Discrete moments of the Riemann zeta function

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PhD

University of York
Mathematics

September 2024

Abstract

An important problem in number theory is to calculate the moments of the Riemann zeta function $\zeta(s)$. Moments have a wide range of applications, for example in calculating proportions of non-trivial zeros $\rho = \beta + i\gamma$ of $\zeta(s)$ that satisfy the Riemann Hypothesis, or that are simple.

Shanks [280] noticed that $\zeta'(\rho)$ is real and positive on average, a strange result when we consider that this is a complex-valued function summed over complex points. Later, it was noticed that this peculiar behaviour continued to higher derivatives, where the sum remains real on average, but oscillates positive and negative depending on whether the order of the derivative is odd or even.

Generalisations of this observation are considered throughout this thesis. These involve sums of the form

$$\sum_{0<t\leq T} \zeta^{(n_1)}\left(\frac{1}{2}+it\right)\dots\zeta^{(n_k)}\left(\frac{1}{2}+it\right),$$

where for integers $n_1, \dots, n_k$, t ranges over either the non-trivial zeros of zeta or the zeros of the derivative of the Hardy Z-function, and $\zeta^{(n)}$ denotes the n^{th} derivative of $\zeta(s)$.

After a comprehensive background on the zeta function, we begin with a simple heuristic for Shanks' observation and its generalisation, giving a clear reason for the oscillating behaviour before giving a rigorous proof of this fact with a full asymptotic expansion. A weighted first moment of this problem is then considered.

We build on the analogy between characteristic polynomials of random matrices and $\zeta(s)$, first noted by Keating and Snaith [211]. We present new conjectures for full asymptotic expansions of the above summation over the non-trivial zeros of $\zeta(s)$ after giving other supporting evidence for the leading order behaviour of these sums.

Finally we consider the above sum over the zeros λ of the derivative of the Hardy Z-function, and show that the behaviour of this sum oscillates in the opposite way to that over the non-trivial zeros, that is, $\zeta'(1/2+i\lambda)$ is real and negative on average.

Acknowledgments

This thesis has only been possible due to the hard work and support of many people.

It goes without saying that a supervisor should be super in many ways, all of which Chris Hughes has been. Your support, encouragement, patience, guidance, kindness, and friendship has never wavered, and I hope to be just 1% as enthusiastic about maths as you are. The sheer amount of time and energy you have invested in me won't go to waste. If I ever need a fun anecdote, I know where to go. Chris considered me a peer from the get-go and shows us all exactly what a supervisor should be.

Several other academics have had a strong influence on my PhD. Hung Bui has always been available for a discussion on maths and has taught me a great deal, much of which has influenced what has appeared in this thesis. It has been a pleasure to already work with you and see how you approach tackling a problem. I am fortunate to have met Nathan Ng while in Canada on a conference. He has been a constant supporter of mine, and I appreciate every discussion we have had, all of which have been productive. A huge thanks also goes to him for being my external examiner and for his close reading of this thesis. I must also give thanks to Jon Keating, who was the first contact I had with academics in this field outside of Chris, and for being so welcoming and generous with his advice. Discussions with Jon on maths and careers have already helped shape my future in the field. I look forward to working with you all in the future.

The other group of people to mention are those involved with the PIMS CRG for L-functions in Analytic Number Theory, particularly the four organisers. I have already mentioned the impact Nathan has had on my PhD, but thanks also goes to Habiba Kadiri, Greg Martin, and Alia Hamieh. They have helped in many ways, from career advice from Habiba, collaborating and publishing a paper with Greg, and the all around support from Alia, particularly in inviting me to Canada in the first place. I have been lucky that the CRG has overlapped with my PhD, and I have benefited massively from interacting with all parts of the CRG.

Many other academics deserve a mention by name, but at the risk of missing people off the list I have only mentioned a few. Thanks goes to everyone I have met and had any conversation or collaboration with, for your welcoming attitude, for your support, for the various invitations to give seminars and attend conferences, and for just being a good bunch of people in general.

The last academics who I want to mention are those based at the University of York, which has been my home for the last few years. Thanks to all those involved in the department, particularly Alet Roux for her encouragement with teaching, the Number Theory group who have been involved with all stages of my PhD, from interviewing me, inviting me to give talks, TAP support, and internal examining of this thesis, and to Sol Lugmayer for expanding my duo with Chris into a trio of people to talk maths with for the last couple of years.

A vast amount of support over these years has come from beyond the world of academia. To Mike, Esai, and Holly, thanks for your friendship, curry and pub visits, and for keeping me in touch with my old life as a teacher. Thanks also goes to Harry and the whole Hayes family, particularly Nick and Suz, for their love and support since I first met them. I look forward to putting a copy of this thesis in your hands and know I appreciate all you have done, treating me as part of the family over the years.

I finally come to the five people who deserve the biggest thanks of all. This thesis is dedicated entirely to you.

To Aza and Edward, thanks for being my siblings. That's all, really. Well, I suppose I should mention the non-stop dirty jokes and comments which would be weird to anyone else, and I look forward to all the others to come over the years ahead. Thanks especially to Aza for teaching me some of our best words in our second language, and to Edward for helping me with maths over the years.

There are no words to describe just how much I owe my parents, Donald and Amanda, for all they have done for me and my siblings. The endless support and love you pour into the three of us can never be repaid, and all I can say is thank you for all you have done and continue to do for us all. While you may not understand a word of my work, you always show an interest and provide the encouragement I need.

Lucy has been by my side since sending me a rose, and for some reason has agreed to move across the country with me for our next big adventure. I look forward to carrying on our evening routine of me summarising my day in under 30 seconds and in two words - I'm stuck! Somehow I spent just enough time being unstuck to put this thesis together over the years, and you played a huge role in this. Thank you for all of your love and support, and I can't wait to see where our future takes us.

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.

Section 1.3.8.2 on the background of joint moments in Chapter 1 can be found in [183], written jointly with Christopher Hughes and Solomon Lugmayer, titled *'The second moment of the Riemann zeta function at its local extrema'*.

Chapter 2 is based heavily on joint work with Christopher Hughes and Greg Martin [184], titled *'A heuristic for discrete mean values of the derivative of the Riemann zeta function'*, which has been published in the journal Integers.

Much of Chapter 3 can be found in a joint paper with Christopher Hughes [186], called *'A discrete mean-value theorem for the higher derivatives of the Riemann zeta function'*, and has appeared in the Journal of Number Theory.

Almost all of the content of Chapter 4 can be found in the paper [262], titled *'A further generalisation of sums of higher derivatives of the Riemann Zeta Function'*, which has been accepted for publication by the International Journal of Number Theory.

Chapter 5 is based heavily on joint work with Christopher Hughes [187], called *'Moments of derivatives of the Riemann zeta function: Characteristic polynomials and the hybrid formula'*, and has been submitted for publication.

Much of Chapter 6 will be in an upcoming paper [185], *'Moments of derivatives of the Riemann zeta function: the Ratios Conjecture'*, written jointly with Christopher Hughes.

Much of Chapter 7 will be found in [263] *'Moments of the Riemann zeta function at its local extrema'*.

Versions of unpublished and upcoming papers have been shared privately with other mathematicians and will all soon be submitted for publication. I was involved in, and contributed to the work and the write up in all of the above papers in an equal manner to any co-authors. Permission has been obtained to include the above in this thesis.

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Notation

We remind the reader of the main notational conventions used in this thesis.

We write $\Re(z)$ and $\Im(z)$ for the real and imaginary parts of a complex number z.

The Riemann zeta function is denoted $\zeta(s)$ for a complex number $s = \sigma + it$ and the n^{th} derivative of $\zeta(s)$ is denoted $\zeta^{(n)}(s)$. A non-trivial zero of $\zeta(s)$ is written as $\rho = \beta + i\gamma$.

We also adopt the ε-notation: each occurrence of ε represents a sufficiently small positive real number which may vary from occurrence to occurrence, potentially even in the same line. We also let δ be some small real number.

We will use the standard asymptotic notations concerning limits at infinity:

- $f(x) = O(g(x))$ as $x \to \infty$ if there exists a positive constant A such that
$$\limsup_{x\to\infty} \left|\frac{f(x)}{g(x)}\right| \le A.$$
- $f(x) = o(g(x))$ as $x \to \infty$ if
$$\lim_{x\to\infty} \left|\frac{f(x)}{g(x)}\right| = 0.$$
- $f(x) = \Omega(g(x))$ as $x \to \infty$ if there exists a positive constant B such that
$$\limsup_{x\to\infty} \left|\frac{f(x)}{g(x)}\right| \ge B.$$
- $f(x) \asymp g(x)$ as $x \to \infty$ if $f(x) = O(g(x))$ and $f(x) = \Omega(g(x))$.
- $f(x) \sim g(x)$ as $x \to \infty$ if
$$\lim_{x\to\infty} \frac{f(x)}{g(x)} = 1.$$
- $f(x) \ll g(x)$ as $x \to \infty$ if $f(x) = O(g(x))$.

Any product or summation with a subscript p denotes a product or summation over the prime numbers p, for example $\prod_p$.

For a real number c we write
$$\frac{1}{2\pi i}\int_{(c)} f(z)\ dz = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} f(z)\ dz.$$

The Prime Number Theorem is discussed at various points throughout this thesis. We write:

- $\pi(x)$ for the number of primes less than or equal to some real number x.
- $\mathrm{Li}(x)$ is the logarithmic integral, given by $\mathrm{Li}(x) = \int_2^x \frac{1}{\log t}\, dt$.
- $\pi(x; q, a)$ for the number of primes congruent to a mod q that are less than or equal to x.

The gamma function $\Gamma(z)$ is defined for all z by

$$\Gamma(z) = \int_0^\infty x^{z-1} e^{-x}\, dx$$

for $\Re(z) > 0$. The gamma function satisfies the functional equation

$$\Gamma(n+1) = n\Gamma(n), \text{ with } \Gamma(1) = 1.$$

The Barnes G-function $G(z)$ is defined for all z by

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

where γ_0 is Euler's constant. The Barnes G-function satisfies the functional equation

$$G(z+1) = \Gamma(z)G(z), \text{ with } G(1) = 1.$$

Arithmetic functions play a big part in this thesis. Let $n \in \mathbb{N}$. If $f, g : \mathbb{N} \to \mathbb{C}$ are two arithmetic functions, the Dirichlet convolution $f * g : \mathbb{N} \to \mathbb{C}$ is defined by

$$(f * g)(n) = \sum_{d|n} f(d) g\left(\frac{n}{d}\right) = \sum_{ab=n} f(a)g(b),$$

where the sum extends over all positive divisors d of n, or equivalently over all distinct pairs (a, b) of positive integers whose product is n. Dirichlet convolution appears naturally when we multiply Dirichlet series, as

$$\left(\sum_{n=1}^{\infty} \frac{f(n)}{n^s}\right)\left(\sum_{n=1}^{\infty} \frac{g(n)}{n^s}\right) = \left(\sum_{n=1}^{\infty} \frac{(f*g)(n)}{n^s}\right).$$

A wide range of arithmetic functions are used throughout this thesis. We have:

- The von Mangoldt function is given by

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

- The Euler totient function $\varphi(n)$ counts the positive integers up to a given integer n that are relatively prime to n.

- The Möbius function is defined by

$$\mu(n) = \begin{cases} 1 & \text{if } n = 1 \\ (-1)^k & \text{if } n = p_1 ... p_k \text{ with the } p_j \text{ distinct} \\ 0 & \text{if } n \text{ is not square-free.} \end{cases}$$

For k a positive integer,

- $\mu_k(n)$ denotes the n^{th} coefficient of the Dirichlet series for $\zeta(s)^{-k}$.
- $d_k(n)$ denotes the n^{th} coefficient of the Dirichlet series for $\zeta(s)^k$.
- $\Lambda_k(n)$ denotes the n^{th} coefficient of the Dirichlet series for $(-1)^k(\zeta'(s)/\zeta(s))^k$.

By our previous comments on Dirichlet convolution, we can describe each of μ_k, d_k and Λ_k via convolutions. For example, we can write

$$\Lambda_k = \underbrace{\Lambda * \Lambda * \Lambda * \cdots * \Lambda}_{k-1 \text{ convolutions}}$$

with the convention that $\Lambda_0(m)$ takes the value 1 if $m = 1$ and 0 otherwise, and where $\Lambda_1(m) = \Lambda(m)$ is the usual von Mangoldt function.

The classical compact groups $U(N), SO(2N), Sp(2N)$ are used in this thesis with their definitions given in Section 1.2.1. The $N \times N$ identity matrix is written as I_N. The characteristic polynomial of an $N \times N$ matrix A from $\{U(N), SO(2N), Sp(2N)\}$ is

$$Z_{N,A}(\theta) = \det(I - Ae^{-i\theta}).$$

Preface

We give an overview of the work presented in this thesis. We consider the problem of moments of derivatives of the Riemann zeta function, and variations thereof. In particular, we will study moments of the form

$$\sum_{0<\gamma\leq T} \zeta^{(n)}(\rho)^k$$

as $T \to \infty$, for integer k, n, where $\zeta^{(n)}(s)$ denotes the n^{th} derivative of the Riemann zeta function $\zeta(s)$ and where $\rho = \beta + i\gamma$ denotes a non-trivial zero of the Riemann zeta function. More generally, we consider moments of mixed derivatives of the form

$$\sum_{0<\gamma\leq T} \zeta^{(n_1)}(\rho) \ldots \zeta^{(n_k)}(\rho)$$

as $T \to \infty$, for integer $n_1, \ldots n_k$. We will also extend this problem to studying moments of derivatives of the Riemann zeta function over different points, as seen in Chapter 7.

Chapter 1

Chapter 1 serves as a comprehensive introduction to the field. Many topics are considered including, but not limited to, the Prime Number Theorem, the Riemann Hypothesis, continuous and discrete moments of the Riemann zeta function, random matrix theory (RMT), and applications of moments.

