.$$

Lemma 2.4.1. *For large T, uniformly for $-1\leq\sigma\leq 2$ we have*

$$J(\sigma,r,T) = \begin{cases} 2\pi r^{1-\sigma}e^{2\pi i r} + E(\sigma,r,T) & \text{if } T<2\pi r\leq 2T \\ E(\sigma,r,T) & \text{if } 2\pi r\leq T \text{ or } 2\pi r>2T, \end{cases} \tag{2.8}$$

where

$$E(\sigma,r,T)=O(T^{1/2-\sigma})+O\left(\frac{T^{3/2-\sigma}}{|T-2\pi r|+T^{1/2}}\right)+O\left(\frac{T^{3/2-\sigma}}{|2T-2\pi r|+T^{1/2}}\right).$$

Proof. This is essentially due to Gonek [26, Lemma 2]. We use Stirling's approximation to expand $\chi(\sigma+it)$ for fixed σ and $t\geq 1$ as

$$\chi(\sigma+it)=\left(\frac{t}{2\pi}\right)^{\frac{1}{2}-\sigma-it}e^{it+i\frac{\pi}{4}}\left(1+O\left(\frac{1}{t}\right)\right). \tag{2.9}$$

This allows us to write our integral as

$$J(\sigma,r,T)=e^{i\pi/4}\int_T^{2T}\left(\frac{t}{2\pi}\right)^{\frac{1}{2}-\sigma}\exp\left[-it\log\left(\frac{t}{2\pi er}\right)\right]\,dt+O(T^{1/2-\sigma}).$$

By [26, Lemma 2], we are able to write (after taking the complex conjugate of what is shown there)

$$e^{i\pi/4}\int_T^{2T}\left(\frac{t}{2\pi}\right)^{\frac{1}{2}-\sigma}\exp\left[-it\log\left(\frac{t}{2\pi er}\right)\right]\,dt=\begin{cases}2\pi r^{1-\sigma}e^{2\pi ir}+E(\sigma,r,T)\\ E(\sigma,r,T),\end{cases} \tag{2.10}$$

where in the first case $T<2\pi r\leq 2T$, and in the second case $2\pi r\leq T$ or $2\pi r>2T$, and where

$$E(\sigma,r,T)=O(T^{1/2-\sigma})+O\left(\frac{T^{3/2-\sigma}}{|T-2\pi r|+T^{1/2}}\right)+O\left(\frac{T^{3/2-\sigma}}{|2T-2\pi r|+T^{1/2}}\right). \tag{2.11}$$

This completes the proof. □

To prove Theorem 13 we use Cauchy's Theorem to write

$$\sum_{T<\gamma\leq 2T}\chi(\rho)X^\rho=\frac{1}{2\pi i}\int_{\mathcal{R}}\frac{\zeta'}{\zeta}(s)\chi(s)X^s\,ds,$$

where $\mathcal{R}$ is the positively oriented rectangular contour with vertices $c+iT, c+2iT, 1-c+2iT, 1-c+iT$, where $c=1+1/\log T$.

We shall restrict T so that both $|T-\gamma|\gg\frac{1}{\log T}$ and $|2T-\gamma|\gg\frac{1}{\log T}$ for all γ, that is, the contour is always a distance $\gg\frac{1}{\log T}$ from the ordinate γ of any zero. This incurs a small error term which we deal with now. It is well-known that there are

$O(\log T)$ zeros between T and $T+1$ (for example, [66, Section 9.2]), and so by (2.9) we see that we incur a cost bounded by

$$O\left(\chi(\beta+iT)X^{\beta}\log T\right)+O\left(\chi(1-\beta+iT)X^{1-\beta}\log T\right)$$
$$=O\left(T^{1/2}\left(\frac{X}{T}\right)^{\beta}\log T\right)+O\left(\frac{X}{T^{1/2}}\left(\frac{T}{X}\right)^{\beta}\log T\right),$$

where $\beta=\max\{\Re(\rho):T\le\Im(\rho)\le T+1\}$, and we consider both the zero at $\beta+i\gamma$ and $1-\beta+i\gamma$, as the dominant contribution changes depending on whether $X\ll T$ or $X\gg T$. Clearly the strength of the zero-free region we may assume will play a role in the strength of the bound we obtain. If we use the trivial bound $\beta<1$ we see this is

$$O\left(\frac{X\log T}{T^{1/2}}\right)+O\left(T^{1/2}\log T\right).$$

The errors considered here will be shown to be absorbed into the errors $E(X,T)$ in (2.7).

Returning to the Cauchy integral, we will consider each piece of the contour in turn. We write

$$\frac{1}{2\pi i}\int_{\mathcal{R}}\frac{\zeta'}{\zeta}(s)\chi(s)X^{s}ds=\frac{1}{2\pi i}\left(\int_{c+iT}^{c+2iT}+\int_{c+2iT}^{1-c+2iT}+\int_{1-c+2iT}^{1-c+iT}+\int_{1-c+iT}^{c+iT}\right)\frac{\zeta'}{\zeta}(s)\chi(s)X^{s}ds$$
$$=I_1+I_2+I_3+I_4. \tag{2.12}$$

We begin by bounding the two horizontal segments before handling the vertical segments, which require a more careful approach.

Lemma 2.4.2. *The integrals along the top and bottom of the contour are uniformly bounded for $X\ge 1, T>1$ by*

$$I_2,I_4=O\left(T^{1/2}(\log T)^2\right)+O\left(\frac{X^{1+1/\log T}(\log T)^2}{T^{1/2}}\right)$$

Proof. By Gonek [26, p. 126], if T is such that $|T-\gamma|\gg\frac{1}{\log T}$ for any zero ordinate γ, then the bound

$$\frac{\zeta'}{\zeta}(\sigma+iT)=O\left((\log T)^2\right)$$

holds uniformly for $-1\le\sigma\le 2$. We also have from (2.9) that

$$|\chi(\sigma+iT)|=\left(\frac{T}{2\pi}\right)^{\frac{1}{2}-\sigma}\left(1+O\left(\frac{1}{T}\right)\right). \tag{2.13}$$

Applying these bounds and trivially estimating the resulting integral by the maximum of the integrand (which is maximised at $\sigma = 1 - c$ if $X \ll T$, and at $\sigma = c$ if $X \gg T$), we have

$$I_2 = O\left((\log T)^2 \left(T^{1/2}\left(\frac{T}{X}\right)^{\frac{1}{\log T}} + \frac{X}{T^{1/2}}\left(\frac{X}{T}\right)^{\frac{1}{\log T}}\right)\right)$$

Now, since $\left(\frac{T}{X}\right)^{\frac{1}{\log T}} < T^{\frac{1}{\log T}} = e$ we deduce that

$$I_2 = O\left(T^{1/2}(\log T)^2\right) + O\left(\frac{X^{1+1/\log T}(\log T)^2}{T^{1/2}}\right)$$

as required. □

Note that in Lemma 2.4.2 the first term dominates if $X \ll T$ and the second term dominates if $X \gg T$. We see also that these two terms collectively dominate the error coming from restricting $|T - \gamma| \gg \frac{1}{\log T}$. This gives the first two terms in the error, $E(X, T)$, given in (2.7).

Lemma 2.4.3. *The integral along the right-hand side of the contour in* (2.12) *is given by*

$$\begin{aligned} I_1 &= \frac{1}{2\pi}\int_T^{2T} \frac{\zeta'}{\zeta}(c+it)\chi(c+it)X^{c+it}\, dt \\ &= -X \sum_{\frac{\pi X}{T} \le n < \frac{2\pi X}{T}} \frac{\Lambda(n)}{n} e^{\frac{2\pi X i}{n}} + O\left(\frac{X \log T}{T^{1/2}}\right). \end{aligned}$$

with the error uniform for $X \ge 1$ and $T > 1$.

Remark. *This result is non-trivial only for $X \gg T$, otherwise the sum over n is empty.*

Proof. Since $c > 1$ we are to the right of $\Re(s) = 1$ and so we can use the Dirichlet series

$$\frac{\zeta'}{\zeta}(c+it) = -\sum_{n=1}^{\infty} \frac{\Lambda(n)}{n^{c+it}}.$$

Swapping the sum and integral transforms I_1 into

$$I_1 = -\frac{1}{2\pi}\sum_{n=1}^{\infty} \Lambda(n)\left(\frac{X}{n}\right)^c \int_T^{2T} \left(\frac{X}{n}\right)^{it} \chi(c+it)\, dt.$$

We now apply Lemma 2.4.1 to the integral in this expression, with $\sigma = c$ and $r = X/n$. Since the main term only arises when $2\pi r \in (T, 2T]$, we are forced into the regime $\pi X/T \leq n < 2\pi X/T$ and so

$$\begin{aligned} I_1 &= -\frac{1}{2\pi} \sum_{n=1}^{\infty} \Lambda(n) \left(\frac{X}{n}\right)^c J\left(c, \frac{X}{n}, T\right) \\ &= -X \sum_{\frac{\pi X}{T} \leq n < \frac{2\pi X}{T}} \frac{\Lambda(n)}{n} e^{2\pi i X/n} + \sum_{n=1}^{\infty} \Lambda(n) \left(\frac{X}{n}\right)^c E\left(c, \frac{X}{n}, T\right). \end{aligned}$$

Observe that the first piece occurs as a main term in Theorem 13. Now we establish an upper bound for the error term,

$$\begin{aligned} \sum_{n=1}^{\infty} \Lambda(n) \left(\frac{X}{n}\right)^c E\left(c, \frac{X}{n}, T\right) &= O\left(X^c \sum_{n=1}^{\infty} \frac{\Lambda(n)}{n^c} T^{-1/2}\right) \\ &\quad + O\left(X^c \sum_{n=1}^{\infty} \frac{\Lambda(n)}{n^c} \frac{T^{1/2}}{|T - 2\pi X/n| + T^{1/2}}\right). \end{aligned}$$

Since $c = 1 + 1/\log T$, the series $\sum \Lambda(n) n^{-c} = -\zeta'/\zeta(c) = O(\log T)$ and so we can easily bound the first error term by

$$O\left(\frac{X^{1+1/\log T} \log T}{T^{1/2}}\right).$$

For the second error term, using $\sum_{n \leq X} \Lambda(n) \ll X$, this is bounded by

$$X^c \int_1^{\infty} n^{-1-1/\log T} \frac{T^{1/2}}{|T - 2\pi X/n| + T^{1/2}}\, dn \ll \frac{X}{T^{1/2}} \int_0^{2\pi X/T} y^{-1+1/\log T} \frac{1}{|1-y| + T^{-1/2}}\, dy$$

coming from letting $y = 2\pi X/(Tn)$. Splitting into regions around the relevant majorants of the integral, and letting the upper limit be infinity, we can bound this by

$$\begin{aligned} \frac{X}{T^{1/2}} \int_0^{1/2} y^{-1+1/\log T} dy + \frac{X}{T^{1/2}} \int_{1/2}^{3/2} \frac{1}{|y-1| + T^{-1/2}} dy + \frac{X}{T^{1/2}} \int_{3/2}^{\infty} \frac{1}{y^2} dy \\ \ll \frac{X \log T}{T^{1/2}} + \frac{X \log T}{T^{1/2}} + \frac{X}{T^{1/2}}. \end{aligned}$$

Note that since

$$\int_0^{2\pi/T} y^{-1+1/\log T} dy \gg \log T$$

the contribution from $y \approx 0$ is a positive proportion of the total bound, so replacing the upper limit from $2\pi X/T$ with ∞ does not cause an overestimate of the total error. $\square$

Lemma 2.4.4. *The integral along the left-hand vertical segment in (2.12) is*

$$I_3 = \begin{cases} -X \displaystyle\sum_{\frac{T}{2\pi X} < n \le \frac{T}{\pi X}} \Lambda(n) e^{2\pi i X n} + E'(X,T) & \text{if } X \le \frac{T}{2\pi} \\ X(\log X) e^{2\pi X i} + E'(X,T) & \text{if } \frac{T}{2\pi} < X \le \frac{T}{\pi} \\ E'(X,T) & \text{if } X > \frac{T}{\pi} \end{cases}$$

where

$$E'(X,T) = O(T^{1/2}\log T) + O\left(\frac{T^{3/2}\log T}{|T - 2\pi X| + T^{1/2}}\right) + O\left(\frac{T^{3/2}\log T}{|2T - 2\pi X| + T^{1/2}}\right).$$

To approach Lemma 2.4.4 we start by taking the logarithmic derivative of functional equation for zeta (2.14) to obtain

$$\begin{aligned} I_3 &= -\frac{1}{2\pi}\int_T^{2T} \frac{\zeta'}{\zeta}(1-c+it)\chi(1-c+it)X^{1-c+it}\,dt \\ &= -\frac{1}{2\pi}\int_T^{2T} \left(-\frac{\zeta'}{\zeta}(c-it) + \frac{\chi'}{\chi}(1-c+it)\right)\chi(1-c+it)X^{1-c+it}\,dt \\ &= \frac{1}{2\pi}\int_T^{2T} \frac{\zeta'}{\zeta}(c-it)\chi(1-c+it)X^{1-c+it}\,dt - \frac{1}{2\pi}\int_T^{2T} \chi'(1-c+it)X^{1-c+it}\,dt \\ &= I_{3,1} + I_{3,2}. \end{aligned}$$

We shall deal with $I_{3,1}$ and $I_{3,2}$ separately, and it is clear that Lemma 2.4.4 follows from Lemmas 2.4.5 and 2.4.6, below.