Chapter 2

In Chapter 2, we look at the history of the first moment of the derivatives of the Riemann zeta function, a problem known as (the Generalised) Shanks' Conjecture. This is an example of the moments problem above with $k = 1$ and n a positive integer. This conjecture, now a theorem, states that on average,

$$\zeta^{(n)}(\rho) \text{ is positive if } n \text{ is odd, and negative if } n \text{ is even in the mean.}$$

We develop a heuristic which is used to non-rigorously prove the leading order behaviour of such moments. The heuristic relies on the Landau–Gonek Theorem, found in [144], which is an explicit formula (one that relates zeta zeros to the prime numbers). This heuristic, that is very basic and easy to use, derives the alternating plus/minus behaviour depending on whether the order of the derivative is odd/even, and even re-derives the correct order of magnitude to leading order. We also consider the question of the first negative moment of the first derivative of the Riemann zeta function.

Chapter 3

Chapter 3 involves the first original rigorous proof in this thesis. We consider the Generalised Shanks' Conjecture and derive a full asymptotic result with lower order terms, and (under the Riemann Hypothesis) a power-saving error term, although the Riemann Hypothesis isn't needed anywhere else in the proof. The result can be stated in the following form.

Theorem. *Let $\rho = \beta + i\gamma$ denote a non-trivial zero of the Riemann zeta function. Then*

$$\sum_{0<\gamma\leq T} \zeta^{(n)}(\rho) = (-1)^{n+1}\frac{1}{n+1}\frac{T}{2\pi}\left(\log\frac{T}{2\pi}\right)^{n+1} + \frac{T}{2\pi}\mathcal{P}_n\left(\log\frac{T}{2\pi}\right) + E_n(T)$$

where $\mathcal{P}_n(x)$ is an explicit polynomial in x of degree n, given in Theorem 3.1, and $E_n(T)$ is given by

$$E_n(T) = O\left(T\mathrm{e}^{-C\sqrt{\log T}}\right)$$

with C is a positive constant. If we assume the Riemann hypothesis, then

$$E_n(T) = O\left(T^{1/2}(\log T)^{n+9/4}\right).$$

This conditional error term improves upon what was previously known due to Fujii in the first derivative case, and the one given in this thesis improves upon the published result that this chapter is based on.

Next, we employ a shifted sum over the non-trivial zeros of the Riemann zeta function of $\zeta(\rho+\alpha)$, where α is a small shift. This shifted sum follows from a result of Fujii's [126]. Using this result, we give an equivalent form of the main result in this chapter.

Theorem. *For $\rho = \beta + i\gamma$ a non-trivial zero of $\zeta(s)$, and where $\zeta^{(n)}(s)$ is the n^{th} derivative of $\zeta(s)$, we have for T sufficiently large,*

$$\begin{aligned}\sum_{0<\gamma\leq T} \zeta^{(n)}(\rho) = n!\sum_{\ell=0}^{n+1}&\frac{(-1)^{n-\ell+1}}{(n-\ell+1)!}\frac{T}{2\pi}\left(\log\frac{T}{2\pi}\right)^{n-\ell+1}\\ &+ n!\sum_{m=0}^{n}\sum_{\ell=0}^{n-m}\frac{(-1)^{n-m-\ell+1}\gamma_m}{(n-m-\ell)!m!}\frac{T}{2\pi}\left(\log\frac{T}{2\pi}\right)^{n-m-\ell}\\ &+ n!A_n\frac{T}{2\pi} + O\left(Te^{-C\sqrt{\log T}}\right),\end{aligned}$$

where the coefficients γ_j *and* A_n *are from the Laurent expansions of* $\zeta(s)$ *and* $\zeta'(s)/\zeta(s)$ *about* $s = 1$, *respectively.*

We end the chapter by briefly discussing the question of the Generalised Shanks' Conjecture over short intervals. That is, we previously sum over the imaginary part of the non-trivial zeros between 0 and T, but we could consider the analogous problem between T and $T + H$, where $T^{1/2+\varepsilon} \ll H \ll T$. This result to leading order is as expected, that is, we can show the following result in an analogous way to the proof of Theorem 3.1.

Theorem. *For* $T^{1/2+\varepsilon} \ll H \ll T$,

$$\sum_{T<\gamma\leq T+H} \zeta^{(n)}(\rho) = (-1)^{n+1}\frac{1}{n+1}\frac{H}{2\pi}(\log T)^{n+1} + O\left(H(\log T)^n\right) + O\left(T^{1/2+\varepsilon}\right).$$

Chapter 4

In Chapter 4, we combine the Landau's Theorem (a non-uniform version of the Landau–Gonek Theorem) with the Generalised Shanks' Conjecture. Specifically, we generalise a result of Fujii's to all derivatives.

Theorem. *For a fixed positive real number* X,

$$\begin{aligned}\sum_{0<\gamma\leq T} \zeta^{(n)}(\rho)X^{\rho} = \\ (-1)^n \Bigg\{ \Delta(X)\frac{T}{2\pi}\left((\log X)^n\left(\frac{1}{2}\log\frac{T}{2\pi} - \frac{1}{2} + \frac{\pi i}{4}\right) - \sum_{mr=X}\Lambda(r)(\log m)^n\right) \\ + X(\log X)^n\left(\frac{1}{2}\log X - \frac{\pi i}{4}\right)\sum_{m\leq\frac{T}{2\pi X}} e^{2\pi i m X} + \frac{X}{2}(\log X)^n \sum_{m\leq\frac{T}{2\pi X}} e^{2\pi i m X}\log m \\ - X\sum_{mr\leq\frac{T}{2\pi X}} e^{2\pi i m r X}\Lambda(r)(\log rX)^n\Bigg\} + E_n(T),\end{aligned}$$

where $\Delta(X)$ *equals* 1 *if* X *is a positive integer and* 0 *otherwise and* $E_n(T)$ *is the error term given in Theorem 3.1.*

When X is a fixed positive integer, this result can be rewritten in a different way. This different way is of interest as the Landau–Gonek Theorem appears quite different (although to the same leading order) depending on whether the term X is a positive integer or a positive real number. This new asymptotic that we derive shows a clear distinction between the behaviour of such sums depending on whether the X is a generic positive real number, or specifically, a positive integer.

Corollary.

$$\sum_{0<\gamma\le T}\zeta^{(n)}(\rho)X^{\rho}=$$

$$(-1)^{n+1}\frac{T}{2\pi}(\log X)^{n}\Bigg\{\sum_{k=0}^{n}\sum_{u=0}^{k+1}\binom{n}{k}\binom{k+1}{u}(-1)^{u}\frac{1}{k+1}\left(\log\frac{T}{2\pi}\right)^{k+1-u}(\log X)^{u-k}$$
$$+\sum_{k=0}^{n}\sum_{l=0}^{k}\sum_{u=0}^{k-l}\binom{n}{k}\binom{k}{l}\binom{k-l}{u}(-1)^{l}l!\left(-1+\sum_{j=0}^{l}\frac{1}{j!}\gamma_j\right)\left(\log\frac{T}{2\pi}\right)^{k-l-u}(\log X)^{u-k}$$
$$+\sum_{k=0}^{n}\binom{n}{k}(-1)^{k+1}k!A_k(\log X)^{-k}-\left(\log\frac{T}{2\pi}-1-\sum_{mr=X}\Lambda(r)(\log m)^{n}\right)\Bigg\}+E_n(T)$$

with the error term $E_n(T)$ as given in Theorem 3.1 and where the coefficients γ_j and A_n are from the Laurent expansions of $\zeta(s)$ and $\zeta'(s)/\zeta(s)$ about $s=1$, respectively.

Chapter 5

We consider higher moments of the derivatives of the Riemann zeta function in Chapter 5. We begin by considering an approach using characteristic polynomials of random unitary matrices, which involves proving rigorously a RMT result, and use it to conjecture a result on the Riemann zeta function. We also consider a hybrid approach to conjecture what the arithmetic term should be in these conjectures.

Conjecture. *Assume the Riemann Hypothesis. For fixed, positive integers $n_1,\ldots,n_k$, the moments of mixed derivatives of $\zeta(s)$, evaluated at the non-trivial zeros of $\zeta(s)$, are given by*

$$\frac{1}{N(T)}\sum_{0<\gamma\le T}\zeta^{(n_1)}\left(\frac{1}{2}+i\gamma\right)\ldots\zeta^{(n_k)}\left(\frac{1}{2}+i\gamma\right)$$
$$\sim(-1)^{n_1+\ldots+n_k+k}\frac{n_1!\ldots n_k!}{(n_1+\ldots+n_k+1)!}\left(\log\frac{T}{2\pi}\right)^{n_1+\ldots+n_k}$$

as $T\to\infty$, where $N(T)$ is the number of non-trivial zeros of $\zeta(s)$ in the critical strip above the real axis up to height T.

A simple corollary is when all the derivatives are equal to each other.

Conjecture. *Assume the Riemann Hypothesis. For $n,k\in\mathbb{N}$, the k^{th} moment of the n^{th} derivative of $\zeta(s)$ is given by*

$$\frac{1}{N(T)}\sum_{0<\gamma\le T}\zeta^{(n)}\left(\frac{1}{2}+i\gamma\right)^{k}\sim(-1)^{k(n+1)}\frac{(n!)^{k}}{(kn+1)!}\left(\log\frac{T}{2\pi}\right)^{kn}$$

as $T\to\infty$.

Using the hybrid model approach, we are able to extend this conjecture beyond integer k to a conjecture over complex k.

Conjecture. *Assume the Riemann Hypothesis. For complex k with $\Re(k) > -3$,*

$$\frac{1}{N(T)} \sum_{0<\gamma\leq T} \zeta'\left(\frac{1}{2}+i\gamma\right)^k \sim \frac{1}{\Gamma(k+2)}\left(\log\frac{T}{2\pi}\right)^k$$

as $T\to\infty$.

This last conjecture suggests some further conjectures for the negative moments, and we find that in the case $k=-1$, they agree with what was previously known, specifically Theorem 2.3. Conjectures for the negative moments in the cases where $k=-2,-3$ are also considered. The chapter ends with a discussion on a certain recurrence relation.

Chapter 6

In Chapter 6 we consider the problem of finding the lower order terms of these asymptotic conjectures via the Ratios Conjecture. A comprehensive overview on the background of the Ratios Conjecture is given, with specific focus given to known applications of the Ratios Conjecture. We have found a new application of the Ratios Conjecture, and describe how to give a full asymptotic expansion for the moments of mixed derivatives of $\zeta(s)$, evaluated at the non-trivial zeros of $\zeta(s)$, first considered in Chapter 5.

Conjecture. *Assume the Riemann Hypothesis. Let α_j be small complex numbers. Assume that $|\Re(\alpha_j)| < \frac{1}{4}$ and $|\Im(\alpha_j)| \ll_\varepsilon T^{1-\varepsilon}$ for every $\varepsilon>0$. For $|\delta|<1/4$, let*

$$A_{\{\alpha_1,\dots,\alpha_k\}}(\delta) := \prod_p \frac{1+F_1(p,\delta)+F_2(p,\delta)+\cdots+F_k(p,\delta)}{(1-p^{-(1+\alpha_1)})\dots(1-p^{-(1+\alpha_k)})}$$

where for $1\leq m\leq k$

$$F_m(p,\delta) = (-1)^m \sum_{\substack{J\subset\{1,\dots,k\}\\ |J|=m}} p^{-\left(m+(m-1)\delta+\sum_{j\in J}\alpha_j\right)}.$$

The discrete moments of shifts of $\zeta(s)$, evaluated at the non-trivial zeros $\rho = 1/2+i\gamma$ of the Riemann zeta function, are given by

$$\sum_{0<\gamma\leq T} \zeta\left(\frac{1}{2}+i\gamma+\alpha_1\right)\dots\zeta\left(\frac{1}{2}+i\gamma+\alpha_k\right)$$
$$= \frac{1}{2\pi}\int_1^T \left(A'_{\{\alpha_1,\dots,\alpha_k\}}(0) + \sum_{j=1}^k W_{\{\alpha_1,\dots,\alpha_k\}\setminus\{\alpha_j\}}(\alpha_j,t)\right)\, dt + O(T^{1/2+\varepsilon}),$$

where

$$W_{\{\alpha_1,\ldots,\alpha_k\}\backslash\{\alpha_j\}}(\alpha_j,t) = \frac{\zeta'(1+\alpha_j)}{\zeta(1+\alpha_j)} - \left(\frac{t}{2\pi}\right)^{-\alpha_j} \zeta(1-\alpha_j) A_{\{\alpha_1,\ldots\alpha_{j-1},0,\alpha_{j+1},\ldots,\alpha_k\}}(-\alpha_j) \prod_{\substack{\ell=1\\ \ell\neq j}}^{k} \frac{\zeta(1+\alpha_\ell-\alpha_j)}{\zeta(1+\alpha_\ell)}.$$

This approach allows us to re-derive the Generalised Shanks' Conjecture asymptotic in an integral form, showing a third way of writing this result in this thesis.

Theorem. *Assume the Riemann Hypothesis. For n a positive integer, $L = \log \frac{t}{2\pi}$, we have*

$$\sum_{0<\gamma\leq T} \zeta^{(n)}\left(\frac{1}{2}+i\gamma\right) = \frac{n!}{2\pi}\int_1^T \left(A_n + \frac{(-1)^{n+1}L^{n+1}}{(n+1)!} + \sum_{m=0}^{n} \frac{(-1)^{m+1}L^m\gamma_{n-m}}{m!(n-m)!}\right) dt + O\left(T^{1/2+\varepsilon}\right),$$

where the coefficients γ_j and A_n are from the Laurent expansions of $\zeta(s)$ and $\zeta'(s)/\zeta(s)$ about $s=1$, respectively.

Additionally, we can now conjecture full asymptotic results for previously unknown moments, such as the second moment for the first derivative of the Riemann zeta function. We explain how to derive this conjecture, and give some numerical proof that we have both captured the full asymptotic, and that the error term is of a reasonable size.