Lemma 2.4.5. *Uniformly for $X \ge 1$ and $T > 1$ we have*

$$\begin{aligned} I_{3,1} &= \frac{1}{2\pi}\int_T^{2T} \frac{\zeta'}{\zeta}(c-it)\chi(1-c+it)X^{1-c+it}\,dt \\ &= -X \sum_{\frac{T}{2\pi X} < n \le \frac{T}{\pi X}} \Lambda(n)e^{2\pi i X n} + O(T^{1/2}\log T). \end{aligned}$$

Proof of Lemma 2.4.5. By using the Dirichlet series for $\frac{\zeta'}{\zeta}(s)$ we are able to write

$$\begin{aligned}
I_{3,1} &= \frac{1}{2\pi}\int_T^{2T} \frac{\zeta'}{\zeta}(c-it)\chi(1-c+it)X^{1-c+it}\, dt \\
&= -\frac{1}{2\pi}\int_T^{2T} \left(\sum_{n=1}^{\infty} \frac{\Lambda(n)}{n^{c-it}}\right) \chi(1-c+it)X^{1-c+it}\, dt \\
&= -\frac{X^{1-c}}{2\pi}\sum_{n=1}^{\infty}\frac{\Lambda(n)}{n^c}\int_T^{2T} \chi(1-c+it)(Xn)^{it}\, dt.
\end{aligned}$$

The integral is in a form which may be handled by Lemma 2.4.1 with $\sigma = 1-c$ and $r = Xn$, where we note that a non-error-term contribution only arises when $2\pi Xn \in (T, 2T]$, that is, $\frac{T}{2\pi X} < n \leq \frac{T}{\pi X}$. We therefore obtain

$$\begin{aligned}
I_{3,1} &= -\frac{X^{1-c}}{2\pi}\sum_{n=1}^{\infty}\frac{\Lambda(n)}{n^c} J(1-c, Xn, T) \\
&= -X \sum_{\frac{T}{2\pi X} < n \leq \frac{T}{\pi X}} \Lambda(n)e^{2\pi i X n} + X^{1-c}\sum_{n=1}^{\infty}\frac{\Lambda(n)}{n^c}E(1-c, Xn, T).
\end{aligned}$$

We now treat the error arising from $I_{3,1}$ in similar way to the treatment in Lemma 2.4.3, namely

$$\begin{aligned}
X^{1-c}\sum_{n=1}^{\infty}\frac{\Lambda(n)}{n^c}E(1-c, Xn, T) &= O\left(X^{-1/\log T}\sum_{n=1}^{\infty}\frac{\Lambda(n)}{n^c}T^{1/2}\right) \\
&\quad + O\left(X^{-1/\log T}\sum_{n=1}^{\infty}\frac{\Lambda(n)}{n^c}\frac{T^{3/2}}{|T-2\pi Xn| + T^{1/2}}\right).
\end{aligned}$$

As before, since $c = 1 + 1/\log T$, the Dirichlet series can be evaluated and the first term is

$$O\left(X^{-1/\log T}T^{1/2}\log T\right)$$

and the second term can be bounded by

$$\begin{aligned}
X^{-1/\log T}\int_1^{\infty} n^{-1-1/\log T}\frac{T^{3/2}}{|T-2\pi Xn| + T^{1/2}}\, dn \\
= T^{1/2}\int_{2\pi X/T}^{\infty} y^{-1-1/\log T}\frac{1}{|1-y| + T^{-1/2}}\, dy
\end{aligned}$$

where this time we substituted $y = 2\pi Xn/T$. If $2\pi X/T > 1+\epsilon$ then the integral is $\ll \int_1^\infty y^{-2-1/\log T} dy \ll 1$, and if $X/T = o(1)$ then there will be a contribution from $y \approx 0$ and from $y \approx 1$. The former contributes

$$\int_{2\pi X/T}^{1/2} y^{-1-1/\log T} dy \ll \log T \left(\frac{2\pi X}{T}\right)^{-1/\log T} \ll \log T$$

and the latter contributes

$$\int_{1/2}^{3/2} \frac{1}{|1-y| + T^{-1/2}}\, dy \ll \log T.$$

These can all be combined uniformly into one error, $O(T^{1/2}\log T)$, which is an overestimate by $\log T$ in the case when $X > T^{\log\log T}$, but is a good bound for the size of X required in our applications. □

Lemma 2.4.6. *We have*

$$\begin{aligned} I_{3,2} &= -\frac{1}{2\pi}\int_T^{2T} \chi'(1-c+it) X^{1-c+it}\, dt \\ &= \begin{cases} X(\log X)e^{2\pi i X} + E'(X,T) & \text{if } T < 2\pi X \le 2T \\ E'(X,T) & \text{if } X \le \frac{T}{2\pi} \text{ or if } X > \frac{T}{\pi} \end{cases} \end{aligned}$$

with

$$E'(X,T) = O(T^{1/2}\log T) + O\left(\frac{T^{3/2}\log T}{|T-2\pi X| + T^{1/2}}\right) + O\left(\frac{T^{3/2}\log T}{|2T-2\pi X| + T^{1/2}}\right)$$

Proof of Lemma 2.4.6. For $s = \sigma + it$ with $|\sigma| \le 2$ and $t > 1$, we have

$$\frac{\chi'}{\chi}(\sigma+it) = -\log\left(\frac{t}{2\pi}\right) + O\left(\frac{1}{t}\right),$$

so upon multiplying through by $\chi(\sigma+it)$ and using (2.13) this yields

$$\chi'(\sigma+it) = -\chi(\sigma+it)\log\left(\frac{t}{2\pi}\right) + O\left(t^{-1/2-\sigma}\right).$$

In our case we have $s = 1-c+it$ and so we can write

$$\begin{aligned} I_{3,2} &= -\frac{1}{2\pi}\int_T^{2T} \left(-\chi(1-c+it)\log\left(\frac{t}{2\pi}\right) + O\left(t^{c-3/2}\right)\right) X^{1-c+it}\, dt \\ &= \frac{1}{2\pi}\int_T^{2T} \chi(1-c+it)\log\left(\frac{t}{2\pi}\right) X^{1-c+it}\, dt + O\left(\int_T^{2T} X^{1-c} t^{c-3/2} dt\right) \end{aligned}$$

Upon integration we see that our error term may be bounded as $O(T^{1/2})$ which is no bigger than the error terms already found in $I_{3,1}$. Finally, a variant of Lemma 2.4.1 with $\sigma = 1-c$ and $r = X$ yields

$$\begin{aligned} I_{3,2} &= \frac{1}{2\pi}\int_T^{2T} \chi(1-c+it)\left(\log\frac{t}{2\pi}\right) X^{1-c+it}\,dt \\ &= \begin{cases} X(\log X)e^{2\pi i X} + E(1-c,X,T)\log T & \text{if } T < 2\pi X \le 2T \\ E(1-c,X,T)\log T & \text{if } X \le \frac{T}{2\pi} \text{ or if } X > \frac{T}{\pi} \end{cases} \end{aligned}$$

where $E(\sigma, r, T)$ is given in Lemma 2.4.1, and we have simply applied that lemma together with an integration by parts (which is the same argument used by Gonek [26, Lemma 3]). $\square$

2.5 Deduction of Shanks' conjecture

In this section we show how Theorem 13 can be used to establish a new proof of Theorem 11, albeit with worse error terms. We begin by recalling the approximate functional equation for $\zeta'(\sigma+it)$ (see [41, Lemma 1], for example), which states that if $0<\alpha<1$ and $s = \sigma + it$

$$\zeta'(s) = -\sum_{n \le \left(\frac{t}{2\pi}\right)^{\alpha}} \frac{\log n}{n^s} + \chi(s) \sum_{n \le \left(\frac{t}{2\pi}\right)^{1-\alpha}} \frac{\log n - \ell(t)}{n^{1-s}} + O\left(t^{-\alpha/2}\log t\right) + O\left(t^{-(1-\alpha)/2}\log t\right) \tag{2.14}$$

where $\ell(t) = \log\frac{t}{2\pi}$.

Taking the sum over non-trivial zeros $\rho = \frac{1}{2} + i\gamma$ with $0 < \gamma \le T$, we have

$$\begin{aligned} \sum_{0<\gamma\le T} \zeta'(\rho) = &-\sum_{0<\gamma\le T}\sum_{n\le\left(\frac{\gamma}{2\pi}\right)^{\alpha}} \frac{\log n}{n^{\rho}} + \sum_{0<\gamma\le T}\sum_{n\le\left(\frac{\gamma}{2\pi}\right)^{1-\alpha}} \frac{\chi(\rho)\log n}{n^{1-\rho}} \\ &- \sum_{0<\gamma\le T}\sum_{n\le\left(\frac{\gamma}{2\pi}\right)^{1-\alpha}} \frac{\chi(\rho)\ell(\gamma)}{n^{1-\rho}} + O\left(T^{1-\alpha/2}\log T\right) + O\left(T^{1/2+\alpha/2}\log T\right) \end{aligned} \tag{2.15}$$

and we label the three sums on the right-hand side A_1, A_2, and A_3 respectively.

We will see that if $0<\alpha<1$ these can all be summed using our results, but first we collect some standard results which we shall need for the evaluation of these sums.

Lemma 2.5.1. *We have the following asymptotic expansions:*

1. $$\sum_{n\le x}\frac{1}{n}=\log x+\gamma_0+O\left(\frac{1}{x}\right),$$

   where γ_0 is Euler's constant.

2. $$\sum_{n\le x}\frac{\log n}{n}=\frac{1}{2}(\log x)^2+\gamma_1+O\left(\frac{\log x}{x}\right),$$

   where the Stieltjes constant γ_1 is given in (2.4).

3. $$\sum_{n\le x}\frac{\Lambda(n)\log n}{n}=\frac{1}{2}(\log x)^2-(\gamma_0^2+2\gamma_1)+O\left(e^{-a\sqrt{\log x}}\right)$$

   for some $a>0$, where the Stieltjes constants γ_0,γ_1 are given in (2.4).

4. *For $C>-1$,*

   $$\sum_{n\le x}n^C\log n=\frac{x^{C+1}\log x}{C+1}-\frac{x^{C+1}}{(C+1)^2}+O(x^C\log x).$$

5. *For $C>-1$,*

   $$\sum_{n\le x}n^C\Lambda(n)\log n=\frac{x^{C+1}\log x}{C+1}-\frac{x^{C+1}}{(C+1)^2}+O(x^{C+1}e^{-a\sqrt{\log x}}),$$

   for some $a>0$.

Proof. We note that parts (1) and (2) are standard and can be found in [1, p.55, 70] respectively. Part (3) is an application of Perron's formula on $\left(\frac{\zeta'}{\zeta}(s)\right)'$. We may obtain (4) using partial summation with $a_n=\log n$, $f(t)=t^C$. From this, another partial summation with $a_n=\Lambda(n)$ and $f(t)=n^C\log n$ establishes (5). □

We handle A_1 first. By swapping the order of summation we may write

$$\begin{aligned}A_1&=-\sum_{0<\gamma\le T}\sum_{n\le\left(\frac{\gamma}{2\pi}\right)^\alpha}\frac{\log n}{n^\rho}\\&=-\sum_{n\le\left(\frac{T}{2\pi}\right)^\alpha}\log n\sum_{2\pi n^{1/\alpha}\le\gamma\le T}\frac{1}{n^\rho}.\end{aligned}$$

Using the Landau-Gonek formula, (2.3), we have

$$
\begin{aligned}
A_1 &= -\sum_{n\le\left(\frac{T}{2\pi}\right)^\alpha} \log n \left(-\frac{T}{2\pi n}\Lambda(n) + \Lambda(n)n^{-1+1/\alpha} + O(\log T\log\log T)\right) \\
&= \frac{T}{2\pi}\sum_{n\le\left(\frac{T}{2\pi}\right)^\alpha} \frac{\Lambda(n)\log n}{n} - \sum_{n\le\left(\frac{T}{2\pi}\right)^\alpha} n^{-1+1/\alpha}\Lambda(n)\log n + O\left(T^\alpha(\log T)^2\log\log T\right) \\
&= \frac{T}{4\pi}\alpha^2\left(\log\frac{T}{2\pi}\right)^2 - \frac{T}{2\pi}\alpha^2\left(\log\frac{T}{2\pi}\right) + \frac{T}{2\pi}(-\gamma_0^2 - 2\gamma_1 + \alpha^2) + O\left(Te^{-a\sqrt{\log T}}\right),
\end{aligned}
\tag{2.16}
$$

having applied Lemma 2.5.1 parts (3) and (5) with the choices $x = \left(\frac{T}{2\pi}\right)^\alpha$ and $C = -1 + 1/\alpha$ (and using that trivially $x^{1/\alpha} = \frac{T}{2\pi}$ and $\log x = \alpha\left(\log\frac{T}{2\pi}\right)$). Note that we need $\alpha < 1$ for the claimed error term in the last line (coming from summing the von Mangoldt function) to dominate the error term in the middle line (coming from the Landau–Gonek formula).

Now we turn to A_2. We have

$$
\begin{aligned}
A_2 &= \sum_{0<\gamma\le T}\sum_{n\le\left(\frac{\gamma}{2\pi}\right)^{1-\alpha}} \frac{\chi(\rho)\log n}{n^{1-\rho}} \\
&= \sum_{n\le\left(\frac{T}{2\pi}\right)^{1-\alpha}} \frac{\log n}{n} \sum_{2\pi n^{1/(1-\alpha)}\le\gamma\le T} \chi(\rho)n^\rho \\
&= -\frac{T}{2\pi}\sum_{n\le\left(\frac{T}{2\pi}\right)^{1-\alpha}} \frac{\log n}{n} + \sum_{n\le\left(\frac{T}{2\pi}\right)^{1-\alpha}} n^{-1+1/(1-\alpha)}\log n \\
&\quad + \sum_{n\le\left(\frac{T}{2\pi}\right)^{1-\alpha}} \left(O\left((\log n)^2\right) + O\left(\frac{\log n}{n}Te^{-a\sqrt{\log T}}\right)\right) \\
&= -\frac{T}{4\pi}(1-\alpha)^2\left(\log\frac{T}{2\pi}\right)^2 + \frac{T}{2\pi}(1-\alpha)^2\left(\log\frac{T}{2\pi}\right) - \frac{T}{2\pi}(\gamma_1 + (1-\alpha)^2) \\
&\quad + O\left(Te^{-a'\sqrt{\log T}}\right),
\end{aligned}
\tag{2.17}
$$

where in passing from the first line to the second we have swapped the order of summation, in passing from the second to the third line we have applied Corollary 15 (with the unconditional error term). To get from the third line to the fourth, we have applied Lemma 2.5.1 parts (2) and (4) with $x = \left(\frac{T}{2\pi}\right)^{1-\alpha}$ and $C = -1 + \frac{1}{1-\alpha}$. Note that we must have $\alpha > 0$ for the claimed error term to be dominant when passing from the third to the fourth line.

Finally we turn to A_3. We have

$$\begin{aligned} A_3 &= -\sum_{0<\gamma\le T}\sum_{n\le\left(\frac{\gamma}{2\pi}\right)^{1-\alpha}} \chi(\rho)\frac{\log\left(\frac{\gamma}{2\pi}\right)}{n^{1-\rho}} \\ &= -\sum_{n\le\left(\frac{T}{2\pi}\right)^{1-\alpha}} \frac{1}{n}\sum_{2\pi n^{1/(1-\alpha)}\le\gamma\le T} \chi(\rho)n^{\rho}\log\frac{\gamma}{2\pi}, \end{aligned}$$

by swapping the order of summation. By Abel summation and Corollary 15 we can easily evaluate this inner sum using

$$\begin{aligned} \sum_{\gamma\le T}\chi(\rho)n^{\rho}\log\frac{\gamma}{2\pi} &= \int_2^T \log\left(\frac{t}{2\pi}\right)\, dS(n,t) \\ &= \log\frac{T}{2\pi}S(n,T) - \int_2^T \frac{1}{t}S(n,t)\, dt \\ &= -\frac{T}{2\pi}\log\frac{T}{2\pi} + \frac{T}{2\pi} + O\left(Te^{-a\sqrt{\log T}}\right), \end{aligned}$$

which we obtain simply by substituting in Corollary 15 and simplifying. Note that since $n = O(T^{1-\alpha})$ with $\alpha > 0$, the claimed error term is the dominant one of the two in the Corollary. Therefore, by substituting this expression into the definition of A_3 and subtracting the terms with $\gamma \le 2\pi n^{\frac{1}{1-\alpha}}$ we deduce

$$A_3 = -\sum_{n\le\left(\frac{T}{2\pi}\right)^{1-\alpha}} \frac{1}{n}\left(-\frac{T}{2\pi}\log\frac{T}{2\pi} + \frac{T}{2\pi} + \frac{1}{1-\alpha}n^{\frac{1}{1-\alpha}}\log n - n^{\frac{1}{1-\alpha}} + O\left(Te^{-a\sqrt{\log T}}\right)\right),$$

and once again applying Lemma 2.5.1 gives

$$\begin{aligned} A_3 = \frac{T}{2\pi}(1-\alpha)\left(\log\frac{T}{2\pi}\right)^2 + \frac{T}{2\pi}(\gamma_0 - 2(1-\alpha))\left(\log\frac{T}{2\pi}\right) - \frac{T}{2\pi}(\gamma_0 + 2(\alpha-1)) \\ + O\left(Te^{-a'\sqrt{\log T}}\right) \quad (2.18) \end{aligned}$$

for any $0 < a' < a$.

We combine A_1, A_2 and A_3 from (2.16), (2.17), and (2.18) respectively into (2.15), to obtain

$$\begin{aligned} \sum_{0<\gamma\le T}\zeta'(\rho) = \frac{T}{4\pi}\left(\log\frac{T}{2\pi}\right)^2 + (\gamma_0 - 1)\frac{T}{2\pi}\left(\log\frac{T}{2\pi}\right) + (1-\gamma_0-\gamma_0^2-3\gamma_1)\frac{T}{2\pi} \\ + O\left(Te^{-a\sqrt{\log T}}\right) \end{aligned}$$

for some $a > 0$. This recovers Theorem 11 with the unconditional error term.

Remark. *If we had assumed the Riemann Hypothesis, then the error terms in Lemma 2.5.1 would be smaller (roughly $x^{1/2}$) and the resulting error terms would look like T^α and $T^{1-\alpha}$ times certain powers of logarithms, and thus be optimised when the approximate functional equation has roughly equal weight in both its pieces, i.e. when $\alpha = 1/2$.*

2.6 DEDUCTION OF THE GENERALISED SHANKS' CONJECTURE

The purpose of this section is to deduce Theorem 12 from Theorem 13. This follows essentially the same approach as that in Section 2.5. We firstly start by recalling the approximate functional equation for $\zeta^{(\nu)}(\sigma + it)$ (see, for example, Equation (36) of [41]), which says that

$$\zeta^{(\nu)}(s) = (-1)^\nu \sum_{n \le \left(\frac{t}{2\pi}\right)^\alpha} \frac{(\log n)^\nu}{n^s} + \chi(s) \sum_{n \le \left(\frac{t}{2\pi}\right)^{1-\alpha}} \frac{(\log n - \ell(t))^\nu}{n^{1-s}} + O\left(t^{-\alpha/2}(\log t)^{\nu+1}\right) + O\left(t^{-(1-\alpha)/2}(\log t)^{\nu+1}\right)$$

for $0 < \alpha < 1$, where $\ell(t) = \log \frac{t}{2\pi}$.

Before proceeding, we shall need the following lemma which is analogous to Lemma 2.5.1.

Lemma 2.6.1. *We have the following asymptotic expansions: For $\nu \ge 0$ and $C > -1$,*

1. $$\sum_{n \le x} \frac{\Lambda(n)(\log n)^\nu}{n} = \frac{(\log x)^{\nu+1}}{\nu+1} + O((\log x)^\nu).$$

2. $$\sum_{n \le x} \Lambda(n) n^C (\log n)^\nu = \frac{x^{C+1}(\log x)^\nu}{C+1} + O\left(x^{C+1}(\log x)^{\nu-1}\right).$$

3. $$\sum_{n \le x} \frac{(\log n)^\nu}{n} = \frac{(\log x)^{\nu+1}}{\nu+1} + O((\log x)^\nu)$$

4. $$\sum_{n \le x} n^C (\log n)^\nu = \frac{x^{C+1}(\log x)^\nu}{C+1} + O\left(x^{C+1}(\log x)^{\nu-1}\right).$$

Proof of Lemma 2.6.1. Part (1) may be found in [43, p.30], from which Part (2) follows by partial summation. Parts (3) and (4) are standard applications of the Euler–Maclaurin summation formula. □

Taking the sum over non-trivial zeros $\rho = \beta + i\gamma$ with $0 < \gamma \leq T$, we have

$$\sum_{0<\gamma\leq T} \zeta^{(\nu)}(\rho) = (-1)^\nu \sum_{0<\gamma\leq T} \sum_{n\leq\left(\frac{\gamma}{2\pi}\right)^\alpha} \frac{(\log n)^\nu}{n^\rho} + \sum_{0<\gamma\leq T} \sum_{n\leq\left(\frac{\gamma}{2\pi}\right)^{1-\alpha}} \frac{\chi(\rho)}{n^{1-\rho}}(\log n - \ell(\gamma))^\nu + O\left(T^{1-\alpha/2}(\log T)^{\nu+1}\right) + O\left(T^{1/2+\alpha/2}(\log T)^{\nu+1}\right)$$

with $0 < \alpha < 1$. We label the two sums on the right-hand side B_1, and B_2, respectively.

For the first term B_1, we may use the Landau–Gonek formula, (2.3), and we have

$$\begin{aligned} B_1 &= (-1)^\nu \sum_{0<\gamma\leq T} \sum_{n\leq\left(\frac{\gamma}{2\pi}\right)^\alpha} \frac{(\log n)^\nu}{n^\rho} \\ &= (-1)^\nu \sum_{n\leq\left(\frac{T}{2\pi}\right)^\alpha} (\log n)^\nu \sum_{2\pi n^{1/\alpha}\leq\gamma\leq T} \frac{1}{n^\rho} \\ &= (-1)^\nu \sum_{n\leq\left(\frac{T}{2\pi}\right)^\alpha} (\log n)^\nu \left(-\frac{T}{2\pi n}\Lambda(n) + \Lambda(n)n^{-1+1/\alpha} + O(\log T \log\log T)\right) \\ &= (-1)^{\nu+1}\frac{T}{2\pi} \sum_{n\leq\left(\frac{T}{2\pi}\right)^\alpha} \frac{\Lambda(n)(\log n)^\nu}{n} + (-1)^\nu \sum_{n\leq\left(\frac{T}{2\pi}\right)^\alpha} \Lambda(n)(\log n)^\nu n^{-1+1/\alpha} \\ &\quad + O\left(T^\alpha(\log T)^{\nu+1}\log\log T\right) \end{aligned}$$

It follows immediately from part (1) of Lemma 2.6.1 that

$$\frac{T}{2\pi} \sum_{n\leq\left(\frac{T}{2\pi}\right)^\alpha} \frac{\Lambda(n)(\log n)^\nu}{n} = \frac{\alpha^{\nu+1}}{\nu+1}\frac{T}{2\pi}\left(\log\frac{T}{2\pi}\right)^{\nu+1} + O\left(T(\log T)^\nu\right).$$

Moreover, from part (2) of the same lemma we see that

$$\sum_{n\leq\left(\frac{T}{2\pi}\right)^\alpha} \Lambda(n)(\log n)^\nu n^{-1+1/\alpha} = O(T(\log T)^\nu)$$

Therefore, if $\alpha < 1$,

$$B_1 = (-1)^{\nu+1} \frac{\alpha^{\nu+1}}{\nu+1} \frac{T}{2\pi} \left(\log \frac{T}{2\pi} \right)^{\nu+1} + O(T (\log T)^{\nu}). \tag{2.19}$$

For B_2 we use the binomial theorem and swap the order of summation to write

$$\begin{aligned} B_2 &= \sum_{0<\gamma\leq T} \sum_{n \leq \left(\frac{\gamma}{2\pi}\right)^{1-\alpha}} \frac{\chi(\rho)}{n^{1-\rho}} (\log n - \ell(\gamma))^{\nu} \\ &= \sum_{j=0}^{\nu} \binom{\nu}{j} (-1)^{\nu-j} \sum_{0<\gamma\leq T} \sum_{n \leq \left(\frac{\gamma}{2\pi}\right)^{1-\alpha}} \frac{\chi(\rho)(\log n)^j \ell(\gamma)^{\nu-j}}{n^{1-\rho}} \\ &= \sum_{j=0}^{\nu} \binom{\nu}{j} (-1)^{\nu-j} \sum_{n \leq \left(\frac{T}{2\pi}\right)^{1-\alpha}} \frac{(\log n)^j}{n} \sum_{2\pi n^{1/(1-\alpha)} \leq \gamma \leq T} \chi(\rho) n^{\rho} \ell(\gamma)^{\nu-j} \end{aligned}$$

We may handle the innermost sum in a similar way as we did for $\nu = 1$, to obtain

$$\begin{aligned} \sum_{2\pi n^{1/(1-\alpha)} \leq \gamma \leq T} \chi(\rho) n^{\rho} \left(\log \frac{\gamma}{2\pi} \right)^{\nu-j} = \left(\log \frac{T}{2\pi} \right)^{\nu-j} S(n,T) + \frac{(\log n)^{\nu-j}}{(1-\alpha)^{\nu-j}} S\left(n, 2\pi n^{1/(1-\alpha)}\right) \\ - (\nu - j) \int_{2\pi n^{1/(1-\alpha)}}^{T} \frac{\left(\log \frac{t}{2\pi}\right)^{\nu-j-1}}{t} S(n,t)\, dt \end{aligned}$$

and using Corollary 15 to evaluate $S(n,T)$ we see this is, for $\alpha > 0$,

$$\begin{aligned} \sum_{2\pi n^{1/(1-\alpha)} \leq \gamma \leq T} \chi(\rho) n^{\rho} \left(\log \frac{\gamma}{2\pi} \right)^{\nu-j} = -\frac{T}{2\pi} \left(\log \frac{T}{2\pi} \right)^{\nu-j} + \frac{n^{1/(1-\alpha)} (\log n)^{\nu-j}}{(1-\alpha)^{\nu-j}} \\ + O\left(T (\log T)^{\nu-j-1}\right) \end{aligned}$$

Part (3) of Lemma 2.6.1 shows

$$\sum_{n \leq \left(\frac{T}{2\pi}\right)^{1-\alpha}} \frac{(\log n)^j}{n} \frac{T}{2\pi} \left(\log \frac{T}{2\pi} \right)^{\nu-j} = \frac{(1-\alpha)^{j+1}}{j+1} \frac{T}{2\pi} \left(\log \frac{T}{2\pi} \right)^{\nu+1}$$

and Part (4) shows

$$\sum_{n \leq \left(\frac{T}{2\pi}\right)^{1-\alpha}} \frac{n^{-1+1/(1-\alpha)} (\log n)^{\nu}}{(1-\alpha)^{\nu-j}} = O\left(T (\log T)^{\nu}\right)$$

We deduce that for $\alpha > 0$

$$B_2 = (-1)^{\nu+1} \sum_{j=0}^{\nu} (-1)^j \binom{\nu}{j} \frac{(1-\alpha)^{j+1}}{j+1} \frac{T}{2\pi} \left(\log \frac{T}{2\pi} \right)^{\nu+1} + O(T(\log T)^{\nu}).$$

It follows from the binomial identity that

$$\sum_{j=0}^{\nu} (-1)^j \binom{\nu}{j} \frac{(1-\alpha)^{j+1}}{j+1} = \frac{1-\alpha^{\nu+1}}{\nu+1}$$

This allows us to simplify B_2 as

$$B_2 = (-1)^{\nu+1} \frac{1-\alpha^{\nu+1}}{\nu+1} \frac{T}{2\pi} \left(\log \frac{T}{2\pi} \right)^{\nu+1} + O(T(\log T)^{\nu}).$$

Finally since $\sum_{0<\gamma\le T} \zeta^{(\nu)}(\rho) = B_1 + B_2$ and inserting B_1 from (2.19), we see that

$$\sum_{0<\gamma\le T} \zeta^{(\nu)}(\rho) = \frac{(-1)^{\nu+1}}{\nu+1} \frac{T}{2\pi} \left(\log \frac{T}{2\pi} \right)^{\nu+1} + O(T(\log T)^{\nu}),$$

which recovers Theorem 12.

— 3 —

The discrete second moment of mixed derivatives of the Riemann zeta function

Abstract

We establish the full asymptotic for the discrete second moment of the Riemann zeta function of mixed derivatives evaluated at the zeta zeros, providing both unconditional and conditional error terms. This was first studied by Gonek, where only the leading order asymptotic was given, later extended by Conrey–Snaith and Milinovich to include the lower order terms for the first derivative. We extend the case of the first derivative to all derivatives.

3.1 Introduction

The central object of this paper is the discrete second moment of mixed derivatives of the Riemann zeta function, given by the sum

$$I(\mu,\nu) := I(\mu,\nu;T) = \sum_{0<\gamma\leq T} \zeta^{(\mu)}(\rho)\zeta^{(\nu)}(1-\rho), \tag{3.1}$$

as $T\to\infty$, where the sum is over non-trivial zeros of zeta $\rho=\beta+i\gamma$, and where $\zeta^{(\mu)}(s)$ denotes the μ^{th} derivative of the Riemann zeta function. We will establish a full asymptotic expansion for this sum, with a power-saving error term under the Riemann Hypothesis.

This type of discrete moment was introduced by Gonek [26], who proved for positive integers μ, ν, a leading order asymptotic of the form

$$\sum_{0<\gamma\le T} \zeta^{(\mu)}(\rho)\zeta^{(\nu)}(1-\rho)$$
$$= (-1)^{\mu+\nu}\left(\frac{1}{\mu+\nu+1} - \frac{1}{(\mu+1)(\nu+1)}\right)\frac{T}{2\pi}\left(\log\frac{T}{2\pi}\right)^{\mu+\nu+2} + O\left(T(\log T)^{\mu+\nu+1}\right) \tag{3.2}$$

as $T \to \infty$.