Conjecture. *Assume the Riemann Hypothesis. For $L = \log\frac{t}{2\pi}$ and $\rho = 1/2+i\gamma$ a non-trivial zero of the Riemann zeta function,*

$$\begin{aligned}\sum_{0<\gamma\leq T} \zeta'\left(\frac{1}{2}+i\gamma\right)^2 = \\ \frac{1}{2\pi}\int_1^T \Bigg(\frac{1}{6}L^3 + \frac{1}{2}L^2\left(2\gamma_0 + A^{(0,0,1)}\right) + \frac{1}{2}L\left(-8\gamma_1 + 4\gamma_0 A^{(0,0,1)} + A^{(0,0,2)} + 2A^{(0,1,1)}\right) \\ + \frac{1}{6}\Big(-12\gamma_0^3 - 36\gamma_0\gamma_1 + 6\gamma_2 - 24\gamma_1 A^{(0,0,1)} + 6\gamma_0 A^{(0,0,2)} + A^{(0,0,3)} \\ +12\gamma_0 A^{(0,1,1)} + 3A^{(0,1,2)} - 3A^{(0,2,1)} + 6A^{(1,1,1)}\Big) + O\left(T^{1/2+\varepsilon}\right) dt\end{aligned}$$

where the γ_m are the coefficients in the Laurent expansion of $\zeta(s)$ about $s=1$ and the $A^{(i,j,k)}$ are arithmetic terms that are various products and sums over primes.

Chapter 7

Chapter 7 involves a different generalisation of the Generalised Shanks' Conjecture. Specifically, rather than summing the derivatives of the Riemann zeta function over the non-trivial zeros of the Riemann zeta function, we instead sum the derivatives of the Riemann zeta function over the local maxima of $|\zeta(s)|$. These local maxima can be written in terms of the local maxima of the Hardy Z-function $Z(t)$. These maxima occur at the (under the Riemann Hypothesis) unique points λ such that $Z'(\lambda) = 0$. This has a natural analogy to a result of Conrey and Ghosh [66].

Theorem. *Assume the Riemann Hypothesis. Write $L = \log T/2\pi$. For λ defined by $Z'(\lambda) = 0$ and $K, n \geq 1$ positive integers, we have*

$$\sum_{0<\lambda\leq T} \zeta^{(n)}\left(\frac{1}{2} + i\lambda\right) = a_{n+1}\frac{T}{2\pi}L^{n+1} + \frac{T}{2\pi}\sum_{\ell=0}^{n} a_{n-\ell}L^{n-\ell} + \frac{T}{2\pi}\sum_{m=1}^{K}\frac{b_m}{L^m} + O\left(\frac{T}{L^{K+1}}\right),$$

as $T \to \infty$ where we give the coefficients a_m, b_m in the statement in Chapter 7.

Recall that for the Generalised Shanks' Conjecture, the average of $\zeta^{(n)}(s)$, summed over the non-trivial zeros of $\zeta(s)$, clearly alternates between positive and negative as n increases. In the case of this theorem, the behaviour is reversed; the average of $\zeta^{(n)}(s)$, summed over the maxima of $|\zeta(s)|$, alternates between negative and positive as n increases. In particular, $\zeta'(1/2 + i\lambda)$ is negative and real in the mean. We also consider the sum of $\zeta(s)$ over these maxima (as it isn't trivially zero here, unlike the case when we sum over the non-trivial zeros of zeta).

Additionally, we sum the $\chi(s)$ factor from the functional equation for $\zeta(s)$ given in (1.1) over both the non-trivial zeros of the Riemann zeta function, and over the local maxima of $|\zeta(s)|$. As with the derivatives of the zeta function, the behaviour is reversed for the $\chi(s)$ factor, whether summed over the non-trivial zeros of zeta (in which case it is negative on average) or the zeros of the derivative of the Hardy Z-function (in which case it is positive on average).

Theorem. *Assume the Riemann Hypothesis. Write $L = \log T/2\pi$. For λ defined by $Z'(\lambda) = 0$ and $K \geq 1$ a positive integer, we have*

$$\sum_{0<\lambda\leq T} \chi\left(\frac{1}{2} + i\lambda\right) = (e^2 - 2)\frac{T}{2\pi} - 4e^2\gamma_0\frac{T}{2\pi}\frac{1}{L} + \frac{T}{2\pi}\sum_{m=2}^{K}\frac{e_m}{L^m} + O_K\left(\frac{T}{L^{K+1}}\right)$$

as $T \to \infty$ where we give the coefficients e_m in the statement in Chapter 7.

In the results where we are comparing the derivatives of the zeta function or the factor $\chi(s)$, the leading order term is of the same order of magnitude, whether we are summing over the non-trivial zeros of the Riemann zeta function, or over the maxima of $|\zeta(s)|$.

— 1 —

Introduction

1.1 THE PRIME NUMBER THEOREM

1.1.1 Historical Background

Mankind has been interested in prime numbers since antiquity, dating back at least to Euclid and his Elements [111]. In Book VII, he defines prime numbers and in Book IX he proves both that there are infinitely many primes, and the Fundamental Theorem of Arithmetic, that every natural number can be factored uniquely as a product of primes.

Since then, mathematicians have wanted to understand everything there is to know about the primes. One question in particular that was of central interest to 18$^{\text{th}}$ and 19$^{\text{th}}$ century mathematicians was the distribution of the prime numbers, a result we now know as the Prime Number Theorem. This result states

$$\pi(x) \sim \frac{x}{\log x}$$

as $x \to \infty$, where $\pi(x)$ denotes the number of primes less than or equal to some real number x.

The Prime Number Theorem was first conjectured by Legendre [221] (up to some erroneous constants), and by Gauss [137], who at the age of 15 would calculate the number of primes in a chiliad (a group of one thousand numbers) whenever he had some spare time. He noted that the primes obey an inverse logarithm law. Gauss restated this conjecture in a different way, writing

$$\pi(x) \sim \mathrm{Li}(x)$$

as $x \to \infty$, where $\mathrm{Li}(x)$ is the logarithmic integral, given by $\mathrm{Li}(x) = \int_2^x \frac{1}{\log t}\, dt$.

This second form is numerically more accurate to the true value of $\pi(x)$. These two forms of the Prime Number Theorem are equivalent as it can be shown that for a positive integer N,

$$\mathrm{Li}(x) = \frac{x}{\log x}\sum_{k=0}^{N}\frac{k!}{(\log x)^k} + O\left(\frac{x}{(\log x)^{N+2}}\right).$$

Among the many celebrated mathematicians who attempted to prove the Prime Number Theorem, it is probably fair to say that Chebyshev [51] came closest before its eventual proof in 1896. He was able to show that if the limit

$$\lim_{x\to\infty}\pi(x)\Big/\frac{x}{\log x}$$

exists, then the limit has to equal 1. Despite not obtaining the full proof of the Prime Number Theorem, he was able to prove Bertrand's Postulate [24], that there exists a prime number between n and $2n$ for any natural number $n \geq 2$.

Despite mathematician's best efforts, a new idea was needed. Enter Georg Friedrich Bernhard Riemann in 1859 and his eponymous function.

1.1.2 The Riemann Zeta Function

Upon his election as a corresponding member to the Berlin Academy in 1859, Riemann presented his seminal (and only) number theoretical paper, 'On the Number of Prime Numbers less than a Given Quantity' [271]. In this paper, Riemann introduces the zeta function that now bears his name.

The Riemann zeta function was originally studied by Euler in relation to solving the Basel problem concerning the infinite sum of inverse squares. Riemann's insight was to consider this function for a complex variable s rather than a real variable s. Riemann defines his zeta function as the Dirichlet series

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

which converges for all complex s with $\Re(s) > 1$.

This Dirichlet series has an Euler product representation, that is, a product over prime numbers given by

$$\zeta(s) = \prod_p \left(1 - \frac{1}{p^s}\right)^{-1}$$

which converges for all complex s with $\Re(s) > 1$, where we write $\prod_p$ to mean a product over all prime numbers p.

Equality between these two ways of writing $\zeta(s)$ is equivalent to the Fundamental Theorem of Arithmetic, and provides a new way to prove that there are infinitely many prime numbers. This second fact follows by letting $s \to 1^+$, and noting that the Dirichlet series representation becomes the harmonic series which we know diverges, and the Euler product representation could only tend to infinity if there were infinitely many terms in the product being multiplied together, which can only happen if there are infinitely many primes.

This connection between the natural numbers and prime numbers underlines the importance of the Riemann zeta function and motivates our study of it. Riemann wrote his paper with the aim to prove the Prime Number Theorem, and introduced many of the fundamental features and properties that we use today.

We will return to the Prime Number Theorem and a sketch of its proof in Section 1.1.4. We now look at the rest of the context of Riemann's paper and consider the results within as these will guide us, as they did Hadamard and de la Vallée Poussin, to the traditional proof of the Prime Number Theorem.

Firstly, Riemann established the meromorphic continuation of $\zeta(s)$ to the whole complex plane, except for a simple pole at $s = 1$ with residue 1. He did this by establishing a functional equation for $\zeta(s)$, an equation that relates the value of zeta at s to that at $1 - s$. He gives two proofs of the functional equation, both of which we write in modern notation. We will sketch one way that Riemann proved the functional equation, and highlight some consequences of the second.

The sketch proof involves the modular form (a complex analytic function on the upper half-plane satisfying certain conditions) called the Jacobi theta function, defined by

$$\theta(x) = \sum_{n=-\infty}^{\infty} e^{-n^2\pi x}.$$

First we note that

$$\zeta(s)\Gamma\left(\frac{s}{2}\right)\pi^{-s/2} = \int_0^\infty x^{s/2-1}\psi(x)\ ds$$

where

$$\psi(x) = \sum_{n=1}^{\infty} e^{-n^2\pi x}$$

and where throughout this thesis $\Gamma(s)$ is the gamma function defined by

$$\Gamma(s) = \int_0^\infty x^{s-1}e^{-x}\ dx$$

for $\Re(s) > 0$. The gamma function satisfies the functional equation

$$\Gamma(n+1) = n\Gamma(n), \text{ with } \Gamma(1) = 1.$$

Clearly

$$\psi(x) = \frac{\theta(x) - 1}{2}$$

and by Poisson summation we may show that $\theta(x)$ satisfies the functional equation

$$\theta(x) = \frac{1}{\sqrt{x}}\theta\left(\frac{1}{x}\right).$$

Using these facts we can show

$$\zeta(s)\Gamma\left(\frac{s}{2}\right)\pi^{-s/2} = \frac{1}{s(s-1)} + \int_1^\infty \left(x^{-s/2-1/2} + x^{s/2-1}\right)\psi(x)\ ds.$$

This integral converges for all s due to the rapid decay of $\psi(x)$, and so the meromorphic continuation follows. Since the integral is unchanged if s is replaced by $1-s$, we have established the formula

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

which is the functional equation for $\zeta(s)$. This is often written as

$$\zeta(s) = \chi(s)\zeta(1-s) \tag{1.1}$$

where

$$\begin{aligned}\chi(s) &= \pi^{s-1/2}\frac{\Gamma(1/2-s/2)}{\Gamma(s/2)} \\ &= 2^s\pi^{s-1}\sin\left(\frac{\pi s}{2}\right)\Gamma(1-s). \qquad (1.2)\end{aligned}$$

Riemann's second proof involves manipulating the integral

$$\zeta(s) = e^{-i\pi s}\Gamma(1-s)\frac{1}{2\pi i}\int_C \frac{x^{s-1}}{e^x-1}\ dx,$$

where C is a certain keyhole contour. Using this representation, it can be shown that for all natural numbers

$$\zeta(-n) = (-1)^n\frac{B_{n+1}}{n+1} \tag{1.3}$$

where the B_n are the Bernoulli numbers, given by the coefficients in the Taylor series

$$\frac{z}{e^z-1} = \sum_{j=0}^{\infty} B_j\frac{z^j}{j!}$$

for $|z| < 2\pi$.

Setting $n = -1+2k$ for integer k in equation (1.3), we may show using the functional equation (1.1) that

$$\zeta(2k) = \frac{(-1)^{k+1}(2\pi)^{2k}B_{2k}}{2(2k)!}.$$

In particular, setting $k = 1$ recovers Euler's solution to the Basel problem, that is, that $\zeta(2) = \pi^2/6$. Many other proofs have followed Euler's original solution. Note that since integer powers of π are transcendental (and so irrational), so is $\zeta(2k)$ for all positive integers k. However, the problem of showing that $\zeta(2k+1)$ is irrational for all positive integers k is still open in general. A special case is due to Apéry, who showed $\zeta(3)$ is irrational [4]. It is still unknown if it is transcendental. There is also no known closed form for $\zeta(3)$ in terms of π.

1.1.3 Zeta Zeros and the Riemann Hypothesis

We subscribe to the philosophy that if we want to understand a complex function, we need to understand its zeros. We now describe the locations of these zeros.

First note that there are no zeros in the plane $\Re(s) > 1$. To see this, note that we have the Euler product representation of $\zeta(s)$ in this region. Since a convergent infinite product of non-zero factors is not zero, we deduce that $\zeta(s)$ is non-zero here.

By the functional equation, $\zeta(s)$ is also non-zero for $\Re(s) < 0$ except where $\chi(s) = 0$. We see that this occurs at the negative even integers, either by (1.2) and noting that this is zero when the sine term is zero, or by (1.3) and noting that the odd Bernoulli numbers are zero for $n \geq 3$. We call these zeros the trivial zeros of $\zeta(s)$.

The only possible location of the zeros are in the region $0 \leq \Re(s) \leq 1$, the critical strip. As we will show in Section 1.1.4, there are no zeros with $\Re(s) = 1$, and so by the functional equation there are none with $\Re(s) = 0$, leaving the region $0 < \Re(s) < 1$. The zeros within the critical strip are called the non-trivial zeros which we will denote by $\rho = \beta + i\gamma$. If there is a non-trivial zero ρ then we automatically have that $1 - \rho$ is also a zero by the functional equation. Also, as $\zeta(s) = \overline{\zeta(\overline{s})}$, $\overline{\rho}$ is also a zero and then so is $1 - \overline{\rho}$, again by the functional equation. Therefore, if we have one zero in the critical strip, in reality we have up to four zeros (see the comments below on the Riemann Hypothesis to see why this number is actually more likely two).