The special case $\mu = \nu$, called the discrete second moment of zeta, is given under the Riemann Hypothesis by

$$\sum_{0<\gamma\le T}\left|\zeta^{(\nu)}\left(\frac{1}{2}+i\gamma\right)\right|^2 = \frac{\nu^2}{(2\nu+1)(\nu+1)^2}\frac{T}{2\pi}\left(\log\frac{T}{2\pi}\right)^{2\nu+2} + O\left(T(\log T)^{2\nu+1}\right) \tag{3.3}$$

as $T \to \infty$.

Conrey and Snaith [6] conjectured under the Riemann Hypothesis that for $\varepsilon > 0$ arbitrary and $L = \log t/2\pi$,

$$\sum_{0<\gamma\le T} |\zeta'(\rho)|^2 = \frac{1}{2\pi}\int_1^T \left(\frac{1}{12}L^4 + \frac{2\gamma_0}{3}L^3 + \left(\gamma_0^2 - 2\gamma_1\right)L^2 - \left(2\gamma_0^3 + 2\gamma_0\gamma_1 + \gamma_2\right)L \right.$$
$$\left. + \left(2\gamma_0^4 + 2\gamma_0^2\gamma_1 + 14\gamma_1^2 + 8\gamma_0\gamma_2 + \frac{10\gamma_3}{3}\right)\right) dt + O\left(T^{1/2+\varepsilon}\right),$$

as $T \to \infty$, where the γ_n are the Stieltjes coefficients from the expansion of $\zeta(s)$ around $s = 1$,

$$\zeta(s) = \frac{1}{s-1} + \gamma_0 - \gamma_1(s-1) + \frac{\gamma_2}{2!}(s-1)^2 + \cdots + (-1)^n\frac{\gamma_n}{n!}(s-1)^n + \cdots.$$

Milinovich [50] proved this conjecture under the assumption of the Riemann Hypothesis, writing the asymptotic as

$$\sum_{0<\gamma\le T}\left|\zeta'\left(\frac{1}{2}+i\gamma\right)\right|^2 = \frac{T}{2\pi}P_4\left(\log\frac{T}{2\pi}\right) + O\left(T^{\frac{1}{2}+\varepsilon}\right) \tag{3.4}$$

as $T \to \infty$, where $P_4(x)$ is a degree four polynomial given by

$$\begin{aligned}P_4(x) = &\frac{1}{12}x^4\\ &+ \left(\frac{2\gamma_0 - 1}{3}\right) x^3\\ &+ \left(1 - 2\gamma_0 + \gamma_0^2 - 2\gamma_1\right) x^2\\ &+ \left(-2 + 4\gamma_0 - 2\gamma_0^2 - 2\gamma_0^3 - 10\gamma_0\gamma_1 + 4\gamma_1 - \gamma_2\right) x\\ &+ \left(\frac{6 + 6\gamma_0(5\gamma_1 + 4\gamma_2 - 2) + 6\gamma_0^2(\gamma_0 + \gamma_0^2 + 6\gamma_1 + 1) - 12\gamma_1 + 42\gamma_1^2 + 3\gamma_2 + 10\gamma_3}{3}\right)\end{aligned}$$

Remark. *The equivalence of Milinovich's result and the conjecture of Conrey and Snaith follows by performing the integral.*

Some examples of other generalisations of the results discussed above are shifted second moment results [21, 20], higher moment conjectures [25, 31, 34, 56], extreme values of derivatives of zeta [55], upper and lower bounds [45, 2] on moments, and negative moments [25, 18, 30, 17, 4].

3.2 Statement of Results

We generalise the results of both (3.2) and (3.4) by proving a full asymptotic expansion for the discrete second moment of mixed derivatives of the Riemann zeta function (3.1), both unconditionally and conditionally under the Riemann Hypothesis.

Theorem 16. *For positive integers μ, ν, we have*

$$\sum_{0<\gamma\leq T} \zeta^{(\mu)}(\rho)\zeta^{(\nu)}(1-\rho) = \frac{T}{2\pi}\mathcal{P}_{\mu,\nu}\left(\log \frac{T}{2\pi}\right) + O\left(Te^{-C\sqrt{\log T}}\right) \tag{3.5}$$

as $T \to \infty$, where C is a positive constant and where $\mathcal{P}_{\mu,\nu}(x)$ is the polynomial of degree $\mu + \nu + 2$ given by

$$\begin{aligned}\mathcal{P}_{\mu,\nu}(x) = (-1)^{\nu} &\sum_{m=0}^{\mu+\nu+2} \sum_{k=0}^{\nu} \binom{\nu}{k} C_1^{(\mu,\nu)}(m,k)x^m\\ &+ (-1)^{\mu} \sum_{m=0}^{\mu+\nu+2} \sum_{k=0}^{\mu} \binom{\mu}{k} \left(C_1^{(\nu,\mu)}(m,k) + C_2^{(\mu,\nu)}(m,k)\right) x^m,\end{aligned} \tag{3.6}$$

where

$$C_1^{(\mu,\nu)}(m,k) = \begin{cases} \dfrac{(-1)^m(\nu-k)}{m!}\displaystyle\sum_{j=0}^{\mu+\nu+1-m}(-1)^{\mu+\nu-j}\frac{(\mu+\nu+1-j)!}{(\mu+k+2-j)!}c_j^{(\mu,k)}+ \\ \quad +\dfrac{c_{\mu+\nu+2-m}^{(\mu,k)}}{(k+m-\nu)!} & m \geq \nu-k \\ \dfrac{(-1)^m(\nu-k)}{m!}\displaystyle\sum_{j=0}^{\mu+k+2}(-1)^{\mu+\nu-j}\frac{(\mu+\nu+1-j)!}{(\mu+k+2-j)!}c_j^{(\mu,k)} & m \leq \nu-k-1 \end{cases}$$

where $c_j^{(\mu,k)}$ *are the Laurent series coefficients around* $s=1$ *of*

$$\frac{\zeta'}{\zeta}(s)\zeta^{(\mu)}(s)\zeta^{(k)}(s)\frac{1}{s} = \sum_{j=0}^{\infty} c_j^{(\mu,k)}(s-1)^{-\mu-k-3+j}, \tag{3.7}$$

and where

$$C_2^{(\mu,\nu)}(m,k) = \begin{cases} \dfrac{(-1)^m(\mu-k+1)}{m!}\displaystyle\sum_{j=0}^{\mu+\nu+1-m}(-1)^{\mu+\nu-j}\frac{(\mu+\nu+1-j)!}{(\nu+k+1-j)!}d_j^{(\nu,k)}+ \\ \quad +\dfrac{d_{\mu+\nu+2-m}^{(\nu,k)}}{(k+m-\mu-1)!} & m \geq \mu-k+1 \\ \dfrac{(-1)^m(\mu-k+1)}{m!}\displaystyle\sum_{j=0}^{\nu+k+1}(-1)^{\mu+\nu-j}\frac{(\mu+\nu+1-j)!}{(\nu+k+1-j)!}d_j^{(\nu,k)} & m \leq \mu-k \end{cases}$$

where $d_j^{(\nu,k)}$ *are the Laurent series coefficients around* $s=1$ *of*

$$\zeta^{(\nu)}(s)\zeta^{(k)}(s)\frac{1}{s} = \sum_{j=0}^{\infty} d_j^{(\nu,k)}(s-1)^{-\nu-k-2+j}.$$

If one assumes the Riemann Hypothesis, the error term may be replaced with $O\left(T^{\frac{1}{2}+\varepsilon}\right)$ *for arbitrary* $\varepsilon > 0$.

We now state several corollaries of this result, with Corollary 17 clearly following immediately from this theorem and with Corollaries 18 and 19 proved in Section 3.6.

Corollary 17. *Assume the Riemann Hypothesis. For ν a positive integer, the discrete second moment of zeta for all derivatives is given by*

$$\sum_{0<\gamma\leq T}\left|\zeta^{(\nu)}\left(\frac{1}{2}+i\gamma\right)\right|^2$$
$$=\frac{T}{2\pi}\sum_{m=0}^{2\nu+2}\left(\sum_{k=0}^{\nu}(-1)^{\nu}\binom{\nu}{k}\left(2C_1^{(\nu,\nu)}(m,k)+C_2^{(\nu,\nu)}(m,k)\right)\right)\left(\log\frac{T}{2\pi}\right)^m+O\left(T^{\frac{1}{2}+\varepsilon}\right),$$

where $C_1^{(\nu,\nu)}(m,k)$ and $C_2^{(\nu,\nu)}(m,k)$ are defined in Theorem 16.

Corollary 18. *Assume the Riemann Hypothesis. In the case $\mu=\nu=1$, (3.5) recovers the polynomial $P_4(x)$ in (3.4).*

Corollary 19. *For μ,ν positive integers, the leading order coefficient of $\mathcal{P}_{\mu,\nu}(x)$ agrees with the leading order given in (3.2).*

As we see in Milinovich's polynomial $P_4(x)$ in (3.4), the coefficients quickly become unwieldy. We give an example of our result for discrete second moment of the second derivative in Appendix .1 by explicitly writing out the polynomial for the second derivative. Finally, in Appendix .2 we demonstrate the theorem by plotting the graphs for the first and second derivatives.

3.3 Brief outline of the proof

For $c=1+\frac{1}{\log T}$ and $\mathcal{R}$ the rectangular contour with vertices $c+i$, $c+iT$, $1-c+iT$, and $1-c+i$, we may use Cauchy's theorem to write

$$\begin{aligned}
I(\mu,\nu) &= \sum_{0<\gamma\leq T}\zeta^{(\mu)}(\rho)\zeta^{(\nu)}(1-\rho)\\
&= \frac{1}{2\pi i}\oint_{\mathcal{R}}\frac{\zeta'}{\zeta}(s)\zeta^{(\mu)}(s)\zeta^{(\nu)}(1-s)\;ds\\
&= \frac{1}{2\pi i}\left(\int_{c+i}^{c+iT}+\int_{c+iT}^{1-c+iT}+\int_{1-c+iT}^{1-c+i}+\int_{1-c+i}^{c+i}\right)\frac{\zeta'}{\zeta}(s)\zeta^{(\mu)}(s)\zeta^{(\nu)}(1-s)\;ds\\
&= I_1(\mu,\nu)+I_2(\mu,\nu)+I_3(\mu,\nu)+I_4(\mu,\nu).
\end{aligned}\tag{3.8}$$

It is immediate that $I_4(\mu,\nu)=O(1)$ since the integral has finite length and bounded integrand. Furthermore, as shown by Gonek [26], we have $I_2(\mu,\nu)=O\left(T^{\frac{1}{2}+\varepsilon}\right)$ with the harmless restriction that T lies a distance $\gg 1/\log T$ from a zero ordinate γ. We shall use this restriction without loss of generality throughout our proof. From this it follows that

$$I(\mu,\nu) = I_1(\mu,\nu) + I_3(\mu,\nu) + O\left(T^{\frac{1}{2}+\varepsilon}\right). \tag{3.9}$$

In Section 3.4 we deal with the right-hand vertical segment $I_1(\mu,\nu)$. The starting point is by introducing a functional equation which allows us to write $\zeta^{(\nu)}(1-s)$ in terms of $\zeta^{(k)}(s)$ for k between 0 and ν. As a consequence we may write $I_1(\mu,\nu)$ as an integral of an absolutely convergent Dirichlet series. We then use the method of stationary phase to rewrite this integral as the sum

$$\sum_{n_1 n_2 n_3 \le \frac{T}{2\pi}} \Lambda(n_1)(\log n_2)^{\mu}(\log n_3)^{k}(\log n_1 n_2 n_3)^{\nu-k},$$

plus a small error that is subsumed by our error term written above.

We evaluate this sum without the $(\log n_1 n_2 n_3)^{\nu-k}$ factor through Perron's formula. This gives the sum as the residue of a Dirichlet series at $s=1$, which in turn is a polynomial of degree $\mu+\nu+2$. Finally we reinsert the logarithmic term via partial summation.

In Section 3.5 we handle the left-hand segment $I_3(\mu,\nu)$. We use another functional equation to relate the left vertical segment of our integral to the right vertical segment, and then follow similar methods to those used in Section 3.4 to establish the asymptotics for the left vertical segment. Combining these two contours, together with the error term that we carry through the proof, gives Theorem 16.

Finally, as mentioned in the introduction, in Section 3.6 we prove some corollaries of our result.

3.4 The right-hand vertical segment

3.4.1 Initial manipulations

We start by writing $I_1(\mu,\nu)$ in a form more amenable to analysis. Recall that

$$I_1(\mu,\nu) = \frac{1}{2\pi}\int_1^T \frac{\zeta'}{\zeta}(c+it)\zeta^{(\mu)}(c+it)\zeta^{(\nu)}(1-c-it)\, dt.$$

We apply the functional equation for $\zeta^{(\nu)}(1-c-it)$ so we can write the resulting expression in terms of convergent Dirichlet series.

Lemma 3.4.1. *[37, Lemma 4] For $s=\sigma+it$, with $\sigma\geq 1$ and $t\geq 1$ we have*

$$\zeta^{(\nu)}(1-s)=(-1)^{\nu}\chi(1-s)\sum_{k=0}^{\nu}\binom{\nu}{k}\left(\log\frac{t}{2\pi}\right)^{\nu-k}\zeta^{(k)}(s)+O\left(t^{\sigma-\frac{3}{2}}(\log t)^{\nu}\right), \tag{3.10}$$

where $\chi(s)$ is the factor from the functional equation $\zeta(s)=\chi(s)\zeta(1-s)$.

Substituting (3.10) into our expression for $I_1(\mu,\nu)$ gives

$$\begin{aligned} &I_1(\mu,\nu)\\ &=\frac{(-1)^{\nu}}{2\pi}\sum_{k=0}^{\nu}\binom{\nu}{k}\int_1^T\frac{\zeta'}{\zeta}(c+it)\zeta^{(\mu)}(c+it)\zeta^{(k)}(c+it)\chi(1-c-it)\left(\log\frac{t}{2\pi}\right)^{\nu-k}dt\\ &\qquad+O\left(T^{\frac{1}{2}+\varepsilon}\right).\end{aligned}$$

Each term in the integrand can be expressed as a Dirichlet series since $\Re(s)=c>1$, namely

$$\frac{\zeta'}{\zeta}(s)=-\sum_{n=1}^{\infty}\frac{\Lambda(n)}{n^s}\text{ and }\zeta^{(\mu)}(s)=(-1)^{\mu}\sum_{n=1}^{\infty}\frac{(\log n)^{\mu}}{n^s},$$

where $\Lambda(n)$ is the von Mangoldt function.

It follows that, by multiplying the Dirichlet series in the integral above together, we can write

$$\begin{aligned}\frac{\zeta'}{\zeta}(s)\zeta^{(\mu)}(s)\zeta^{(k)}(s)&=(-1)^{\mu+k+1}\left(\sum_{n_1=1}^{\infty}\frac{\Lambda(n_1)}{n_1^s}\right)\left(\sum_{n_2=1}^{\infty}\frac{(\log n_2)^{\mu}}{n_2^s}\right)\left(\sum_{n_3=1}^{\infty}\frac{(\log n_3)^{k}}{n_3^s}\right)\\ &=\sum_{n=1}^{\infty}\frac{A_n^{(\mu,k)}}{n^s}\end{aligned}$$

where

$$A_n^{(\mu,k)}:=(-1)^{\mu+k+1}\sum_{n_1n_2n_3=n}\Lambda(n_1)(\log n_2)^{\mu}(\log n_3)^{k}. \tag{3.11}$$

The integral $I_1(\mu,\nu)$ can then be written as

$$\begin{aligned}&I_1(\mu,\nu)\\ &=\frac{(-1)^{\nu}}{2\pi}\sum_{k=0}^{\nu}\binom{\nu}{k}\int_1^T\chi(1-c-it)\left(\log\frac{t}{2\pi}\right)^{\nu-k}\left(\sum_{n=1}^{\infty}\frac{A_n^{(\mu,k)}}{n^{c+it}}\right)dt+O\left(T^{\frac{1}{2}}(\log T)^{\nu}\right).\end{aligned}$$

We now use a lemma due to Gonek [26, Lemma 5] which comes from the method of stationary phase which will permit us to write this integral as a sum, which we shall subsequently evaluate via the method of Perron.

Lemma 3.4.2. *Let $\{a_n\}_{n=1}^{\infty}$ be a sequence of complex numbers that satisfy $a_n \ll n^{\varepsilon}$ for arbitrary $\varepsilon > 0$. Let $c = 1 + \frac{1}{\log T}$, and let m be a non-negative integer. Then for $T \geq 1$ we have*

$$\frac{1}{2\pi}\int_1^T \chi(1-c-it)\left(\log\frac{t}{2\pi}\right)^m\left(\sum_{n=1}^{\infty}\frac{a_n}{n^{c+it}}\right)dt = \sum_{1\leq n\leq\frac{T}{2\pi}} a_n(\log n)^m + O\left(T^{c-\frac{1}{2}}(\log T)^m\right).$$

Then by Lemma 3.4.2, we can rewrite $I_1(\mu,\nu)$ as the sum

$$I_1(\mu,\nu) = (-1)^{\nu}\sum_{k=0}^{\nu}\binom{\nu}{k}\sum_{n\leq\frac{T}{2\pi}} A_n^{(\mu,k)}(\log n)^{\nu-k} + O\left(T^{\frac{1}{2}+\varepsilon}\right). \tag{3.12}$$

3.4.2 Evaluating the inner sum without the logarithm

Throughout this section we set $Y = \frac{T}{2\pi}$ for notational convenience.

We now evaluate the sum in (3.12). One could use Perron's formula, relying on the Dirichlet series expansion

$$\sum_{n=1}^{\infty}\frac{A_n^{(\mu,k)}(\log n)^{\nu-k}}{n^s} = (-1)^{\nu-k}\frac{d^{\nu-k}}{ds^{\nu-k}}\left(\frac{\zeta'}{\zeta}(s)\zeta^{(\mu)}(s)\zeta^{(k)}(s)\right).$$

However it turns out to be simpler and more convenient to use Perron's formula to calculate $\sum_{n\leq Y} A_n^{(\mu,k)}$ without any logarithms, and then use partial summation to reinsert them later.

We start by using a truncated version of Perron's formula.

Lemma 3.4.3. *Let $A_n^{(\mu,k)}$ be given by (3.11). For $2 \leq V \leq Y$, as $Y \to \infty$,*

$$\sum_{n\leq Y} A_n^{(\mu,k)} = \frac{1}{2\pi i}\int_{c-iV}^{c+iV}\frac{\zeta'}{\zeta}(s)\zeta^{(\mu)}(s)\zeta^{(k)}(s)\frac{Y^s}{s}\,ds + R_1(Y,V),$$

where

$$R_1(Y,V) = O\left(\frac{Y}{V}(\log Y)^{\mu+k+3}\right).$$

Proof. Bounding $R_1(Y,V)$ is all we need to do to prove the lemma, since the integral comes directly from Perron's formula (and the truncation gives the error term). By [53, Cor 5.3] we can bound the remainder as

$$\begin{aligned} R_1(Y,V) &\ll \sum_{\frac{Y}{2}<n<2Y} |A_n^{(\mu,k)}| \min\left(1, \frac{Y}{V|Y-n|}\right) + \frac{4^c+Y^c}{V} \sum_{n\geq 1} \frac{|A_n^{(\mu,k)}|}{n^c} \\ &= A+B, \end{aligned} \tag{3.13}$$

say. To evaluate the error, we start by giving an upper bound for $A_n^{(\mu,k)}$. Note that $\Lambda(n) \leq \log n$ with equality holding if and only if n is prime. We bound $A_n^{(\mu,k)}$ crudely by

$$\left|A_n^{(\mu,k)}\right| \leq \sum_{n_1 n_2 n_3 = n} (\log n)(\log n)^{\mu}(\log n)^k = (\log n)^{\mu+k+1} d_3(n),$$

where $d_3(n)$ is the 3-fold divisor function. Bounding A in (3.13) by the maximum of $A_n^{(\mu,k)}$ and using the notation $\ell = |Y-m|$,

$$\begin{aligned} A &\ll (\log Y)^{\mu+k+1} \sum_{\frac{Y}{2}<m<2Y} d_3(m) \min\left(1, \frac{Y}{V\ell}\right) \\ &\ll (\log Y)^{\mu+k+1} \sum_{\ell \leq Y} \frac{Y}{V}\frac{1}{\ell} d_3(\ell) \\ &\ll \frac{Y}{V}(\log Y)^{\mu+k+4}, \end{aligned}$$

using the fact that $\sum_{\ell\leq Y} \frac{d_3(\ell)}{\ell} \ll (\log Y)^3$ (see, for example, [53, p.43]).

Next we turn to bounding B in (3.13). Since $c = 1 + \frac{1}{\log T}$ the Dirichlet series converges, and so

$$B = \frac{4^c+Y^c}{V}\left|\frac{\zeta'}{\zeta}(c)\zeta^{(\mu)}(c)\zeta^{(k)}(c)\right| \ll \frac{Y}{V}(\log Y)^{\mu+k+3},$$

using the fact that $Y = \frac{T}{2\pi}$ and also that

$$\frac{\zeta'}{\zeta}\left(1+\frac{1}{\log T}\right) \ll \log T, \tag{3.14}$$

and

$$\zeta^{(\mu)}\left(1+\frac{1}{\log T}\right) \ll (\log T)^{\mu+1} \tag{3.15}$$

as required. □

Next we write the integral in Lemma 3.4.3 in terms of the residue of the integrand at $s = 1$. We obtain an error term from completing the contour into a rectangle which we will deal with in Lemma 3.4.4. We remark that this lemma is the only place where we get different errors depending on whether we assume the Riemann Hypothesis or not, so we shall consider both cases separately.

Lemma 3.4.4. *For $Y = \frac{T}{2\pi}$, as $V, Y \to \infty$, we have*

$$\frac{1}{2\pi i}\int_{c-iV}^{c+iV} \frac{\zeta'}{\zeta}(s)\zeta^{(\mu)}(s)\zeta^{(k)}(s)\frac{Y^s}{s}\, ds = \operatorname*{Res}_{s=1}\left(\frac{\zeta'}{\zeta}(s)\zeta^{(\mu)}(s)\zeta^{(k)}(s)\frac{Y^s}{s}\right) + \mathcal{E}_1(Y,V),$$

where $\mathcal{E}_1(\mu,k;Y)$ is given by

1. $\mathcal{E}_1(\mu,k;Y) = \left(Ye^{-C\sqrt{\log Y}}\right)$ *unconditionally for a positive constant C*
2. $\mathcal{E}_1(\mu,k;Y) = \left(Y^{\frac{1}{2}+\varepsilon}\right)$ *under the Riemann Hypothesis.*

Proof of Lemma 3.4.4. We consider the positively oriented rectangular contour with vertices at $c \pm iV, c' \pm iV$, where $\frac{1}{2} < c' < 1$ is large enough that no zeros of zeta with $|\gamma| \le V$ lie on or to the right of the c' line. Therefore the only pole contained within this contour is at $s = 1$, and by Cauchy's Residue Theorem,

$$\begin{aligned}\operatorname*{Res}_{s=1}&\left(\frac{\zeta'}{\zeta}(s)\zeta^{(\mu)}(s)\zeta^{(k)}(s)\frac{Y^s}{s}\right)\\ &= \frac{1}{2\pi i}\left(\int_{c-iV}^{c+iV} + \int_{c+iV}^{c'+iV} + \int_{c'+iV}^{c'-iV} + \int_{c'-iV}^{c-iV}\right)\frac{\zeta'}{\zeta}(s)\zeta^{(\mu)}(s)\zeta^{(k)}(s)\frac{Y^s}{s}\, ds.\end{aligned}$$

By rearranging this expression and switching the orientation of some of the integrals we have that the desired integral is equal to

$$\begin{aligned}\frac{1}{2\pi i}\int_{c-iV}^{c+iV} \frac{\zeta'}{\zeta}(s)\zeta^{(\mu)}(s)\zeta^{(k)}(s)\frac{Y^s}{s}\, ds &= \operatorname*{Res}_{s=1}\left(\frac{\zeta'}{\zeta}(s)\zeta^{(\mu)}(s)\zeta^{(k)}(s)\frac{Y^s}{s}\right)\\ &+ \frac{1}{2\pi i}\left(\int_{c'+iV}^{c+iV} + \int_{c'-iV}^{c'+iV} - \int_{c'-iV}^{c-iV}\right)\frac{\zeta'}{\zeta}(s)\zeta^{(\mu)}(s)\zeta^{(k)}(s)\frac{Y^s}{s}\, ds.\end{aligned}$$

The result will follow from finding appropriate bounds for the three line integrals. We consider the conditional and unconditional cases separately as they involve different values of c' and different bounds for zeta.

The unconditional case

As noted in Titchmarsh [66, p.54], there exists some absolute constant $C > 0$ such that for $c' = 1 - \frac{C}{\log V}$, any zero of $\zeta(s)$ lies a distance $\gg \frac{1}{\log V}$ away from the line between $c' - iV$ and $c' + iV$.

Therefore, on the two horizontal pieces we may apply the bound of Gonek [26, §2] which applies uniformly for $-1 \le \sigma \le 2$

$$\frac{\zeta'}{\zeta}(\sigma \pm iV) \ll (\log V)^2.$$

We also use the convexity bounds inside and to the right of the critical strip

$$\zeta^{(\mu)}(\sigma \pm iV) \ll \begin{cases} V^{\frac{1}{2}(1-\sigma)}(\log V)^{\mu+1} & \text{if } 0 \le \sigma \le 1 \\ (\log V)^{\mu+1} & \text{if } \sigma \ge 1, \end{cases} \tag{3.16}$$

which may be established by using Ivic's bound for $\nu = 1$ [39] and applying Cauchy's estimate for derivatives of analytic functions around a disc of radius $1/\log V$ with centre at $\sigma + iV$.

With these bounds we deduce that

$$\frac{1}{2\pi i}\int_{c'\pm iV}^{c\pm iV} \frac{\zeta'}{\zeta}(s)\zeta^{(\mu)}(s)\zeta^{(k)}(s)\frac{Y^s}{s}\,d\sigma \ll (\log V)^{\mu+k+4}\frac{Y^c}{V}(c-c') \ll \frac{Y}{V}(\log V)^{\mu+k+3},$$

where we have used the fact that $c - c' \ll \frac{1}{\log V}$ and $Y^c = \ll Y$.

Now we turn to the vertical segment of the contour. Away from the pole, we can use the same bounds as above, and for $t \approx 0$ we bound the terms in the integral by the appropriate Laurent expansions, (3.14) and (3.15). Therefore on the line $s = c' + it$, $-V \le t \le V$, we can bound the integral by

$$Y^{c'}(\log V)^{\mu+k+4} + \int_1^V (\log V)^{\mu+k+4}\frac{Y^{c'}}{t}\,dt \ll Y^{c'}(\log V)^{\mu+k+5}.$$

Since $Y^{c'} = Y\exp\left(-\frac{C\log Y}{\log V}\right)$ this completes the proof of the unconditional case.

The conditional case

Under the assumption of the Riemann Hypothesis, we can both shift the line of integration further to the left without crossing any zeros, and also use better (conditional) bounds on zeta and its derivatives. Specifically we shift the contour to just to the right of the critical line, letting $c' = \frac{1}{2} + \frac{1}{\log V}$, and we use $\zeta^{(n)}(s) \ll t^{\varepsilon}$ for arbitrary $\varepsilon > 0$.

At any point on the vertical segment the closest zero is $\geq \frac{1}{\log V}$ away, so we have $\frac{\zeta'}{\zeta}(s) \ll (\log V)^2$ and so the vertical integral is bounded by

$$Y^{\frac{1}{2}} \exp\left(\frac{\log Y}{\log V}\right) V^{\varepsilon}$$

for arbitrary $\varepsilon > 0$.

The horizontal segments are dealt with similarly to before, only this time the length of integration is bounded and we will bound terms like $\log V$ by V^{ε} since that's sufficient for our purposes. The two horizontal pieces are bounded by

$$\frac{Y}{V} V^{\varepsilon}$$

and this completes the proof in the conditional case. □

Completion of the proof of Lemma 3.4.4

Using Lemma 3.4.3, thus far in Lemma 3.4.4 we have shown that

$$\sum_{n \leq Y} A_n^{(\mu,k)} = \operatorname*{Res}_{s=1}\left(\frac{\zeta'}{\zeta}(s)\zeta^{(\mu)}(s)\zeta^{(k)}(s)\frac{Y^s}{s}\right) + R_1(Y,V) + \mathcal{E}_1(V,Y).$$

where we now pick an optimal V in terms of Y, depending on whether we are bounding the error terms conditionally or unconditionally.