While complex analysis hadn't reached an appropriate level of maturity when Riemann presented his paper, he predicted that the zeta function should have a third representation (beyond the infinite series and product over primes) as a product over its zeros. He was proved true by Hadamard in 1893 [154] who showed that $\zeta(s)$ satisfies a Hadamard product given by

$$\zeta(s) = \frac{e^{(\log(2\pi)-1-\gamma_0/2)s}}{2(s-1)\Gamma(1+s/2)} \prod_{\rho} \left(1 - \frac{s}{\rho}\right) e^{s/\rho},$$

where γ_0 is Euler's constant and the product is over all non-trivial zeros of $\zeta(s)$. In this way, the primes are related to the zeros of $\zeta(s)$ in a fundamental way which we see through the different representations of the zeta function. This is a theme that we come back to repeatedly through what are known as explicit formulae.

As with odd values of zeta, Euler's constant γ_0 has a host of open questions. For example, we do not know whether it is irrational or transcendental. One way of defining Euler's constant is as the limiting difference between the harmonic series and the natural logarithm, given by

$$\lim_{n\to\infty} \left\{ \sum_{k=1}^{n} \frac{1}{n} - \log n \right\} = \gamma_0.$$

Another way of defining Euler's constant, as we will see many times throughout this thesis, is from the Laurent expansion of the Riemann zeta function about $s = 1$, where

$$\lim_{s\to 1}\left\{\zeta(s) - \frac{1}{s-1}\right\} = \gamma_0.$$

The final representation that we mention, although don't use it in this thesis, is that we can write Euler's constant as

$$-\Gamma'(1) = \gamma_0.$$

Finally, we can count the number of zeros within regions of the critical strip, typically above the real axis up to some height T. As before, Riemann stated the formula in his 1859 paper, and later von Mangoldt proved it [305]. Through the argument principle, they showed that this count of zeros,

$$N(T) = \#\{\rho = \beta + i\gamma \ : \ 0 < \beta < 1,\ 0 \le \gamma \le T\}, \tag{1.4}$$

is given by the Riemann–von Mangoldt formula,

$$N(T) = \frac{T}{2\pi}\log\frac{T}{2\pi} - \frac{T}{2\pi} + \frac{7}{8} + S(T) + O\left(\frac{1}{T}\right), \tag{1.5}$$

with

$$S(T) = \frac{1}{\pi}\arg\zeta\left(\frac{1}{2} + it\right) \ll \log T,$$

where the argument is defined by continuous variation from $+\infty + iT$ to $1/2 + iT$, starting with the value 0.

1.1.3.1 The Riemann Hypothesis

Why did we say that for each zero in the critical strip, there are 'up to' four zeros in total? This is because if the real part of the zero equals $1/2$, then there are only two zeros, ρ and $\overline{\rho}$. If a zero has real part $1/2$, we say it lies on the critical line. Indeed, we believe that all non-trivial zeros have this property, a conjecture first made by Riemann in his 1859 paper, which we now call the Riemann Hypothesis and one that has taken on a life of its own. Due to its significance, we state it separately below. We will often assume the truth of this conjecture in this thesis.

Conjecture 1.1 (Riemann Hypothesis)**.** *All non-trivial zeros of $\zeta(s)$ have real part $1/2$.*

The Riemann Hypothesis remains an open question to this day. It is considered one of, if not the most, important questions in mathematics. It appears on the list of the seven Millennium Problems set by the Clay Institute and comes with a prize of $1 million for whoever can prove it. A full description can be found in [34] and in [58].

While we do not have a proof of this problem, some partial progress has been made. Numerically, all zeros that we have computed lie on the critical line - at time of writing, this is the first 10^{13} zeros [264], along with several billion other zeros higher up the critical line [259]. The Riemann zeta function is just one of a wider class of functions, called L-functions, each of which has its own representation as a Dirichlet series, Euler product, a meromorphic continuation, a functional equation, and a Riemann Hypothesis and each of which has all of its known zeros on the critical line.

In 1914, Hardy [163] showed that there are infinitely many zeros on the critical line. Selberg [276] improved this to show that a positive proportion lie on the line, and Min [238] gave an explicit constant for this proportion, showing that at least $1/14,074,731$ of the zeros of $\zeta(s)$ lie on the line. Levinson [222] improved this to show that at least one-third of the zeros lie on the line through a method that now carries his name. Conrey [56] improved this to two-fifths, and the current record is due to Pratt, Robles, Zaharescu and Zeindler [265] who showed that just over five-twelfths lie on the line. A more detailed discussion of these results can be found in Section 1.3.7.3.

In addition to these partial results, in the theory of algebraic varieties over finite fields, the analogous Riemann Hypothesis (one of the Weil Conjectures) was proved true by Deligne [309, 99, 100] giving us further evidence for the truth of the Riemann Hypothesis in general.

Many equivalent forms of the Riemann Hypothesis are known, some of which we discuss later in this thesis.

While the Riemann Hypothesis answers the question of the horizontal distribution of the zeros, we can also ask questions on the vertical distribution of the zeros, a topic we come to in Section 1.2.2.

1.1.4 A proof of the Prime Number Theorem

We have given a summary of most of Riemann's paper in the previous section, but he went further still. We now sketch his arguments, and those of Hadamard [155] and de la Vallée Poussin [95] in proving the Prime Number Theorem (combined with some modern ideas that simply the proofs).

An explicit formula is one that relates zeros of an L-function to prime numbers. Riemann was able to establish an explicit formula for a function related to $\pi(x)$. We do this in a more modern way by establishing an explicit formula for a related, more mathematically natural function, the Chebyshev-ψ function, defined by

$$\psi(x) = \sum_{n \leq x} \Lambda(n) = \sum_{\substack{p^k \leq x \\ p \text{ prime}}} \log p \tag{1.6}$$

where

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

is the von Mangoldt function. While this new way of counting primes (and prime powers) may seem odd at first glance, it is actually mathematically natural. This is because the logarithmic derivative of $\zeta(s)$ is given by

$$\frac{\zeta'}{\zeta}(s) = -\sum_{n=2}^{\infty} \frac{\Lambda(n)}{n^s}$$

for $\Re(s) > 1$. Then we can show that the Prime Number Theorem is equivalent to

$$\psi(x) \sim x$$

as $x \to \infty$. By Perron's formula,

$$\psi(x) = -\frac{1}{2\pi i} \int_{(c)} \frac{\zeta'}{\zeta}(s) \frac{x^s}{s} \, ds$$

where $c > 1$, $\int_{(c)}$ denotes an integral up the vertical line $\Re(s) = c$, and where we are ignoring various technicalities, error terms, and whether x is an integer. Then move the line of integration to the left and compute residues. We have residues at $s = 1$ giving a contribution of x, at the trivial and non-zeros of $\zeta(s)$ giving a contribution of $-\sum_z x^z/z$, and at $s = 0$ giving a contribution of $-\log(2\pi)$. Overall, again ignoring technicalities and error terms, we have

$$\psi(x) = x - \sum_{\zeta(z)=0} \frac{x^z}{z} - \log(2\pi).$$

We can split the sum over zeros into trivial and non-trivial zeros. Recalling that the trivial zeros occur at $z = -2n$ for n a natural number, we have

$$\sum_{n=1}^{\infty} \frac{1}{2nx^{2n}} = -\frac{1}{2} \log\left(1 - \frac{1}{x^2}\right)$$

which vanishes as $x \to \infty$. Therefore we have for large x,

$$\psi(x) \sim x - \sum_{\rho} \frac{x^\rho}{\rho},$$

as $x \to \infty$, where the sum is over the non-trivial zeros of $\zeta(s)$ and is conditionally convergent (the sum over zeros should be taken in increasing order of imaginary part in complex conjugate pairs).

The Prime Number Theorem would then follow if we could show there are no non-trivial zeros with $\Re(\rho) = 1$. This is the step that Hadamard and de la Vallée Poussin completed in 1896. Taking logarithms of the Euler product for $\zeta(s)$, we have

$$\log \zeta(s) = \sum_{p \text{ prime}} \sum_{k=1}^{\infty} \frac{1}{k} p^{-ks}$$

so writing $s = \sigma + it$,

$$|\zeta(s)| = \exp\left(\sum_{p \text{ prime}} \sum_{k=1}^{\infty} \frac{\cos(kt \log p)}{kp^{k\sigma}} \right).$$

Then for $\sigma > 1$,

$$\zeta(\sigma)^3 |\zeta(\sigma + it)|^4 |\zeta(\sigma + 2it)| = \exp\left(\sum_{p \text{ prime}} \sum_{k=1}^{\infty} \frac{3 + 4\cos(kt \log p) + \cos(2kt \log p)}{kp^{k\sigma}} \right) \geq 1$$

since $3 + 4\cos\theta + \cos 2\theta = 2(1 + \cos\theta)^2 \geq 0$.

Since we have a simple pole at $s = 1$, as $\sigma \to 1^+$, $\zeta(\sigma)^3 = O((\sigma - 1)^3)$. If we assume for a contradiction that there is some $t \neq 0$ with $\zeta(1 + it) = 0$, then $|\zeta(\sigma + it)|^4 = O((\sigma - 1)^{-4})$. We make no assumptions about $|\zeta(\sigma + 2it)|$ but as we know it isn't a pole, it is just $O(1)$. Combining this, as $\sigma \to 1^+$, we have

$$\zeta(\sigma)^3 |\zeta(\sigma + it)|^4 |\zeta(\sigma + 2it)| = O(\sigma - 1),$$

contradicting that this should be positive for $\sigma > 1$. Therefore $\zeta(s)$ does not vanish on $\Re(s) = 1$ and so the Prime Number Theorem follows.

We note that this is the only shrinking of the critical strip that has been proved since Riemann introduced his function. We cannot say unconditionally that there are no non-trivial zeros with $\Re(\rho) = 1 - \varepsilon$ for any $\varepsilon > 0$. However some zero-free regions are known, regions where $\zeta(s) \neq 0$ inside the critical strip. Note that for each region, as $T \to \infty$, each is equivalent to the fact that $\zeta(s)$ does not vanish on $\Re(s) = 1$. For sufficiently large t with $c > 0$ a positive constant, we have $\zeta(\sigma + it) \neq 0$ when

$$\sigma \geq 1 - \frac{c}{\log |t|},$$

which is due to de la Vallée Poussin [96], with improvements due to Littlewood [226], Chudakov [54], and Korobov [217] and Vinogradov [303]. Explicit versions of zero-free regions can be found in [117, 206].

We finish this section by mentioning two further points regarding the Prime Number Theorem. Firstly, if we want to write this as a full asymptotic rather than just to leading order, then de la Vallée Poussin showed in 1899 [96] that unconditionally for $C > 0$ that

$$\pi(x) = \mathrm{Li}(x) + O(xe^{-C\sqrt{\log x}}), \tag{1.7}$$

with a further slight improvement by Korobov [217] and Vinogradov [303] who showed using their zero-free region for $\zeta(s)$ that for $C > 0$,

$$\pi(x) = \mathrm{Li}(x) + O\left(x \exp\left(-C(\log x)^{3/5}(\log\log x)^{-1/5}\right)\right).$$

These error terms in the Prime Number Theorem follow from the zero-free regions discussed above.

If we assume the Riemann Hypothesis then von Koch showed in 1901 [304] that

$$\pi(x) = \mathrm{Li}(x) + O(x^{1/2}\log x).$$

This power of 1/2 on the x in the error term is exactly the 1/2 in the real part of the zeta zeros (to the extent that if we prove this is the true error term without assuming the Riemann Hypothesis, then we have proved Riemann was correct in making his hypothesis). If we have any zeros off the line, then von Koch [304] showed that the error term becomes $O(x^{\Theta}\log x)$, where

$$\Theta = \sup_{\rho} \Re(\rho)$$

which satisfies $1/2 \leq \Theta \leq 1$.

Finally, it appeared that it was always the case that $\mathrm{Li}(x) > \pi(x)$, displaying what we call Chebyshev bias (see Section 1.4.3.4), with numerical evidence supporting this. However Littlewood [224] showed that $\mathrm{Li}(x) - \pi(x)$ changes sign infinitely often. Skewes [283, 284] showed under the Riemann Hypothesis that the first time this happens is by $x \approx 10^{10^{10^{34}}}$. The best known upper bound for this first sign change is by $x \approx 1.397166161527 \times 10^{316}$, calculated in [286]. While a fascinating topic in its own right which we revisit later, it serves as a warning that just because we have what seems to be overwhelming numerical evidence, what we really need are rigorous proofs.

1.1.4.1 The Prime Number Theorem in Arithmetic Progressions

While we will mainly only consider the Riemann zeta function in this thesis, it belongs to a wider class of functions called L-functions. We mention one specific type, called Dirichlet L-functions. To understand what these are, we being with a Dirichlet character χ mod q (where q is a positive integer) which is an arithmetic function $\chi : \mathbb{Z} \to \mathbb{C}$ that satisfies

1. $\chi(n+q) = \chi(n)$ for all $n \in \mathbb{Z}$
2. $\chi(n) = 0$ if $(n, q) \neq 1$
3. $\chi(mn) = \chi(m)\chi(n)$ for all $m, n \in \mathbb{Z}$
4. $\chi(1) = 1$.

There are exactly $\varphi(q)$ distinct Dirichlet characters mod q, where $\varphi(q)$ is the Euler totient function which counts the number of positive integers less than or equal to q that are coprime to q.

A Dirichlet L-function associated with a Dirichlet character $\chi \bmod q$ has Dirichlet series representation

$$L(s,\chi) = \sum_{n=1}^{\infty} \frac{\chi(n)}{n^s}$$

which converges for all complex s with $\Re(s) > 1$. As with the Riemann zeta function, it has an Euler product representation given by

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

which converges for all complex s with $\Re(s) > 1$.

The principal character χ_0 is given by

$$\chi_0(n) = \begin{cases} 1 & \text{if } (n,q) = 1 \\ 0 & \text{otherwise.} \end{cases}$$

The associated L-function is

$$L(s,\chi_0) = \zeta(s) \prod_{p|q} \left(1 - p^{-s}\right).$$

A Dirichlet L-function satisfies a function equation of the form

$$L(s,\chi) = F(s)L(1-s,\overline{\chi})$$

where $F(s)$ is a certain function (similar to the term in the functional equation for the Riemann zeta function) and $\overline{\chi}$ is the complex conjugate of χ. This shows that $L(s,\chi)$ has an analytic continuation to the whole complex plane for $\chi \neq \chi_0$ and a meromorphic continuation with a simple pole if $\chi = \chi_0$.