In the unconditional case, we can choose $V = \exp(\sqrt{C \log Y})$ to optimise the error terms. This then gives an error term of

$$R_1(Y,V) + \mathcal{E}_1(V,Y) \ll Y e^{-\sqrt{C \log Y}} (\log Y)^{\frac{\mu+k+5}{2}} \ll Y \exp(-\tilde{C}\sqrt{\log Y})$$

for some $\tilde{C} > 0$.

In the conditional case, we take $V = Y$ and find

$$R_1(Y,V) + \mathcal{E}_1(V,Y) \ll Y^{\frac{1}{2}+\varepsilon},$$

for arbitrary $\varepsilon > 0$, as stated in Lemma 3.4.4.

We now compute the residue term. In the following lemma we will write the residue in terms of the Laurent coefficients of our triple Dirichlet series given in (3.11) around $s = 1$.

Lemma 3.4.5. *We have*

$$\mathrm{Res}_{s=1}\left(\frac{\zeta'}{\zeta}(s)\zeta^{(\mu)}(s)\zeta^{(k)}(s)\frac{Y^s}{s}\right) = Y\sum_{j=0}^{\mu+k+2}\frac{c_j^{(\mu,k)}}{(\mu+k+2-j)!}(\log Y)^{\mu+k+2-j}, \quad (3.17)$$

where $c_j^{\mu,k}$ are the Laurent series coefficients around $s=1$ of

$$\frac{\zeta'}{\zeta}(s)\zeta^{(\mu)}(s)\zeta^{(k)}(s)\frac{1}{s} = \sum_{j=0}^{\infty}c_j^{(\mu,k)}(s-1)^{-\mu-k-3+j}. \quad (3.18)$$

Proof. The function $\frac{\zeta'}{\zeta}(s)\zeta^{(\mu)}(s)\zeta^{(k)}(s)\frac{1}{s}$ has a pole of order $\mu+k+3$ at $s=1$. We write this expansion as the series given in (3.18).

The expansion of Y^s about $s=1$ is

$$Y^s = Y\left(1+(s-1)\log Y+\frac{(s-1)^2}{2!}(\log Y)^2+\cdots+\frac{(s-1)^k}{k!}(\log Y)^k+\cdots\right).$$

and so the residue of $\frac{\zeta'}{\zeta}(s)\zeta^{(\mu)}(s)\zeta^{(k)}(s)\frac{Y^s}{s}$ is given by the sum of

$$\frac{c_j^{(\mu,k)}}{(\mu+k+2-j)!}(\log Y)^{\mu+k+2-j}$$

for each $j=0,\ldots,\mu+k+2$. □

3.4.3 Reinserting the logarithm in the inner sum

Throughout this section we set $Y=\frac{T}{2\pi}$ for notational convenience.

Lemma 3.4.6. *For $0\le k\le\nu$, we have that*

$$\sum_{n\le Y}A_n^{(\mu,k)}(\log n)^{\nu-k} = Y\sum_{m=0}^{\mu+\nu+2}C_1^{(\mu,\nu)}(m,k)(\log Y)^m + O\left(Ye^{-C\sqrt{\log Y}}\right),$$

where for $m\ge\nu-k$,

$$C_1^{(\mu,\nu)}(m,k) = \frac{(-1)^m(\nu-k)}{m!}\sum_{j=0}^{\mu+\nu+1-m}(-1)^{\mu+\nu-j}\frac{(\mu+\nu+1-j)!}{(\mu+k+2-j)!}c_j^{(\mu,k)}+\frac{c_{\mu+\nu+2-m}^{(\mu,k)}}{(k+m-\nu)!}$$

and for $m<\nu-k$

$$C_1^{(\mu,\nu)}(m,k) = \frac{(-1)^m(\nu-k)}{m!}\sum_{j=0}^{\mu+k+2}(-1)^{\mu+\nu-j}\frac{(\mu+\nu+1-j)!}{(\mu+k+2-j)!}c_j^{(\mu,k)}$$

Remark. *The differences in the two expressions for $C_1^{(\mu,\nu)}(m,k)$ are the extra term for larger m, and the different upper limit on the j-sums. Those two upper limits are the same when $m = \nu - k - 1$. Finally, when $m = \mu+\nu+2$, which is the largest it can be, the j-sum is empty.*

Proof. We have shown using Lemmas 3.4.3, 3.4.4 and 3.4.5 that

$$\sum_{n\le Y} A_n^{(\mu,k)} = Y \sum_{j=0}^{\mu+k+2} \frac{c_j^{(\mu,k)}}{(\mu+k+2-j)!}(\log Y)^{\mu+k+2-j} + O\left(Ye^{-C\sqrt{\log Y}}\right).$$

By partial summation we have

$$\sum_{n\le Y} A_n^{(\mu,k)}(\log n)^{\nu-k} = \left(\sum_{n\le Y} A_n^{(\mu,k)}\right)(\log Y)^{\nu-k} - (\nu-k)\int_1^Y \left(\sum_{n\le t} A_n^{(\mu,k)}\right)\frac{(\log t)^{\nu-k-1}}{t}\,dt. \tag{3.19}$$

Clearly

$$\left(\sum_{n\le Y} A_n^{(\mu,k)}\right)(\log Y)^{\nu-k} = Y\sum_{j=0}^{\mu+k+2}\frac{c_j^{(\mu,k)}}{(\mu+k+2-j)!}(\log Y)^{\mu+\nu+2-j} + O\left((\log Y)^{\nu-k} Ye^{-C\sqrt{\log Y}}\right),$$

where $C > 0$ isn't necessarily the same constant throughout. Relabelling the sum so $m = \mu+\nu+2-j$ (to help make the power of $\log Y$ clear), the first piece on the right-hand side of (3.19) is

$$\sum_{n\le Y} A_n^{(\mu,k)}(\log Y)^{\nu-k} = Y\sum_{m=\nu-k}^{\mu+\nu+2}\frac{c_{\mu+\nu+2-m}^{(\mu,k)}}{(m+k-\nu)!}(\log Y)^m + O\left(Ye^{-C\sqrt{\log Y}}\right). \tag{3.20}$$

Next, note that the second term in (3.19) is

$$(\nu-k)\sum_{j=0}^{\mu+k+2}\frac{c_j^{(\mu,k)}}{(\mu+k+2-j)!}\int_1^Y (\log t)^{\mu+\nu+1-j}\,dt + O\left(Ye^{-C\sqrt{\log Y}}\right). \tag{3.21}$$

Note that, by repeated integration by parts,

$$\int_1^Y (\log t)^n\,dt = (-1)^n n! Y\sum_{m=0}^{n}\frac{(-1)^m(\log Y)^m}{m!} + O(1), \tag{3.22}$$

so using (3.22) with $n = \mu + \nu + 1 - j$ we have that

$$\int_1^Y \left(\sum_{n \le t} A_n^{(\mu,k)} \right) \frac{(\log t)^{\nu-k-1}}{t} \, dt$$
$$= \sum_{j=0}^{\mu+k+2} \frac{c_j^{(\mu,k)}}{(\mu+k+2-j)!} (-1)^{\mu+\nu+1-j} (\mu+\nu+1-j)! Y \sum_{m=0}^{\mu+\nu+1-j} \frac{(-1)^m (\log Y)^m}{m!}$$
$$+ O\left(Y e^{-C\sqrt{\log Y}} \right).$$

Next swap the order of summation in the double sum to give

$$Y \sum_{m=0}^{\nu-k-1} \frac{(-1)^m (\log Y)^m}{m!} \sum_{j=0}^{\mu+k+2} \frac{c_j^{(\mu,k)}}{(\mu+k+2-j)!} (-1)^{\mu+\nu+1-j} (\mu+\nu+1-j)!$$
$$+ Y \sum_{m=\nu-k}^{\mu+\nu+1} \frac{(-1)^m (\log Y)^m}{m!} \sum_{j=0}^{\mu+\nu+1-m} \frac{c_j^{(\mu,k)}}{(\mu+k+2-j)!} (-1)^{\mu+\nu+1-j} (\mu+\nu+1-j)! \tag{3.23}$$

Combining the pieces (3.20), (3.21), and (3.23) gives

$$\sum_{n \le Y} A_n^{(\mu,k)} (\log n)^{\nu-k} = Y \sum_{m=\nu-k}^{\mu+\nu+2} \frac{c_{\mu+\nu+2-m}^{(\mu,k)}}{(m+k-\nu)!} (\log Y)^m$$
$$+ (\nu-k) Y \sum_{m=0}^{\mu+\nu+1} \frac{(-1)^m (\log Y)^m}{m!} \sum_{j=0}^{\min\{\mu+\nu+1-m\,,\,\mu+k+2\}} (-1)^{\mu+\nu-j} \frac{(\mu+\nu+1-j)!}{(\mu+k+2-j)!} c_j^{(\mu,k)}$$
$$+ O\left(Y e^{-C\sqrt{\log Y}} \right) \tag{3.24}$$

for some $C > 0$, as required. □

Finally, since $I_1(\mu, \nu)$ is equal to

$$(-1)^\nu \sum_{k=0}^{\nu} \binom{\nu}{k} \sum_{n \le \frac{T}{2\pi}} A_n^{(\mu,k)} (\log n)^{\nu-k} + O\left(T^{\frac{1}{2}+\varepsilon} \right),$$

we have by Lemma 3.4.6 that

$$I_1(\mu,\nu) = (-1)^\nu \frac{T}{2\pi} \sum_{m=0}^{\mu+\nu+2} \sum_{k=0}^{\nu} \binom{\nu}{k} C_1^{(\mu,\nu)}(m,k) \left(\log \frac{T}{2\pi} \right)^m + O\left(T e^{-C\sqrt{\log T}} \right) \tag{3.25}$$

with the $C_1^{\mu,\nu}(m,k)$ given in the statement of Lemma 3.4.6.

3.5 The left-hand vertical segment

The evaluation of the left-hand segment $I_3(\mu,\nu)$ follows closely that that of $I_1(\mu,\nu)$, so in this section we give the overview and highlight where the differences between the two calculations lie.

3.5.1 Initial manipulations

We start by writing $I_3(\mu,\nu)$, given in (3.8), in a form which relates $I_3(\mu,\nu)$ to $I_1(\mu,\nu)$. We have

$$I_3(\mu,\nu) = -\frac{1}{2\pi}\int_1^T \frac{\zeta'}{\zeta}(1-c+it)\zeta^{(\mu)}(1-c+it)\zeta^{(\nu)}(c-it)\ dt.$$

By [26, Lemma 6] we have (where $t \neq 0$)

$$\frac{\zeta'}{\zeta}(1-s) = -\log\left(\frac{|t|}{2\pi}\right) - \frac{\zeta'}{\zeta}(s) + O\left(\frac{1}{1+|t|}\right). \tag{3.26}$$

so

$$\begin{aligned} I_3(\mu,\nu) &= \frac{1}{2\pi}\int_1^T \left(\log\left(\frac{t}{2\pi}\right) + \frac{\zeta'}{\zeta}(c-it) + O\left(\frac{1}{1+|t|}\right)\right)\zeta^{(\mu)}(1-c+it)\zeta^{(\nu)}(c-it)\ dt \\ &= \overline{J(\mu,\nu)} + \overline{I_1(\nu,\mu)} + O\left(T^{\frac{1}{2}+\varepsilon}\right), \end{aligned} \tag{3.27}$$

where the overline denotes complex conjugate, and where we write for $s = c+it$

$$J(\mu,\nu) = \frac{1}{2\pi}\int_1^T \left(\log\frac{t}{2\pi}\right)\zeta^{(\mu)}(1-s)\zeta^{(\nu)}(s)\ dt.$$

We have already evaluated $I_1(\mu,\nu)$ (although note that μ and ν are switched here). It therefore only remains to compute $J(\mu,\nu)$. This follows a similar approach, the difference being only minor technical details (in particular, we have a logarithm term in our integrand in place of the logarithmic derivative of zeta in $I_1(\mu,\nu)$).

Remark. *We will evaluate $J(\mu,\nu)$ explicitly in terms of the Stieltjes coefficients to be consistent with our approach for $I_1(\mu,\nu)$. However, an alternative approach would be to adapt Ingham's approach [38], which yields*

$$J(\mu,\nu) = \int_1^T \left(\log\frac{t}{2\pi}\right)\frac{\partial^{\mu+\nu}}{\partial\alpha^{\mu+\nu}}\left(\zeta(1+\alpha) + \left(\frac{t}{2\pi}\right)^{-\alpha}\zeta(1-\alpha)\right)\Bigg|_{\alpha=0} dt + O\left(T^{1/2+\epsilon}\right).$$

3.5.2 Initial Manipulations of $J(\mu,\nu)$

We start by using Lemma 3.4.1 on $\zeta^{(\mu)}(1-s)$ to write $J(\mu,\nu)$ as

$$\frac{(-1)^\mu}{2\pi}\sum_{k=0}^{\mu}\binom{\mu}{k}\int_1^T \zeta^{(\nu)}(c+it)\zeta^{(k)}(c+it)\chi(1-c-it)\left(\log\frac{t}{2\pi}\right)^{\mu-k+1} dt+O\left(T^{\frac{1}{2}+\varepsilon}\right).$$

Since we are in the region $\Re(s)=c>1$ we can make use of the Dirichlet series representations of these terms, namely

$$\zeta^{(\nu)}(s)\zeta^{(k)}(s)=\sum_{n=1}^{\infty}\frac{B_n^{(\nu,k)}}{n^s}$$

where

$$B_n^{(\nu,k)}=(-1)^{\nu+k}\sum_{n_1n_2=n}(\log n_1)^\nu(\log n_2)^k$$

so that

$$J(\mu,\nu)=\frac{(-1)^\mu}{2\pi}\sum_{k=0}^{\mu}\binom{\mu}{k}\int_1^T \chi(1-c-it)\left(\log\frac{t}{2\pi}\right)^{\mu-k+1}\sum_{n=1}^{\infty}\frac{B_n^{(\nu,k)}}{n^{c+it}}\,dt+O\left(T^{\frac{1}{2}+\varepsilon}\right).$$

Next, by applying Lemma 3.4.2 we have

$$J(\mu,\nu)=(-1)^\mu\sum_{k=0}^{\mu}\binom{\mu}{k}\sum_{n\le\frac{T}{2\pi}}B_n^{(\nu,k)}(\log n)^{\mu-k+1}+O\left(T^{\frac{1}{2}+\varepsilon}\right). \qquad (3.28)$$

3.5.3 Evaluating the inner sum

Throughout this section we we set $Y=\frac{T}{2\pi}$ for notational convenience.

We have the following lemmas, closely resembling Lemmas 3.4.3 and 3.4.4. The key difference here is that we don't have a $\zeta'/\zeta(s)$ term (or, equivalently, we don't need to perform a sum over primes), meaning we don't need to split the error term depending on whether we assume the Riemann Hypothesis or not, as we do in Lemma 3.4.4.

Lemma 3.5.1. *As $Y\to\infty$ we have*

$$\sum_{n\le Y}B_n^{(\nu,k)}=\operatorname*{Res}_{s=1}\left(\zeta^{(\nu)}(s)\zeta^{(k)}(s)\frac{Y^s}{s}\right)+O\left(Y^{\frac{1}{2}+\varepsilon}\right). \qquad (3.29)$$

Proof. As in Lemma 3.4.3 we have for $2 \le V \le Y$, as $Y \to \infty$ we have

$$\sum_{n \le Y} B_n^{(\nu,k)} = \frac{1}{2\pi i} \int_{c-iV}^{c+iV} \zeta^{(\nu)}(s)\zeta^{(k)}(s)\frac{Y^s}{s} ds + O\left(\frac{Y}{V}(\log Y)^{\nu+k+2}\right).$$

Similar to Lemma 3.4.4, we shift the contour to the vertical line $c' = 1/2$, noting that the integrand has no singularities other than at $s = 1$. On the two horizontal pieces $\sigma \pm iV$ we use the unconditional convexity bounds for $\zeta^{(\mu)}(\sigma + iV)$ given in (3.16), giving an error of size

$$\int_{1/2}^{1} V^{(1-\sigma)}(\log V)^{\mu+\nu+2}\frac{Y^\sigma}{V} d\sigma \ll \frac{Y}{V}V^\epsilon.$$

The vertical contour on the line $c' = 1/2$ is bounded by

$$\ll \int_1^V \left|\zeta^{(\mu)}(\tfrac{1}{2} + it)\right| \left|\zeta^{(\mu)}(\tfrac{1}{2} + it)\right| \frac{Y^{1/2}}{t} dt$$
$$\ll Y^{1/2} \left(\int_1^V \frac{\left|\zeta^{(\mu)}(\frac{1}{2} + it)\right|^2}{t}\right)^{1/2} \left(\int_1^V \frac{\left|\zeta^{(\nu)}(\frac{1}{2} + it)\right|^2}{t}\right)^{1/2} \ll Y^{1/2}V^\epsilon$$

the last inequality following from Ingham's [38] evaluation of the second moment of derivatives of zeta on the critical line. Picking any V satisfying $\sqrt{Y} \le V \le Y$ produces the desired error, and proves the lemma. □

Evaluating the residue in (3.29) can be done in a similar way to Lemma 3.4.5.

Lemma 3.5.2. *We have*

$$\operatorname*{Res}_{s=1}\left(\zeta^{(\nu)}(s)\zeta^{(k)}(s)\frac{Y^s}{s}\right) = Y \sum_{j=0}^{\nu+k+1} \frac{d_j^{(\nu,k)}}{(\nu + k + 1 - j)!}(\log Y)^{\nu+k+1-j}$$

where $d_j^{(\nu,k)}$ are the Laurent series coefficients around $s = 1$ of

$$\zeta^{(\nu)}(s)\zeta^{(k)}(s)\frac{1}{s} = \sum_{j\ge 0} d_j^{(\nu,k)}(s-1)^{-\nu-k-2+j}.$$

By combining Lemma 3.5.1 and 3.5.2 we have

$$\sum_{n \le Y} B_n^{(\nu,k)} = Y \sum_{j=0}^{\nu+k+1} \frac{d_j^{(\nu,k)}}{(\nu + k + 1 - j)!}(\log Y)^{\nu+k+1-j} + O\left(Y^{\frac{1}{2}+\varepsilon}\right).$$

The next lemma is analogous to what was proved in Lemma 3.4.6, where we reinsert the logarithm in the sum above.

Lemma 3.5.3. *For $k = 0, 1, \ldots, \mu$ we have that*

$$\sum_{n \le Y} B_n^{(\nu,k)} (\log n)^{\mu-k+1} = Y \sum_{m=0}^{\mu+\nu+2} C_2^{(\mu,\nu)}(m,k)(\log Y)^m + O\left(Y^{\frac{1}{2}+\varepsilon}\right),$$

where for $m \ge \mu - k + 1$,

$$C_2^{(\mu,\nu)}(m,k) = \frac{(-1)^m(\mu-k+1)}{m!} \sum_{j=0}^{\mu+\nu+1-m} (-1)^{\mu+\nu-j} \frac{(\mu+\nu+1-j)!}{(\nu+k+1-j)!} d_j^{(\nu,k)} + \frac{d_{\mu+\nu+2-m}^{(\nu,k)}}{(k+m-\mu-1)!}$$

and for $m \le \mu - k$,

$$C_2^{(\mu,\nu)}(m,k) = \frac{(-1)^m(\mu-k+1)}{m!} \sum_{j=0}^{\nu+k+1} (-1)^{\mu+\nu-j} \frac{(\mu+\nu+1-j)!}{(\nu+k+1-j)!} d_j^{(\nu,k)}$$

Remark. *In the case when $m = \mu + \nu + 2$ (which is the largest m can be), the sum in $C_2^{(\mu,\nu)}(m,k)$ is empty.*

Proof. As with the right hand vertical segment in Lemma 3.4.6, we use partial summation to reinsert the logarithmic term. By the partial summation formula we have

$$\sum_{n \le Y} B_n^{(\nu,k)} (\log n)^{\mu-k+1} = \left(\sum_{n \le Y} B_n^{(\nu,k)}\right)(\log Y)^{\mu-k+1} - (\mu-k+1)\int_1^Y \left(\sum_{n \le t} B_n^{(\nu,k)}\right) \frac{(\log t)^{\mu-k}}{t}\, dt.$$

The first term is

$$\left(\sum_{n \le Y} B_n^{(\nu,k)}\right)(\log Y)^{\mu-k+1} = Y \sum_{j=0}^{\nu+k+1} \frac{d_j^{(\nu,k)}}{(\nu+k+1-j)!}(\log Y)^{\mu+\nu+2-j} + O\left(Y^{\frac{1}{2}+\varepsilon}\right)$$
$$= Y \sum_{m=\mu-k+1}^{\mu+\nu+2} \frac{d_{\mu+\nu+2-m}^{(\nu,k)}}{(m+k-\mu-1)!}(\log Y)^m + O\left(Y^{\frac{1}{2}+\varepsilon}\right)$$

and the second is equal to

$$-(\mu-k+1) \sum_{j=0}^{\nu+k+1} \frac{d_j^{(\nu,k)}}{(\nu+k+1-j)!} \int_1^Y (\log t)^{\mu+\nu+1-j} dt + O\left(Y^{\frac{1}{2}+\varepsilon}\right)$$

and using (3.22), this evaluates to

$$-(\mu-k+1)\sum_{j=0}^{\nu+k+1}\frac{d_j^{(\nu,k)}}{(\nu+k+1-j)!}(-1)^{\mu+\nu+1-j}(\mu+\nu+1-j)!Y\sum_{m=0}^{\mu+\nu+1-j}\frac{(-1)^m(\log Y)^m}{m!}$$

Swapping the order of summation, the double sum is

$$(\mu-k+1)Y\sum_{m=0}^{\mu-k}\frac{(-1)^m(\log Y)^m}{m!}\sum_{j=0}^{\nu+k+1}(-1)^{\mu+\nu-j}\frac{(\mu+\nu+1-j)!}{(\nu+k+1-j)!}d_j^{(\nu,k)}$$
$$+(\mu-k+1)Y\sum_{m=\mu-k+1}^{\mu+\nu+1}\frac{(-1)^m(\log Y)^m}{m!}\sum_{j=0}^{\mu+\nu+1-m}(-1)^{\mu+\nu-j}\frac{(\mu+\nu+1-j)!}{(\nu+k+1-j)!}d_j^{(\nu,k)}.$$

Combining the two pieces gives the formula for $C_2^{(\mu,\nu)}(m,k)$ and completes the proof. □

Applying Lemma 3.5.3 to (3.28) we have

$$J(\mu,\nu)=(-1)^\mu\frac{T}{2\pi}\sum_{m=0}^{\mu+\nu+2}\sum_{k=0}^{\mu}\binom{\mu}{k}C_2^{(\mu,\nu)}(m,k)\left(\log\frac{T}{2\pi}\right)^m+O\left(T^{\frac{1}{2}+\varepsilon}\right). \tag{3.30}$$

Switching the role of μ and ν in (3.25), we have that

$$I_1(\nu,\mu)=(-1)^\mu\frac{T}{2\pi}\sum_{m=0}^{\mu+\nu+2}\sum_{k=0}^{\mu}\binom{\mu}{k}C_1^{(\nu,\mu)}(m,k)\left(\log\frac{T}{2\pi}\right)^m+O\left(Te^{-C\sqrt{\log T}}\right) \tag{3.31}$$

so combining $\overline{J(\mu,\nu)}$ and $\overline{I_1(\nu,\mu)}$ in (3.27) gives

$$I_3(\mu,\nu)=(-1)^\mu\frac{T}{2\pi}\sum_{m=0}^{\mu+\nu+2}\sum_{k=0}^{\mu}\binom{\mu}{k}\left(C_1^{(\nu,\mu)}(m,k)+C_2^{(\mu,\nu)}(m,k)\right)\left(\log\frac{T}{2\pi}\right)^m$$
$$+O\left(Te^{-C\sqrt{\log T}}\right) \tag{3.32}$$

Substituting (3.25) and (3.32) into (3.9), we deduce that

$$I(\mu,\nu)=(-1)^\nu\frac{T}{2\pi}\sum_{m=0}^{\mu+\nu+2}\sum_{k=0}^{\nu}\binom{\nu}{k}C_1^{(\mu,\nu)}(m,k)\left(\log\frac{T}{2\pi}\right)^m$$
$$+(-1)^\mu\frac{T}{2\pi}\sum_{m=0}^{\mu+\nu+2}\sum_{k=0}^{\mu}\binom{\mu}{k}\left(C_1^{(\nu,\mu)}(m,k)+C_2^{(\mu,\nu)}(m,k)\right)\left(\log\frac{T}{2\pi}\right)^m+O\left(Te^{-C\sqrt{\log T}}\right),$$

completing the proof of Theorem 16.

3.6 Proof of the Corollaries

As already noted, Corollary 17 follows immediately from Theorem 16.

Proof of Corollary 18. We show that our theorem with $\mu = \nu = 1$ recovers precisely Milinovich's full asymptotic expansion for the first derivative, stated in (3.4).

Theorem 16 states that, under the Riemann Hypothesis,

$$\sum_{0<\gamma\le T} \left|\zeta'\left(\frac{1}{2}+i\gamma\right)\right|^2$$
$$= \frac{T}{2\pi}\sum_{m=0}^{4}(-2C_1^{(1,1)}(m,0) - C_2^{(1,1)}(m,0) - 2C_1^{(1,1)}(m,1) - C_2^{(1,1)}(m,1))\left(\log\frac{T}{2\pi}\right)^m$$
$$+ O\left(T^{\frac{1}{2}+\varepsilon}\right).$$

We now calculate the various terms in this expansion. We have

$$C_1^{(1,1)}(m,0) = \begin{cases} c_0^{(1,0)} - c_1^{(1,0)} + c_2^{(1,0)} - c_3^{(1,0)} & \text{if } m=0 \\ -c_0^{(1,0)} + c_1^{(1,0)} - c_2^{(1,0)} + c_3^{(1,0)} & \text{if } m=1 \\ \frac{1}{2}c_0^{(1,0)} - \frac{1}{2}c_1^{(1,0)} + c_2^{(1,0)} & \text{if } m=2 \\ -\frac{1}{6}c_0^{(1,0)} + \frac{1}{2}c_1^{(1,0)} & \text{if } m=3 \\ \frac{1}{6}c_0^{(1,0)} & \text{if } m=4 \end{cases}$$

where $c_j^{(1,0)}$ are the coefficients of

$$\frac{\zeta'(s)^2}{s} = \frac{c_0^{(1,0)}}{(s-1)^4} + \frac{c_1^{(1,0)}}{(s-1)^3} + \frac{c_2^{(1,0)}}{(s-1)^2} + \frac{c_3^{(1,0)}}{(s-1)} + \ldots$$

and where

$$C_2^{(1,1)}(m,0) = \begin{cases} 6d_0^{(1,0)} - 4d_1^{(1,0)} + 2d_2^{(1,0)} & \text{if } m=0 \\ -6d_0^{(1,0)} + 4d_1^{(1,0)} - 2d_2^{(1,0)} & \text{if } m=1 \\ 3d_0^{(1,0)} - 2d_1^{(1,0)} + d_2^{(1,0)} & \text{if } m=2 \\ -d_0^{(1,0)} + d_1^{(1,0)} & \text{if } m=3 \\ \frac{1}{2}d_0^{(1,0)} & \text{if } m=4 \end{cases}$$

where $d_j^{(1,0)}$ are the coefficients of

$$\frac{\zeta'(s)\zeta(s)}{s} = \frac{d_0^{(1,0)}}{(s-1)^3} + \frac{d_1^{(1,0)}}{(s-1)^2} + \frac{d_2^{(1,0)}}{(s-1)} + \dots$$

and where

$$C_1^{(1,1)}(m,1) = \begin{cases} c_4^{(1,1)} & \text{if } m=0 \\ c_3^{(1,1)} & \text{if } m=1 \\ \frac{1}{2}c_2^{(1,1)} & \text{if } m=2 \\ \frac{1}{6}c_1^{(1,1)} & \text{if } m=3 \\ \frac{1}{24}c_0^{(1,1)} & \text{if } m=4 \end{cases}$$

where $c_j^{(1,1)}$ are the coefficients of

$$\frac{\zeta'(s)^3}{\zeta(s)}\frac{1}{s} = \frac{c_0^{(1,1)}}{(s-1)^5} + \frac{c_1^{(1,1)}}{(s-1)^4} + \frac{c_2^{(1,1)}}{(s-1)^3} + \frac{c_3^{(1,1)}}{(s-1)^2} + \frac{c_4^{(1,1)}}{(s-1)} + \dots$$

and where

$$C_2^{(1,1)}(m,1) = \begin{cases} d_0^{(1,1)} - d_1^{(1,1)} + d_2^{(1,1)} - d_3^{(1,1)} & \text{if } m=0 \\ -d_0^{(1,1)} + d_1^{(1,1)} - d_2^{(1,1)} + d_3^{(1,1)} & \text{if } m=1 \\ \frac{1}{2}d_0^{(1,1)} - \frac{1}{2}d_1^{(1,1)} + d_2^{(1,1)} & \text{if } m=2 \\ -\frac{1}{6}d_0^{(1,1)} + \frac{1}{2}d_1^{(1,1)} & \text{if } m=3 \\ \frac{1}{6}d_0^{(1,1)} & \text{if } m=4 \end{cases}$$

where $d_j^{(1,1)}$ are the coefficients of

$$\frac{\zeta'(s)^2}{s} = \frac{d_0^{(1,1)}}{(s-1)^4} + \frac{d_1^{(1,1)}}{(s-1)^3} + \frac{d_2^{(1,1)}}{(s-1)^2} + \frac{d_3^{(1,1)}}{(s-1)} + \dots$$

which we note are the same as $c_j^{(1,0)}$ in this special case.