Dirichlet L-functions have trivial zeros at $s = 0, -2, -4, \ldots$ if $\chi(-1) = 1$ and at $s = -1, -3, -5, \ldots$ if $\chi(-1) = -1$, and have their non-trivial zeros in the critical strip. They are believed to satisfy a Generalised Riemann Hypothesis, that is, it is believed that all non-trivial zeros of any Dirichlet L-function lie on the critical line.

We can ask many of the questions for Dirichlet L-functions that we do for the Riemann zeta function. Most are not considered in this thesis, but a general survey of such questions can be found in [2].

Part of the reason to mention Dirichlet L-functions at this point is to talk about their connection with prime numbers. Just as with using the Riemann zeta function to study prime numbers, Dirichlet L-functions can be used to study the prime numbers in arithmetic progressions. Questions of these forms are what led Dirichlet to first consider these functions. We mention two such results briefly, but many more questions about primes in arithmetic progressions can be considered, and we mention a few at other points in this introduction.

First, we start with Dirichlet's theorem on primes in arithmetic progressions [105]. It states that if $(a, q) = 1$, then there are infinitely many prime numbers congruent to $a \bmod q$. He proved this by showing through the orthogonality of Dirichlet characters that

$$\sum_{\substack{p \le x \\ p \equiv a \bmod q}} \frac{1}{p} = \frac{1}{\varphi(q)} \sum_{p \le x} \frac{1}{p} + O(1)$$

where $(a, q) = 1$. Since the sum of the reciprocal of the primes diverges, his result follows. In particular, he was required to show

$$\sum_{p \le x} \frac{\chi(p)}{p} = O(1)$$

for all $\chi \neq \chi_0$. He noticed through the Euler product representation for Dirichlet L-functions that

$$\log L(1, \chi) = \sum_{p} \frac{\chi(p)}{p} + O(1).$$

Since $L(s, \chi)$ is analytic at $s = 1$ for $\chi \neq \chi_0$, it was sufficient to show that $L(1, \chi) \neq 0$.

Finally, we write $\pi(x; q, a)$ for the number of primes congruent to $a \bmod q$ that are less than or equal to x. These primes equidistribute between equivalence classes in the way we expect from the Prime Number Theorem, that is, for $(a, q) = 1$, we expect

$$\pi(x; q, a) \sim \frac{1}{\varphi(q)} \frac{x}{\log x}$$

as $x \to \infty$ for fixed q, a fact that de la Vallée Poussin [95] proved in 1896.

1.2 RANDOM MATRIX THEORY

Random Matrix Theory (RMT) can be thought of as the probabilistic study of matrices whose entries are random variables. It has been used in a wide range of applications across mathematics and physics, including in particular the study of spectra of heavy atoms. Most surprisingly, it has found applications in number theory in a way that we describe in this section and throughout this thesis. There are many books on RMT, for example [231].

1.2.1 The Classical Compact Groups

The central objects of study in this section are randomly chosen elements of the classical compact matrix groups, namely the unitary, orthogonal, and symplectic groups. Writing I_N for the $N \times N$ identity matrix, we define these three groups together with some basic properties below.

1. **Unitary Group** $U(N)$**:** The unitary group is the group of of all $N \times N$ complex matrices U such that
$$UU^\dagger = U^\dagger U = I_N$$
where $U^\dagger$ is the complex transpose of U.

   The eigenvalues lie on the unit circle in the complex plane. We write them as $e^{i\theta_1}, ..., e^{i\theta_N}$ where $\theta_j \in [0, 2\pi)$.

2. **Orthogonal Group** $O(N)$**:** The orthogonal group is the group of all $N \times N$ complex matrices O such that
$$OO^T = O^T O = I_N$$
where O^T is the transpose of O.

   The special orthogonal group is the subgroup with $\det O = 1$.

   Specialising to the group of even dimensional special orthogonal matrices $SO(2N)$, the eigenvalues come in complex conjugate pairs, written as $e^{i\theta_1}, e^{-i\theta_1}, ..., e^{i\theta_N}, e^{-i\theta_N}$ where $\theta_j \in [0, \pi]$.

3. **Symplectic Group** $Sp(2N)$**:** The symplectic group is the group of all $2N \times 2N$ complex matrices $S \in U(N)$ such that
$$SJS^T = J$$
where
$$J = \begin{pmatrix} 0 & I_N \\ -I_N & 0 \end{pmatrix}.$$
The eigenvalues come in complex conjugate pairs, denoted $e^{i\theta_1}, e^{-i\theta_1}, \ldots, e^{i\theta_N}, e^{-i\theta_N}$ where $\theta_j \in [0, \pi]$.

Each of the classical compact groups we have considered is a compact Lie group. This means that they have a unique invariant probability measure under the action of the group, called Haar measure. The unitary, orthogonal, and symplectic group ensemble is the group attached with its respective Haar measure. The unitary group with Haar measure is also known as the Circular Unitary Ensemble and is the key group ensemble that we focus on in this thesis. Note that the orthogonal/symplectic group with Haar measure is not the Circular Orthogonal/Symplectic Ensemble.

The calculation of the joint probability density of the eigenangles under Haar measure is due to Weyl [311]. We list the three joint probability densities here for completeness.

1. **Unitary** $U(N)$**:**
$$\frac{1}{N!(2\pi)^N} \prod_{1 \le j < k \le N} \left| e^{i\theta_j} - e^{i\theta_k} \right| \prod_{n=1}^{N} d\theta_n$$

2. **Even Special Orthogonal** $SO(2N)$**:**

$$\frac{2^{(N-1)^2}}{N!\pi^N}\prod_{1\le j<k\le N}(\cos\theta_j-\cos\theta_k)^2\prod_{n=1}^{N}d\theta_n$$

3. **Symplectic** $Sp(2N)$**:**

$$\frac{2^{N^2}}{N!\pi^N}\prod_{1\le j<k\le N}(\cos\theta_j-\cos\theta_k)^2\prod_{n=1}^{N}\sin^2\theta_n d\theta_n$$

These joint probability densities are used in the Weyl integration formula. Weyl's integration formula relates the average of a class function (a function which is symmetric in all of its variables) over a matrix ensemble to a multidimensional integral of the same function, over the eigenvalues of the matrices in that ensemble. In the unitary case, this is defined by

$$\mathbb{E}_{\mathbb{N}}\left\{f(\theta_1,...,\theta_N)\right\}=\frac{1}{N!(2\pi)^N}\int_0^{2\pi}...\int_0^{2\pi}f(\theta_1,...,\theta_N)\prod_{1\le j<k\le N}\left|e^{i\theta_j}-e^{i\theta_k}\right|^2\prod_{n=1}^{N}d\theta_n \quad (1.8)$$

where $\mathbb{E}_{\mathbb{N}}$ denotes expectation with respect to the Circular Unitary Ensemble of an $N\times N$ matrix, the θ_n are the eigenangles of an $N\times N$ unitary matrix, and $f(\theta_1,...,\theta_N)$ is a class function.

One of the major themes in this thesis are calculations relating to the characteristic polynomial of a matrix A from one of our groups above. For our purposes, we define the characteristic polynomial of such a matrix from one of these groups to be

$$Z_{N,A}(\theta)=\det(I-Ae^{-i\theta}) \quad (1.9)$$

where A is from one of $U(N), SO(2N), Sp(2N)$. When it is clear which group we are working with we drop the subscript A. In the unitary case, the characteristic polynomial can be written as

$$Z_N(\theta)=\prod_{n=1}^{N}\left(1-e^{i(\theta_n-\theta)}\right)$$

and in the even special orthogonal or symplectic cases, the characteristic polynomial can be written as

$$Z_N(\theta)=\prod_{n=1}^{N}\left(1-e^{i(\theta_n-\theta)}\right)\left(1-e^{-i(\theta_n+\theta)}\right).$$

Note that the characteristic polynomial, its derivative, and the logarithmic derivative are all class functions, and so Weyl's integration formula will be useful in our study of these functions.

1.2.2 Random Matrix Theory meets Number Theory: Act I

The connection between RMT and number theory can be traced directly back to a single conversation at the Institute of Advanced Studies in Princeton in 1972, as described in [209]. Hugh Montgomery was visiting the IAS and was introduced to the physicist Freeman Dyson by Sarvadaman Chowla. When Dyson asked Montgomery what he was working on, Montgomery told him about his work on the vertical distributions of the zeros of $\zeta(s)$, in particular on a result on the pair correlation of the zeros. Dyson instantly recognised the result as being identical to that of the pair correlation of the eigenvalues of random unitary matrices. This chance meeting at a time when Montgomery had just completed this work together with Dyson's insight from his work on nuclei of heavy atoms was the birth of the future fruitful investigation into the links between RMT and the Riemann zeta function. While Riemann's original manuscript was the first epoch-making paper that kick started our interest in the zeta function, it is fair to say that Montgomery's paper on pair correlation was the second.

Montgomery [239] was one of the first to consider the vertical distribution of the zeros of $\zeta(s)$ under the assumption of the the Riemann Hypothesis. To motivate this problem, Montgomery considered the function

$$F(\alpha, T) = \left(\frac{T}{2\pi}\log T\right)^{-1} \sum_{0<\gamma,\gamma'\leq T} T^{i\alpha(\gamma-\gamma')} w(\gamma-\gamma')$$

where $w(u) = 4/(4+u^2)$ is a weight function, α is real and $T \geq 2$.

Montgomery observed that $F(\alpha, T)$ is a real-valued even function in α, and proved the following about $F(\alpha, T)$.

Theorem 1.2 (Montgomery)**.** *Assume the Riemann Hypothesis. Then*

$$F(\alpha, T) = (1+o(1))T^{-2\alpha}\log T + \alpha + o(1) \tag{1.10}$$

uniformly for $0 \leq \alpha \leq 1-\varepsilon$ *for any fixed* $\varepsilon > 0$*, as* $T \to \infty$*.*

Later, Mueller and Heath-Brown noted that F is non-negative (see [52]) and Goldston and Montgomery [142] showed Montgomery's Theorem 1.2 holds uniformly for $0 \leq \alpha \leq 1$.

Using a quantitative form of the Hardy–Littlewood twin prime hypothesis, Montgomery conjectured that for $\alpha \geq 1$,

$$F(\alpha, T) = 1 + o(1) \tag{1.11}$$

as $T \to \infty$, uniformly in α.

Combining this conjecture with his Theorem 1.2, as $F(\alpha, T)$ is even in α,

$$\lim_{T\to\infty} F(\alpha, T) = \begin{cases} |\alpha| + \delta(\alpha) & \text{if } |\alpha| \leq 1 \\ 1 & \text{if } |\alpha| \geq 1 \end{cases} \tag{1.12}$$

where $\delta(\alpha)$ is the Dirac delta function.

Now rescale the zeros so they have unit mean spacing, that is,

$$w_n = \frac{\gamma_n}{2\pi} \log \frac{\gamma_n}{2\pi}$$

where the γ_n are the ordinates of the non-trivial zeros of $\zeta(s)$, ordered by height above the real axis.

Assuming his conjecture and taking the Fourier transform of $F(\alpha, T)$, Montgomery [239] was lead to his conjecture known as the Pair Correlation Conjecture.

Conjecture 1.3 (Pair Correlation Conjecture)**.** *For fixed $a < b$,*

$$\lim_{T\to\infty} \frac{1}{N(T)} \sum_{\substack{\gamma,\gamma' \in [0,T] \\ a \le w_m - w_n \le b}} 1 = \int_a^b \left(1 - \left(\frac{\sin \pi x}{\pi x}\right)^2\right) dx + \delta(a,b)$$

where

$$\delta(a,b) = \begin{cases} 1 & \text{if } 0 \in [a,b] \\ 0 & \text{otherwise.} \end{cases}$$

This term reflects the fact that if $a \le 0 \le b$, then the sum includes the terms $\gamma = \gamma'$.

There is considerable numerical support for this conjecture, initiated by Odlyzko [257, 258]. Higher correlations have since been studied. The three-point correlation of zeta zeros by Hejhal [178] matches the three-point correlation of $U(N)$. Rudnick and Sarnak [275] then showed that the n-level correlations of zeros of principal L-functions match the analogous results from the RMT side. Both of these works are based on appropriate restrictions on the Fourier transform of the test function. Avoiding this issue, Bogomolny and Keating [30, 31] obtain the above conjectures heuristically, including all lower order terms that arise from arithmetical considerations. We will note later that the Ratios Conjecture [87] recovers these full asymptotics as discussed in Section 6.1. A key feature of these heuristics is that they do not restrict the support of the Fourier transform. Bogomolny and Leboeuf [32] have extended this heuristic to calculate the pair correlation for Dirichlet L-functions, which again agree with what we see from the $U(N)$ result.

From the RMT side, to state Dyson's theorem [107, 108, 109] we let $U \in U(N)$ with eigenvalues $e^{i\theta_1}, ..., e^{i\theta_N}$. We rescale the eigenphases to have unit mean density to give

$$\phi_j = \theta_j \frac{N}{2\pi}.$$

Theorem 1.4 (Dyson)**.** *For a test function f such that $f(x) \to 0$ as $|x| \to \infty$, the pair correlation of eigenvalues tends to a sine kernel as $N \to \infty$. That is,*

$$\lim_{N\to\infty} \mathbb{E}_N \left\{ \frac{1}{N} \sum_{m,n \le N} f(\phi_m - \phi_n) \right\} = \int_{-\infty}^{\infty} f(x) \left(\delta(x) + 1 - \left(\frac{\sin \pi x}{\pi x}\right)^2\right) dx$$

where $\mathbb{E}_N$ denotes the expected value taken over $U(N)$ with respect to Haar measure.

Taking the test function to be $f(x) \equiv 1$ for $x \in [a,b]$ and 0 otherwise gives

$$\mathbb{E}_N \left\{ \frac{1}{N} \sum_{\substack{\phi_m, \phi_n \leq N \\ a < \phi_m - \phi_n < b}} 1 \right\} = \int_a^b \left(1 - \left(\frac{\sin \pi x}{\pi x} \right)^2 \right) \, dx + \delta(a,b)$$

as $N \to \infty$, with $\delta(a,b)$ defined as in Conjecture 1.3.