Evaluating the Laurent coefficients $c_j^{(1,k)}$ and $d_j^{(1,k)}$ and inserting them into $C_1(m,k)$ and $C_2(m,k)$ yields (3.4). □

Proof of Corollary 19. By explicitly evaluating the highest-order term in the polynomial in Theorem 16 we can recover the leading order coefficient, first found by Gonek.

By Theorem 16 we have that the leading order is given by taking the $m = \mu+\nu+2$ term in (3.6), that is,

$$(-1)^{\nu}\sum_{k=0}^{\nu}\binom{\nu}{k}C_1^{(\mu,\nu)}(\mu+\nu+2,k)$$
$$+(-1)^{\mu}\sum_{k=0}^{\mu}\binom{\mu}{k}\left(C_1^{(\nu,\mu)}(\mu+\nu+2,k)+C_2^{(\mu,\nu)}(\mu+\nu+2,k)\right). \quad (3.33)$$

At the very top power , the sum over j pieces in C_1, C_2 are empty and so only the first terms remain,

$$C_1^{(\mu,\nu)}(\mu+\nu+2,k) = \frac{c_0^{(\mu,k)}}{(k+\mu+2)!} = \frac{(-1)^{\mu+k+1}\mu!k!}{(k+\mu+2)!}$$
$$C_1^{(\nu,\mu)}(\mu+\nu+2,k) = \frac{c_0^{(\nu,k)}}{(k+\nu+2)!} = \frac{(-1)^{\nu+k+1}\nu!k!}{(k+\nu+2)!}$$
$$C_2^{(\mu,\nu)}(\mu+\nu+2,k) = \frac{d_0^{(\nu,k)}}{(k+\nu+1)!} = \frac{(-1)^{\nu+k}\nu!k!}{(k+\nu+1)!}.$$

Substituting these values into (3.33) gives

$$(-1)^{\nu}\sum_{k=0}^{\nu}\binom{\nu}{k}\frac{(-1)^{\mu+k+1}\mu!k!}{(k+\mu+2)!}+(-1)^{\mu}\sum_{k=0}^{\mu}\binom{\mu}{k}\left(\frac{(-1)^{\nu+k+1}\nu!k!}{(k+\nu+2)!}+\frac{(-1)^{\nu+k}\nu!k!}{(k+\nu+1)!}\right)$$

and evaluating these sums completes the proof of Corollary 19. □

.1 THE SECOND DERIVATIVE

Employing Mathematica, we evaluated the full asymptotic polynomial for the second derivative. This demonstrates the complexity when writing the result out in full.

We have

$$\sum_{0<\gamma\leq T}\left|\zeta''\left(\frac{1}{2}+i\gamma\right)\right|^2 = \frac{T}{2\pi}\sum_{m=0}^{6}A_j\left(\log\frac{T}{2\pi}\right)^j$$

where the coefficients A_j are given in Table .1.

Similarly, we have

$$\sum_{0<\gamma\le T} \zeta'\left(\frac{1}{2}+i\gamma\right)\zeta''\left(\frac{1}{2}-i\gamma\right) = \frac{T}{2\pi}\sum_{m=0}^{5} B_j\left(\log\frac{T}{2\pi}\right)^j$$

where the coefficients B_j are given in Table .2.

.2 Graphical illustration

We illustrate the power of our result by plotting the graphs for $\mu=\nu=1$ in Figure .1 and $\mu=\nu=2$ in Figure .2, in each figure showing the full sum

$$\sum_{0<\gamma\le T}\left|\zeta^{(\nu)}\left(\frac{1}{2}+i\gamma\right)\right|^2,$$

the sum minus the leading order asymptotic term, and the sum minus the full asymptotic as given in Theorem 16. Even though we only plot this over the first 100,000 zeros, the graphs clearly demonstrate the power of the result.

Similarly in Figure .3 we plot the graph for $\mu=1$ and $\nu=2$. The true sum is not real, but the imaginary parts are very small compared to the real parts, and we show

$$\Im \sum_{0<\gamma\le T} \zeta'\left(\frac{1}{2}+i\gamma\right)\zeta''\left(\frac{1}{2}-i\gamma\right)$$

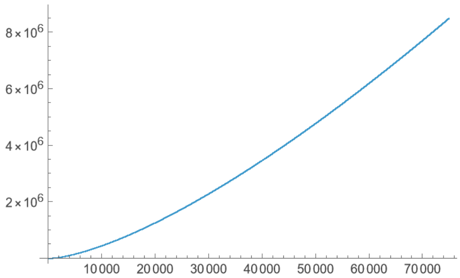
as well as the error coming from subtracting the full asymptotic from the real part of the sum.

A_6	$\frac{4}{45}$
A_5	$-\frac{8}{15}+\frac{11\gamma_0}{15}$
A_4	$\frac{8}{3}-\frac{11\gamma_0}{3}+\gamma_0^2-\frac{8\gamma_1}{3}$
A_3	$-\frac{32}{3}+\frac{44\gamma_0}{3}-4\gamma_0^2-\frac{8\gamma_0^3}{3}+\frac{32\gamma_1}{3}-12\gamma_0\gamma_1+\frac{2\gamma_2}{3}$
A_2	$32-44\gamma_0+12\gamma_0^2+8\gamma_0^3+4\gamma_0^4-32\gamma_1+36\gamma_0\gamma_1+24\gamma_0^2\gamma_1+24\gamma_1^2-2\gamma_2+16\gamma_0\gamma_2+\frac{8\gamma_3}{3}$
A_1	$-64+88\gamma_0-24\gamma_0^2-16\gamma_0^3-8\gamma_0^4+64\gamma_1-72\gamma_0\gamma_1-48\gamma_0^2\gamma_1-8\gamma_0^3\gamma_1-48\gamma_1^2-24\gamma_0\gamma_1^2+4\gamma_2-32\gamma_0\gamma_2-12\gamma_0^2\gamma_2-32\gamma_1\gamma_2-\frac{16\gamma_3}{3}-8\gamma_0\gamma_3-\frac{4\gamma_4}{3}$
A_0	$64-88\gamma_0+24\gamma_0^2+16\gamma_0^3+8\gamma_0^4-8\gamma_0^6-64\gamma_1+72\gamma_0\gamma_1+48\gamma_0^2\gamma_1+8\gamma_0^3\gamma_1-48\gamma_0^4\gamma_1+48\gamma_1^2+24\gamma_0\gamma_1^2-72\gamma_0^2\gamma_1^2-16\gamma_1^3-4\gamma_2+32\gamma_0\gamma_2+12\gamma_0^2\gamma_2-16\gamma_0^3\gamma_2+32\gamma_1\gamma_2-24\gamma_0\gamma_1\gamma_2+4\gamma_2^2+\frac{16\gamma_3}{3}+8\gamma_0\gamma_3+8\gamma_1\gamma_3+\frac{4\gamma_4}{3}+2\gamma_0\gamma_4+\frac{14\gamma_5}{15}$

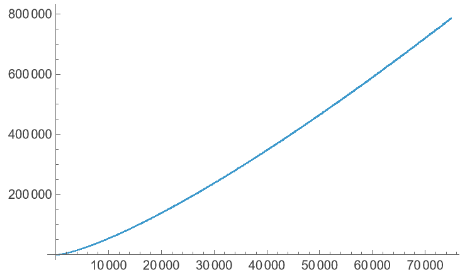
Table .1: The coefficients of the asymptotic degree-6 polynomial for the absolute value squared of the second derivative, $\left|\zeta''\left(\frac{1}{2}+i\gamma\right)\right|^2$.

B_5	$-\frac{1}{12}$
B_4	$\frac{5}{12}-\frac{2\gamma_0}{3}$
B_3	$-\frac{5}{3}+\frac{8\gamma_0}{3}-\gamma_0^2+2\gamma_1$
B_2	$5-8\gamma_0+3\gamma_0^2+2\gamma_0^3-6\gamma_1+10\gamma_0\gamma_1+\gamma_2$
B_1	$-10+16\gamma_0-6\gamma_0^2-4\gamma_0^3-2\gamma_0^4+12\gamma_1-20\gamma_0\gamma_1-12\gamma_0^2\gamma_1-14\gamma_1^2-2\gamma_2-8\gamma_0\gamma_2-\frac{10\gamma_3}{3}$
B_0	$10-16\gamma_0+6\gamma_0^2+4\gamma_0^3+2\gamma_0^4-12\gamma_1+20\gamma_0\gamma_1+12\gamma_0^2\gamma_1+14\gamma_1^2+2\gamma_2+8\gamma_0\gamma_2+\frac{10\gamma_3}{3}$

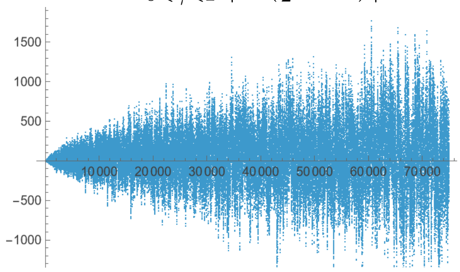
Table .2: The coefficients of the asymptotic degree-5 polynomial for the mixed first and second derivative, $\zeta'\left(\frac{1}{2}+i\gamma\right)\zeta''\left(\frac{1}{2}-i\gamma\right)$.



(a) $\sum_{0<\gamma<T} \left|\zeta'\left(\frac{1}{2}+i\gamma\right)\right|^2$

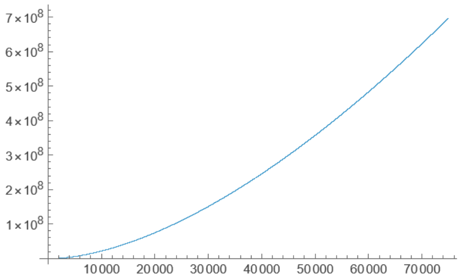


(b) $\sum_{0<\gamma<T} \left|\zeta'\left(\frac{1}{2}+i\gamma\right)\right|^2 - \frac{1}{24\pi}T\left(\log\frac{T}{2\pi}\right)^4$

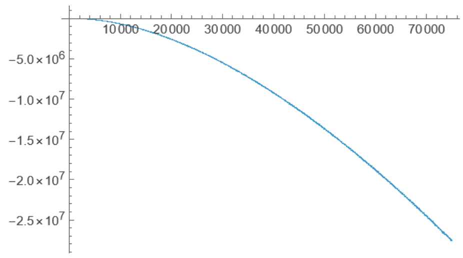


(c) $\sum_{0<\gamma<T} \left|\zeta'\left(\frac{1}{2}+i\gamma\right)\right|^2$ minus the full asymptotic given in (3.4).

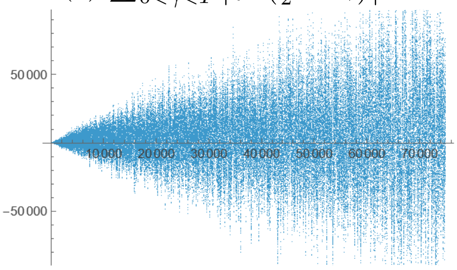
Figure .1: The first derivative



(a) $\sum_{0<\gamma<T} \left|\zeta''\left(\frac{1}{2}+i\gamma\right)\right|^2$

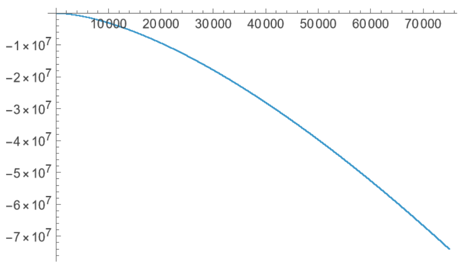


(b) $\sum_{0<\gamma<T} \left|\zeta''\left(\frac{1}{2}+i\gamma\right)\right|^2 - \frac{4}{90\pi}T\left(\log\frac{T}{2\pi}\right)^6$

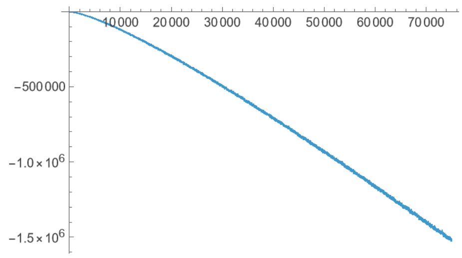


(c) $\sum_{0<\gamma<T} \left|\zeta''\left(\frac{1}{2}+i\gamma\right)\right|^2$ minus the full asymptotic given in Appendix .1

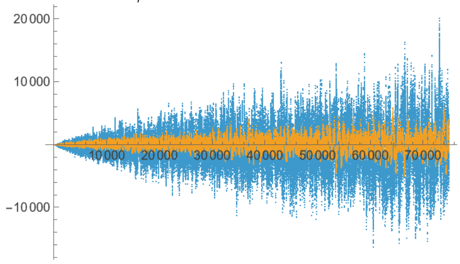
Figure .2: The second derivative



(a) $\Re \sum_{0<\gamma<T} \zeta'\left(\frac{1}{2}+i\gamma\right)\zeta''\left(\frac{1}{2}-i\gamma\right)$



(b) $\Re \sum_{0<\gamma<T} \zeta'\left(\frac{1}{2}+i\gamma\right)\zeta''\left(\frac{1}{2}-i\gamma\right) - \frac{1}{24\pi} T \left(\log \frac{T}{2\pi}\right)^5$



(c) $\Re \sum_{0<\gamma<T} \zeta'\left(\frac{1}{2}+i\gamma\right)\zeta''\left(\frac{1}{2}-i\gamma\right)$ minus the full asymptotic given in Appendix .1 (blue), and also $\Im \sum_{0<\gamma<T} \zeta'\left(\frac{1}{2}+i\gamma\right)\zeta''\left(\frac{1}{2}-i\gamma\right)$ (orange).

Figure .3: The mixed first and second derivatives

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