Comparing Montgomery's Theorem with the RMT result of Dyson makes it obvious why Dyson made his remarks at the IAS. If Montgomery's Pair Correlation Conjecture is true then this suggests there is a spectral interpretation for the Riemann zeta-function as an infinite dimensional operator, which is known as the Hilbert–Pólya conjecture. The idea of randomly choosing large matrices and averaging them should capture information about this one specific matrix related to the zeta function, even if we can't prove the Hilbert–Pólya conjecture. We have evidence supporting this conjecture beyond just the numerical. The strongest theoretical evidence comes from the function field setting as it is possible to provide a spectral interpretation of the zeros in terms of certain eigenvalues, as previously mentioned when discussing the Weil Conjectures.

1.3 CONTINUOUS MOMENTS OF THE RIEMANN ZETA FUNCTION

We saw in Section 1.1 how important it is to understand the Riemann zeta function for our understanding of the distribution of prime numbers. This interest in understanding the primes through the zeros of the Riemann zeta function has led us to ask questions about properties of the zeta function for its own sake.

One such question concerns the size of $\zeta(s)$, either for exceptional values, or on average. We will focus on the average in this thesis but will mention large values occasionally. Averages typically split into two main types that are traditionally considered, with a further one being the main topic of this thesis. The two types that have previously been studied deeply are those called continuous and discrete moments. The third kind is a variant of the typical discrete moments, with a general overview of these moments given in the Preface to this thesis, and with the full details starting in Chapter 2.

The continuous moments are integrals of the form

$$I_{2k}(T) = \int_0^T \left| \zeta \left(\frac{1}{2} + it \right) \right|^{2k} \, dt$$

and the discrete moments are sums of the form

$$J_{2k,n}(T) = \sum_{0 < \gamma \leq T} \left| \zeta^{(n)} \left(\frac{1}{2} + i\gamma \right) \right|^{2k}$$

where the γ are the ordinates of the non-trivial zeros of $\zeta(s)$ and $\zeta^{(n)}(s)$ denotes the n^{th} derivative of $\zeta(s)$.

We can also consider continuous moments of derivatives of $\zeta(s)$, as mentioned in (1.16). For further examples of these moments, see [192, 55, 157].

Additionally, some authors use the convention of writing k rather than $2k$ in the subscripts for the labels of the moments moments, particularly for the discrete case. Some also divide the continuous moments by the length of the integral T and the discrete moments by the number of zeros in the sum $N(T)$. For consistency throughout this thesis we will endeavour to use our convention, although in some places (notably after conjecturing a zeta result from an RMT result) it makes more sense to divide by this length/number of zeros.

1.3.1 The Lindelöf Hypothesis

Why might we want to know about the averages of $\zeta(s)$? The initial motivation came from attempts to prove the Lindelöf Hypothesis, which concerns the size of $\zeta(s)$ on the critical line. We state it as follows.

Conjecture 1.5 (Lindelöf Hypothesis)**.** *For $t > 0$, for every $\varepsilon > 0$,*

$$\zeta\left(\frac{1}{2} + it\right) = O(t^{\varepsilon})$$

as $t \to \infty$.

We note that the Riemann Hypothesis implies the Lindelöf Hypothesis but the converse is not believed to be true. This is because the Lindelöf Hypothesis is equivalent to a less stringent condition on the zeta zeros than the Riemann Hypothesis. The reason that the Riemann Hypothesis implies the Lindelöf Hypothesis is because Littlewood [227] showed that the Riemann Hypothesis implies

$$\left|\zeta\left(\frac{1}{2} + it\right)\right| \ll \exp\left(\frac{c\log t}{\log\log t}\right) \tag{1.13}$$

for some $c > 0$.

It can be shown, for example in Section 13.2 of [298], that the Lindelöf Hypothesis is equivalent to the statement that

$$I_{2k}(T) = O\left(T^{1+\varepsilon}\right)$$

for every $\varepsilon > 0$ and all positive integers k, giving our first clear motivation for studying moments.

1.3.2 Continuous Moment Results

There are only two proven asymptotic formulae for continuous moments, beyond the trivial $k = 0$ case. The second moment is due to Hardy and Littlewood [164] in 1918 where they showed to leading order that

$$I_2(T) \sim T \log T \tag{1.14}$$

as $T \to \infty$. In 1926 Ingham [192] considered a shifted second moment of $\zeta(s)$ with $|\alpha|, |\beta| < 1/2$ and showed that for every $\varepsilon > 0$,

$$\int_0^T \zeta\left(\frac{1}{2} + it + \alpha\right) \zeta\left(\frac{1}{2} - it + \beta\right) \, dt = \\ \int_0^T \left(\zeta(1+\alpha+\beta) + \left(\frac{t}{2\pi}\right)^{-\alpha-\beta} \zeta(1-\alpha-\beta)\right) \left(1 + O(t^{-1/2+\varepsilon})\right) \, dt. \tag{1.15}$$

This idea of using small shifts has proved to be incredibly useful in recent years in obtaining full asymptotics, including lower order terms. In this case, Ingham was able to show that

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

with improvements in the error term being made since then, for example in Heath-Brown–Huxley [175] and Watt [308]. The size of the shifts has been increased by Bettin [25], who showed we may take the shifts α, β with $\Re(\alpha), \Re(\beta) \ll 1/\log T$ and $\Im(\alpha), \Im(\beta) \ll T^{2-\varepsilon}$, for any $\varepsilon > 0$. He conjectures that the imaginary parts may be of size up to $T^{4-\varepsilon}$ for any $\varepsilon > 0$, but not larger due to Omega results for the error term in $I_2(T)$. (We say that $f(x) = \Omega(g(x))$ for some functions f, g if the lim sup of $|f(x)/g(x)|$ is positive as $x \to \infty$.) For some Omega results, see [190, 191], where it is shown that the error term is $\Omega_\pm\left(T^{1/4}\right)$. It is believed that the correct size of the error term is $T^{1/4} \log T$.

As well as allowing us to extract lower order terms, this shifted second moment allows us to write asymptotics for mixed moments of the derivatives of $\zeta(s)$. In particular Ingham's result shows for fixed $m, n \in \mathbb{N}$,

$$\int_0^T \zeta^{(m)}\left(\frac{1}{2} + it\right) \zeta^{(n)}\left(\frac{1}{2} - it\right) \, dt = \frac{(-1)^{m+n}}{m+n+1} T(\log T)^{m+n+1} + O\left(T(\log T)^{m+n}\right). \tag{1.16}$$

At the same time as proving this second moment result, Ingham [192] showed that the fourth moment satisfies to leading order

$$I_4(T) \sim \frac{1}{2\pi^2} T(\log T)^4 \tag{1.17}$$

as $T \to \infty$. Later Heath-Brown [172] showed that the lower order terms are given by

$$I_4(T) = \sum_{n=0}^{4} a_n T \left(\log \frac{T}{2\pi}\right)^n + O\left(T^{7/8+\varepsilon}\right)$$

with a_4 as in Ingham's result, an explicit a_3, and for some implicit computable constants a_n and for all $\varepsilon > 0$. An equivalent form is given as a residue by Conrey [57], and a shifted version of the fourth moment was studied by Motohashi [247]. Improvements to the error term for Heath-Brown's result have been made, for example by Zavorotnyi [317] and by Ivić-Motohashi [200]. Motohashi [246] also showed that error term is $\Omega_{\pm}\left(T^{1/2}\right)$.

Other than these two moments, a smoothed version has also been calculated for the first two moments. We write

$$\tilde{I}_{2k}(T) = \int_0^\infty \left|\zeta\left(\frac{1}{2} + it\right)\right| e^{-\delta t} \, dt$$

where δ is small.

For the second moment, Kober [216] showed that

$$\tilde{I}_2(T) \sim \frac{1}{\delta} \log \frac{1}{\delta}$$

as $\delta \to 0$. For the fourth moment, Titchmarsh [296] showed

$$\tilde{I}_4(T) \sim \frac{1}{2\pi^2 \delta} \left(\log \frac{1}{\delta}\right)^4$$

as $\delta \to 0$ with Atkinson [10] giving lower order terms in 1941. A different method was used to obtain this full asymptotic in Motohasi [245]. It is possible to use a Tauberian theorem to switch between the smoothed and unsmoothed versions to leading order, but not to lower order.

Returning to our standard continuous moments $I_{2k}(T)$, almost 70 years went by before any new results were even conjectured. In 1992, Conrey and Ghosh [68] conjectured that

$$I_6(T) \sim \frac{42}{9!} \prod_p \left\{ \left(1 - \frac{1}{p}\right)^4 \left(1 + \frac{4}{p} + \frac{1}{p^2}\right) \right\} T (\log T)^9$$

as $T \to \infty$. In 1998 Conrey and Gonek [76] conjectured that

$$I_8(T) \sim \frac{24024}{16!} \prod_p \left\{ \left(1 - \frac{1}{p}\right)^9 \left(1 + \frac{9}{p} + \frac{9}{p^2} + \frac{1}{p^3}\right) \right\} T (\log T)^{16}$$

as $T \to \infty$, as well as rederiving the conjecture for the sixth moment in a different way. However, the methods used didn't generalise to higher moments. Indeed, for $k \geq 5$, the method predicts that $I_{2k}(T)$ is negative, which is clearly false from its definition. In Section 1.3.6 we will discuss recent developments that fix this method and predict exactly the moments that we have come to expect.

It became a folklore conjecture after a result of Conrey and Ghosh [65] that the moments should be of the form

$$I_{2k}(T) \sim a_k g_k T (\log T)^{k^2} \tag{1.18}$$

as $T \to \infty$. The arithmetic factor a_k is given by

$$a_k = \prod_p \left(1 - \frac{1}{p}\right)^{k^2} \sum_{m=0}^{\infty} \left(\frac{\Gamma(m+k)}{m!\Gamma(k)}\right)^2 p^{-m} \tag{1.19}$$

and $g_k(k^2)!$ is an integer whenever k is a positive integer. Note that while the arithmetic term is written as an infinite sum, it can be rewritten in a way to show it is actually finite. To do this, write this arithmetic term as

$$a_k = \prod_p \left(1 - \frac{1}{p}\right)^{k^2} \sum_{m=0}^{\infty} d_k^2(p^m) p^{-m}$$

where $d_k(n)$ denotes the n^{th} coefficient of the Dirichlet series for $\zeta(s)^k$. As Conrey and Ghosh [65] showed $a_k = a_{1-k}$, it follows that

$$a_k = \prod_p \left(1 - \frac{1}{p}\right)^{(k-1)^2} \sum_{m=0}^{\infty} d_{1-k}^2(p^m) p^{-m}.$$

Since

$$d_k(p^m) = \binom{k+m-1}{m} = (-1)^m \binom{-k}{m},$$

we have

$$a_k = \prod_p \left(1 - \frac{1}{p}\right)^{(k-1)^2} \sum_{m=0}^{k-1} \binom{k-1}{m}^2 p^{-m}.$$

It is then clear how the arithmetic terms in the sixth and eighth moments conjectures arise.

The issue however is that even without rigorous results for the sixth and eighth moments, there didn't seem to be a way to predict what the value of the geometric factor g_k should be. This all changed with the third epoch-making work on the Riemann zeta function after Riemann and Montgomery, that of Keating and Snaith, which we discuss in Section 1.3.3.

1.3.2.1 Upper and Lower Bounds

There is a huge amount of literature on the subject of upper and lower bounds of continuous moments. We give a brief summary below. We know that for $k > 0$,

$$T(\log T)^{k^2} \ll I_{2k}(T) = \int_0^T \left|\zeta\left(\frac{1}{2} + it\right)\right|^{2k} dt \ll T(\log T)^{k^2}.$$

Here the lower bound holds unconditionally for all $k > 0$ and the upper bound holds unconditionally for $0 < k \leq 2$ and conditionally on the Riemann Hypothesis for all $k > 2$.

For the lower bounds, Ramachandra [268] established the bound for all even natural numbers and Heath-Brown [174] extended this to all positive rational rational numbers.

Under the Riemann Hypothesis, Conrey and Ghosh showed that the folklore conjecture (1.18) was of the right form, showing

$$I_{2k}(T) \geq \left(\frac{a_k}{\Gamma(k^2+1)} + o(1)\right) T(\log T)^{k^2}.$$

This result was improved by Balasubramanian and Ramachandra [16], and later by Soundararajan [288]. Radziwiłł and Soundararajan [267] obtained unconditional lower bounds of the correct form for $k \geq 1$ and Heap and Soundararajan [170] completed this by showing unconditional bounds of the correct form hold for $0 < k \leq 1$.

For the unconditional upper bounds, Heath-Brown [174] showed that they hold for $k = 1/n$ for positive integer n, while Bettin, Chandee and Radziwiłł [27] showed the same result but for $k = 1 + 1/n$. Heap, Radziwiłł, and Soundararajan [169] showed this is the correct upper bound for $0 < k \leq 2$.

For the conditional upper bounds on the Riemann Hypothesis, Soundararajan [291] showed that the upper bound is of the form $C_k T(\log T)^{k^2+\varepsilon}$ for all $\varepsilon > 0$, while Harper [166] managed to remove the ε from this result, showing that the upper bound is of the expected form and believed to be sharp.

1.3.3 Random Matrix Theory meets Number Theory: Act II

On the centenary of the proof of the Prime Number Theorem, a conference was held in Seattle, Washington in 1996 celebrating the proof and gathering all the experts to discuss the Riemann Hypothesis. Among those in attendance was Jon Keating who, at the time, was primarily a physicist who worked in RMT. While some work had been done to investigate the connection between RMT and number theory as highlighted by Dyson, such as numerical evidence of Odlyzko [257, 258] and the n-level correlations of Rudnick and Sarnak [275], it hadn't been fully exploited or investigated and was treated more as a curiosity than a serious avenue of investigation. Shortly before this, the sixth moment had been conjectured by Conrey and Ghosh [68], and Keating was challenged by Peter Sarnak to use RMT to rederive the known and conjectured moments, as described in [209].

With this challenge in mind, after the conference Keating returned to Bristol and together with his new PhD student Nina Snaith, investigated the moments problem from a RMT perspective. They had one hint of a starting point, the one Dyson had highlighted — the eigenvalues of random unitary matrices behave statistically like the zeros of $\zeta(s)$. If the non-trivial zeros of the zeta function are by definition the zeros of $\zeta(s)$, then what is the function that the eigenvalues are the zeros of? This is the characteristic polynomial of the matrix. Perhaps it might then be possible to model moments of $\zeta(s)$ by the moments of characteristic polynomials.

Recall in (1.9) that the characteristic polynomial of $U \in U(N)$ is given by

$$\begin{aligned} Z_N(\theta) &= \det(I - Ue^{-i\theta}) \\ &= \prod_{n=1}^{N} \left(1 - e^{i(\theta_n - \theta)}\right). \end{aligned}$$

Then for a fixed $\theta \in [0, 2\pi)$, the $2k^{\text{th}}$ moments of Z_N are given by

$$M_N(2k) = \mathbb{E}_N \left\{ \prod_{n=1}^{N} \left|1 - e^{i(\theta_n - \theta)}\right|^{2k} \right\} = \int_{U(N)} |Z_N(\theta)|^{2k} \, d\,\text{Haar}$$

where $d\,$Haar is Haar measure on $U(N)$.

By the Weyl integration formula (1.8), we have

$$M_N(2k) = \frac{1}{N!(2\pi)^N} \int_0^{2\pi} ... \int_0^{2\pi} \prod_{1 \le j < k \le N} \left|e^{i\theta_j} - e^{i\theta_k}\right|^2 \prod_{n=1}^{N} \left|1 - e^{i(\theta_n - \theta)}\right|^{2k} d\theta_n. \quad (1.20)$$

This may be evaluated using Selberg's integral. This can be found in various places, for example [277], Chapter 17 of [231] and Chapter 8 of [3].

Theorem 1.6 (Selberg)**.** *Let* $n \in \mathbb{N}$ *and let* $a, b, \alpha, \beta, \gamma \in \mathbb{C}$ *with* $\Re(a, b, \alpha, \beta) > 0$, $\Re(\alpha + \beta) > 1$*, and*

$$-\frac{1}{n} < \Re(\gamma) < \min\left(\frac{\Re(\alpha)}{n-1}, \frac{\Re(\beta)}{n-1}, \frac{\Re(\alpha + \beta + 1)}{2(n-1)}\right)$$

Then

$$\begin{aligned} J(a, b, \alpha, \beta, \gamma, n) &= \int_{-\infty}^{\infty} ... \int_{-\infty}^{\infty} \prod_{1 \le j < k \le N} |x_j - x_k|^{2\gamma} \prod_{j=1}^{n} (a + ix_j)^{-\alpha} (b - ix_j)^{-\beta} \, dx_1 ... dx_n \\ &= \frac{(2\pi)^n}{(a+b)^{(\alpha+\beta)n - \gamma n(n-1) - n}} \prod_{j=0}^{n-1} \frac{\Gamma(1 + \gamma + j\gamma)\Gamma(\alpha + \beta - (n - 1 + j)\gamma - 1)}{\Gamma(1 + \gamma)\Gamma(\alpha - j\gamma)\Gamma(\beta - j\gamma)}. \end{aligned}$$

Then write (1.20) in terms of absolute values of sine-functions and set $\theta = 0$ which we can do thanks to the rotational invariance of Haar measure on $U(N)$. After a change of variables, Keating and Snaith obtain for $\Re(2k) > -1$,

$$\begin{aligned} M_N(2k) &= \frac{2^{N^2 + 2kN}}{N!(2\pi)^N} J(1, 1, N + k, N + k, 1, N) \\ &= \prod_{n=1}^{N} \frac{\Gamma(n)\Gamma(n + 2k)}{\Gamma(n + k)^2} \end{aligned} \quad (1.21)$$

Note that (1.21) has a meromorphic continuation in k to the rest of the complex plane.

Since this is a theorem for finite N, we may take $N \to \infty$ after using the definition of the Barnes G-function in (1.21) and expanding its asymptotics to give

$$M_N(2k) = \frac{G^2(k+1)}{G(2k+1)} N^{k^2} + O\left(N^{k^2-1}\right) \tag{1.22}$$

where $G(z)$ is the Barnes G-function defined by Barnes in [19] for all z by

$$G(z+1) = (2\pi)^{z/2} \exp\left(-\frac{1}{2}(z^2 + \gamma_0 z^2 + z)\right) \prod_{n=1}^{\infty} \left(1 + \frac{z}{n}\right)^n e^{-z+z^2/2n} \tag{1.23}$$

where γ_0 is Euler's constant. The Barnes G-function satisfies the functional equation

$$G(z+1) = \Gamma(z)G(z), \text{ with } G(1) = 1.$$

When k is an integer, the leading order coefficient in (1.22) simplifies to

$$\frac{G^2(k+1)}{G(2k+1)} = \prod_{n=0}^{k-1} \frac{n!}{(n+k)!}.$$

We also know for integer k that $M_N(2k)$ is a polynomial in N of degree k^2. Finally, this ratio times $(k^2)!$ is an integer, a result first proved in [59].

Keating and Snaith wanted to establish the value distribution of the real and imaginary parts of the logarithm of $Z_N(\theta)$, which was part of the motivation for studying $M_N(2k)$. Note that this is precisely the generating function for the moments of the real part, and the imaginary parts may be computed in a similar manner. They showed [211] that as $N \to \infty$, that the real and imaginary parts tend independently to Gaussian random variables.

Theorem 1.7 (Keating–Snaith)**.** *Let $B \subset \mathbb{C}$. Then for fixed $\theta \in [0, 2\pi)$,*

$$\lim_{N\to\infty} \text{Haar}\left\{ A \in U(N) \ : \ \frac{\log Z_N(\theta)}{\sqrt{\frac{1}{2}\log N}} \in B \right\} = \frac{1}{2\pi} \iint_B e^{-\frac{1}{2}(x^2+y^2)} \, dx \, dy,$$

where the measure of the set is taken to be the usual Haar measure on $U(N)$.

This should be compared with the Selberg Central Limit Theorem [278] for $\zeta(s)$, which shows that the real and imaginary parts of the logarithm of $\zeta(s)$ independently tend to a Gaussian random variable.

Theorem 1.8 (Selberg)**.** *Let $B \subset \mathbb{C}$,*

$$\lim_{T\to\infty} \frac{1}{T} \text{meas}\left\{ T \le t \le 2T \ : \ \frac{\log \zeta(\frac{1}{2}+it)}{\sqrt{\frac{1}{2}\log\log \frac{t}{2\pi}}} \in B \right\} = \frac{1}{2\pi} \iint_B e^{-\frac{1}{2}(x^2+y^2)} \, dx \, dy,$$

where the measure of the set is taken to be Lebesgue measure.

The similarity between these two theorems is impossible to miss. Compare the mean densities of the zeta zeros at height T, which is $\frac{1}{2\pi}\log\frac{T}{2\pi}$, to the mean density of eigenangles of an $N \times N$ unitary matrix, which is $\frac{N}{2\pi}$. Setting them equal to each other gives

$$N = \log\frac{T}{2\pi}.$$

With this connection the two central limit theorems are consistent. This scaling has really paved the way for us to understand $\zeta(s)$ through RMT.

To test the predictions of RMT against the Riemann zeta function results, we show plots the real and imaginary parts of the two Central Limit Theorems, with the graphs found in [287, 211]. These graphs have been standardised so as to be compared with the Gaussian of mean zero and variance one. While neither graph matches the asymptotic standard Gaussian limit, the RMT results agree extremely closely to the number theoretic results convincingly well.

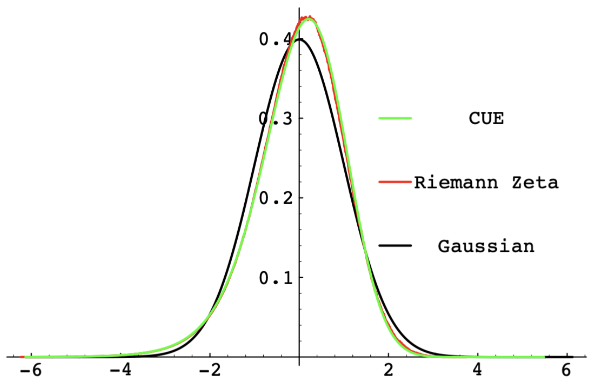

Figure 1.1: A comparison of the Circular Unitary Ensemble value distribution for $\Re(\log Z_N)$ with $N = 42$, Odlyzko's data for the distribution of $\Re(\log\zeta)$ near the $10^{20\text{th}}$ zero ($T \approx 10^{19}$) and the standard Gaussian, all scaled to have unit variance.

Given this identification, it should be simple to transform the moments $M_N(2k)$ into conjectural moments of $\zeta(s)$. This works for $k = 0$ and for $k = 1$, but we have a problem when we consider $k = 2$. In this case, one might think that we would have $\frac{1}{12}T(\log T)^4$ for the fourth moment, but this disagrees with Ingham's result (1.17). What has gone wrong? As we consider higher moments from this approach and compare them with their conjectural results, we see that the arithmetic term is missing. We say colloquially that RMT doesn't know about primes (for example, there is no Euler product equivalent in RMT). Instead, treating our quotient of Barnes G-functions as g_k in the folklore conjecture

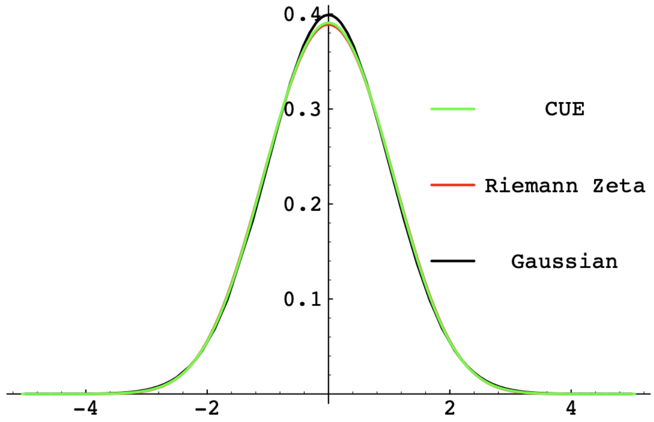

Figure 1.2: A comparison of the Circular Unitary Ensemble value distribution for $\Im(\log Z_N)$ with $N = 42$, Odlyzko's data for the distribution of $\Im(\log \zeta)$ near the $10^{20\text{th}}$ zero ($T \approx 10^{19}$) and the standard Gaussian, all scaled to have unit variance.

(1.18), and using the identification $N = \log \frac{T}{2\pi}$ in their moments calculation, Keating and Snaith were led to the following conjecture, first given in [211].

Conjecture 1.9 (Keating–Snaith)**.** *For k fixed with $\Re(k) > -1/2$,*

$$I_{2k}(T) = \int_0^T \left|\zeta\left(\frac{1}{2} + it\right)\right|^{2k} dt \sim a_k \frac{G^2(k+1)}{G(2k+1)} T(\log T)^{k^2}$$

as $T \to \infty$, with a_k defined in (1.19) *and G is the Barnes G-function defined in* (1.23)*.*

We note that this conjecture is consistent with all known and conjectured results. Indeed, this result and the eighth moment conjecture were announced at the same conference in the 1998 Vienna conference on the Riemann Hypothesis - fortunately, the two conjectures agreed with one another! We also note that Keating and Snaith went further, and also formulated moments conjectures for other L-functions from RMT results over the Orthogonal and Symplectic groups in [210].

Two questions remain: how can one make the arithmetic factor a_k appear naturally, and what are the lower order terms implied in the Keating–Snaith conjecture?

1.3.4 The Hybrid Model

Keating and Snaith were able to obtain the geometric term g_k solely through RMT methods, but as discussed, the arithmetic term a_k doesn't appear. Conversely, we can obtain the arithmetic term a_k solely through relatively simple number theoretical methods, but then the geometric term g_k disappears. We want a model for the moments of $\zeta(s)$ that treats both the arithmetic and geometric terms equally. Rather than considering $\zeta(s)$ as just an Euler product over primes or just a Hadamard product over zeros, Gonek, Hughes and Keating [149] consider a hybrid model where they write $\zeta(s)$ as a product over primes and over zeros. They write

$$\zeta(s) = P_X(s)Z_X(s)(1+\mathcal{E})$$

where $P_X(s)$ is a product over primes given by

$$P_X(s) = \exp\left(\sum_{n\leq X} \frac{\Lambda(n)}{\log n}\frac{1}{n^s}\right),$$

where $\Lambda(n)$ is the von Mangoldt function, $Z_X(s)$ is a product over zeros given by

$$Z_X(s) = \exp\left(-\sum_{\rho_n} U((s-\rho_n)\log X)\right),$$

where $U(z)$ is given in (5.12), X is a mediating variable, and $\mathcal{E}$ is an error term. Letting $X\to\infty$ gives the Euler product over primes only, and letting $X\to 0$ gives the Hadamard product over zeros only. A balanced value of X gives the hybrid approach.

Next they assume that the moments of $\zeta(s)$ can be written as moments of the primes part multiplied by moments of the zeros part, a result they call the Splitting Conjecture. Specifically, they conjecture that the following holds.

Conjecture 1.10 (Splitting Conjecture)**.** *Let $X, T\to\infty$ with $X = O((\log T)^{2-\varepsilon})$. Then for $k > -1/2$, we have*

$$\frac{1}{T}\int_0^T \left|\zeta\left(\frac{1}{2}+it\right)\right|^{2k} dt \sim \left(\frac{1}{T}\int_0^T \left|P_X\left(\frac{1}{2}+it\right)\right|^{2k} dt\right)\left(\frac{1}{T}\int_0^T \left|Z_X\left(\frac{1}{2}+it\right)\right|^{2k} dt\right).$$

The conjecture was shown to hold for $k=1$ and $k=2$ to leading order. The behaviour of the moments of the prime part is calculated rigorously, with

$$\frac{1}{T}\int_0^T \left|P_X\left(\frac{1}{2}+it\right)\right|^{2k} dt \sim a_k(e^{\gamma_0}\log X)^{k^2}$$

as $X, T\to\infty$ where γ_0 is Euler's constant and a_k is given in (1.19). They also conjecture an asymptotic for the zeros part using RMT, showing

$$\frac{1}{T}\int_0^T \left|Z_X\left(\frac{1}{2}+it\right)\right|^{2k} dt \sim \frac{G^2(k+1)}{G(2k+1)}\left(\frac{\log T}{e^{\gamma_0}\log X}\right)^{k^2}$$

as $X, T\to\infty$.

Combining these terms and using the Splitting Conjecture recovers the Conjecture 1.9, with the arithmetic term now appearing naturally. Note that the hybrid model has been extended in various settings to other L-functions, including the derivative of the Riemann zeta function (see Chapter 5 and [187]). For a collection of the literature on the hybrid model, see [40].

1.3.4.1 Extreme Values of the Riemann zeta function

Recall the Lindelöf Hypothesis asserts that for $t > 0$, for every $\varepsilon > 0$, that $\zeta(1/2 + it) \ll t^{\varepsilon}$. With the assumption of the Riemann Hypothesis, it has been shown [49] that

$$\zeta\left(\frac{1}{2} + it\right) = O\left(\exp\left(\left(\frac{\log 2}{2} + o(1)\right)\frac{\log t}{\log\log t}\right)\right)$$

as $t \to \infty$.

The best known unconditional lower bound can be found in [94] and is given by

$$\max_{t\in[0,T]}\left|\zeta\left(\frac{1}{2} + it\right)\right| \geq \exp\left((\sqrt{2} + o(1))\sqrt{\frac{\log T \log\log\log T}{\log\log T}}\right),$$

as $T \to \infty$.

The true order of $|\zeta(1/2 + it)|$ remains elusive. Using the hybrid model, Farmer, Gonek and Hughes [113] have conjectured the following result concerning the extreme values achieved by the Riemann zeta function on the critical line.

Conjecture 1.11 (Farmer–Gonek–Hughes)**.**

$$\max_{t\in[0,T]}\left|\zeta\left(\frac{1}{2} + it\right)\right| = \exp\left(\left(\frac{1}{\sqrt{2}} + o(1)\right)\sqrt{\log T \log\log T}\right)$$

where the $o(1)$ term tends to zero as $T \to \infty$.

Motivated by the goal of understanding the global maximum order of $|\zeta(1/2 + it)|$, Fyodorov, Hiary, and Keating [130, 131] considered the problem of the local maximum size of the zeta function in randomly chosen intervals of constant length on the critical line. They obtained a precise conjecture for the distribution of this maximum over short intervals. This conjecture has been supported by numerical data [129, 1], something that the conjectures for zeta over large intervals cannot claim due to the length of the interval being calculated over.

Conjecture 1.12 (Fyodorov–Hiary–Keating)**.** *If t is chosen uniformly from $[T, 2T]$, then*

$$\max_{|h|\leq 1}\log\left|\zeta\left(\frac{1}{2} + it + ih\right)\right| = \log\log T - \frac{3}{4}\log\log\log T + X_T,$$

where the random variable X_T is $O(1)$ in size and converges weakly, as $T \to \infty$, to a sum of two independent Gumbel random variables.

As is often the case with understanding the Riemann zeta function, the Fyodorov–Hiary–Keating conjecture was motivated by a connection with random matrices and log-correlated processes, with a summary found in [13]. Much progress has been made on the conjecture in recent years, with sharp upper and lower bounds from the zeta function side found in [6, 7], while the RMT side can be found in [261], confirming the conjecture for both number theory and RMT. These papers also form a good summary of the field, a discussion of which takes us too far from the main aim of this thesis.

1.3.5 Lower Order Terms for Moments

By being guided through analogous results in RMT for the classical compact groups [60], the paper of Conrey, Farmer, Keating, Rubinstein and Snaith [61] developed what is now known as the recipe, a method for determining full asymptotics for moments of $\zeta(s)$ and other L-functions for integer moments. They showed that

$$I_{2k}(T) = \int_0^T \left|\zeta\left(\frac{1}{2}+it\right)\right|^{2k} \, dt = \int_0^T P_k\left(\log \frac{t}{2\pi}\right) \, dt + O\left(T^{1/2+\varepsilon}\right)$$

where P_k is a polynomial of degree k^2 given by a certain residue. We note that they conjecture the error term here to be the correct size for general k (see Section 1.3.2 for a discussion for $k = 2, 4$). However, for other L-functions it can be shown that the recipe misses main terms of the size $O\left(T^{1-\delta}\right)$ for $0 < \delta < 1/2$, as shown in [318, 102, 104].

Conrey, Farmer, Keating, Rubinstein and Snaith [61] begin with integrals of the form

$$\int_0^\infty \left(\prod_{\alpha \in A} \zeta\left(\frac{1}{2}+it+\alpha\right)\right)\left(\prod_{\beta \in B} \zeta\left(\frac{1}{2}-it+\beta\right)\right) \psi\left(\frac{t}{T}\right) \, dt \tag{1.24}$$

where A, B are sets of size k of 'shifts' and ψ is a smooth function of compact support. Letting the shifts tend to zero recovers the $2k^{\text{th}}$ moments.

The recipe is exactly what it sounds like – a non-rigorous method to follow to calculate moments. The rough idea is as follows: we ignore error terms throughout, and write each $\zeta(s)$ term using the approximate functional equation,

$$\zeta(s) \sim \sum_{n \leq \sqrt{t/2\pi}} \frac{1}{n^s} + \chi(s) \sum_{m \leq \sqrt{t/2\pi}} \frac{1}{m^{1-s}}. \tag{1.25}$$

Now keep only the non-oscillatory terms, which is when we can pair off a $\chi(s)$ term with a $\chi(1-s)$ term. Note that

$$\chi(s+\alpha)\chi(1-s+\beta) \sim \left(\frac{t}{2\pi}\right)^{-\alpha-\beta}. \tag{1.26}$$

Then we keep only the diagonal terms, which are those where the imaginary parts disappear, ignoring all off-diagonal terms. In this way we recover the polynomial and can integrate it to give the full asymptotic result.

At the same time and independently, Diaconu, Goldfeld and Hoffstein [103] used a multiple Dirichlet series approach to obtain the same conjectures. We note that this approach does predict the missing terms from the recipe of size $O\left(T^{1-\delta}\right)$ for $0 < \delta < 1/2$. All these approaches are consistent for the main terms which are of size T and larger.

1.3.6 Recent Developments

The development of these conjectures has come from a fruitful link between RMT and number theory. However, as we saw earlier for the first four moments, we can obtain the same results and conjectures from number theoretical approaches which fail for $k \geq 5$ as they predict negative values. The approach taken is to write $\zeta(s)$ as a Dirichlet polynomial and calculate moments of these.

In a series of five papers, Conrey and Keating [78, 79, 80, 81, 84] showed how to fix this approach by taking long Dirichlet polynomials, much longer than were previously considered to avoid missing any terms. They showed that (1.24) can be calculated either by multiple contour integrals as in the recipe, or by considering Dirichlet series

$$\prod_{\alpha \in A} \zeta\left(\frac{1}{2} + it + \alpha\right) = \sum_{n=1}^{\infty} \frac{\tau_A(n)}{n^s}$$

and considering divisor sum correlations, where the arithmetic function $\tau_A(n)$ is defined by the Euler product expansion of the left-hand side of the equation. For the first time, they united the RMT and number theoretic approaches and showed that either approach gives exactly the same result. They also showed that in a further two papers [82, 83], the Ratios Conjecture (as seen later in Section 6.1) can also be derived in this way.

While this approach is still conjectural, some progress has been made. For example, in their series of papers, Conrey and Keating showed that what we call the 1-swap terms for moments of $\zeta(s)$ are a consequence of formulas for correlations of divisor sums. Hamieh and Ng [161] have made this rigorous, under the assumption of the asymptotic formulae for correlations of divisor sums, which come from applying the delta method of Duke, Friedlander and Iwaniec [106] to the sum

$$\sum_{\substack{m,n=1 \\ m-n=h}}^{\infty} \tau_A(m)\tau_B(n)f(m,n)$$

for suitable f and ignoring the error terms.

Knowing the results and methods from this approach has proved to be incredibly fruitful. Ng [255], assuming a certain ternary divisor conjecture, has recovered the full asymptotic formula predicted by the recipe for the sixth moment. Specifically, he recovered the analogous shifted form for the sixth moment that Ingham did for the second moment in (1.15). Also, Ng, Shen and Wong [256], assuming a quaternary ternary divisor conjecture, have recovered the leading order term for the eighth moment. Their approach is yet to be extended to higher order moments.

Additionally, the problem of negative continuous moments has come to the fore recently. For $k > 0$ and $\alpha > 0$, let

$$I_{-2k}(\alpha, T) = \int_0^T \left| \zeta\left(\frac{1}{2} + \alpha + it\right) \right|^{-2k} dt.$$

Gonek [145] made the following conjecture for various ranges of k and α.

Conjecture 1.13 (Gonek)**.** *Let $k > 0$. Uniformly for $\frac{1}{\log T} \leq \alpha \leq 1$, we have*

$$I_{-2k}(\alpha, T) \asymp T \left(\frac{1}{\alpha}\right)^{k^2}$$

and uniformly for $0 < \alpha \leq \frac{1}{\log T}$, we have

$$I_{-2k}(\alpha, T) \asymp \begin{cases} T(\log T)^{k^2} & \text{if } k < 1/2 \\ T \log \frac{e}{\alpha \log T} (\log T)^{k^2} & \text{if } k = 1/2 \\ T(\alpha \log T)^{1-2k} (\log T)^{k^2} & \text{if } k > 1/2. \end{cases}$$

More recent RMT computations due to Berry and Keating [23], and due to Forrester and Keating [120] suggest that certain corrections to Gonek's conjecture is due in some ranges. Namely, when $\alpha \leq 1/\log T$, RMT computations contradict Gonek's prediction for the negative moments when $k \geq 3/2$. In particular, the RMT predictions suggest certain transition regimes when k is half an odd positive integer. Gonek's conjecture already captures the first transition at $k = 1/2$ featuring a logarithmic correction, and in this case the two conjectures do agree. Interpreted correctly, the following conjectures have been made on the number theory side, based on the aforementioned RMT calculations.

Conjecture 1.14 (Berry–Keating, Forrester–Keating, Bui–Florea)**.** *Let $k > 0$. Uniformly for $\frac{1}{\log T} \leq \alpha \leq 1$, we have*

$$I_{-2k}(\alpha, T) \sim a(k) T \left(\frac{1}{\alpha}\right)^{k^2}$$

and uniformly for $0 < \alpha \leq \frac{1}{\log T}$, we have

$$I_{-2k}(\alpha, T) \sim \begin{cases} a(k) T (\log T)^{k^2} (\alpha \log T)^{-j(2k-j)} & \text{if } j - 1/2 < k < j + 1/2 \\ a(k) T \log \frac{e}{\alpha \log T} (\log T)^{k^2} (\alpha \log T)^{-j(j-1)} & \text{if } k = j - 1/2 \text{ for } j \geq 1 \end{cases}$$

and where

$$a(k) = \prod_p \left(1 - \frac{1}{p^{1+2\alpha}}\right)^{k^2} \left(1 + \sum_{j=1}^{\infty} \frac{\mu_k(p^j)^2}{p^{(1+2\alpha)j}}\right),$$

where $\mu_k(n)$ denotes the n^{th} coefficient of the Dirichlet series for $\zeta(s)^{-k}$.

Various progress on the zeta function side has been made by Bui and Florea [43]. Additionally, results on negative moments of quadratic Dirichlet L–functions have been proved in the function field setting in [44, 116]. Problems relating to negative continuous moments are of interest due to their relation to the Ratios Conjecture, described in detail in Chapter 6.

1.3.7 Applications of Moments

1.3.7.1 Sub-convexity of $\zeta(s)$

We have already discussed the initial motivation for studying moments, that of proving the Lindelöf Hypothesis. As always, $\varepsilon > 0$ isn't necessarily the same throughout. From the approximate functional equation (1.25), we obtain the convexity bound

$$\left|\zeta\left(\frac{1}{2}+it\right)\right| \ll (1+|t|)^{1/4+\varepsilon}.$$

Going beyond the convexity bound involves showing cancellation in the exponential sums in the approximate functional equation (1.25). This is an active area of research, starting with Weyl [310], and Hardy and Littlewood (unpublished) who showed that

$$\left|\zeta\left(\frac{1}{2}+it\right)\right| \ll (1+|t|)^{1/6+\varepsilon}.$$

The exponent 1/6 is a consequence of Weyl's differencing method for estimating exponential sums, first introduced in 1916. The best known result is due to Bourgain [37] who showed that

$$\left|\zeta\left(\frac{1}{2}+it\right)\right| \ll (1+|t|)^{13/84+\varepsilon}.$$

Sharp moment estimates encode Lindelöf on average, and in some cases, can also yield pointwise sub-convexity estimates. Moments encode this information. For example Ingham's fourth moment (1.17) yields the convexity bound above, while Heath-Brown's result [171]

$$\int_0^T \left|\zeta\left(\frac{1}{2}+it\right)\right|^{12} dt \ll T^{2+\varepsilon}$$

implies (and is stronger than) the sub-convexity bound of Weyl, Hardy and Littlewood.

1.3.7.2 Twisted and Mollified Moments

Another type of moment question is that of twisted, or mollified moments, which are integrals of the form

$$\int_0^T \left|\zeta\left(\frac{1}{2}+it\right)\right|^{2k} \left|M_N\left(\frac{1}{2}+it\right)\right|^2 dt$$

where

$$M_N(s) = \sum_{n=1}^{N} \frac{a(n)}{n^s}$$

and the coefficients satisfy $a(n) \ll n^{\varepsilon}$ for all $\varepsilon > 0$.

Bohr and Landau [33] were the first to consider such questions, with the aim to calculate a zero-density estimate for zeta, described in Section 1.3.7.4. They used a mollified moment, one where the coefficients in $M_N(s)$ are given by $a(n) = \mu(n)$ where $\mu(n)$ is the Möbius function, defined by

$$\mu(n) = \begin{cases} 1 & \text{if } n = 1 \\ (-1)^k & \text{if } n = p_1...p_k \text{ with the } p_j \text{ distinct primes} \\ 0 & \text{if } n \text{ is not square-free.} \end{cases} \tag{1.27}$$

This sum $M_N(s)$ is essentially an approximation to $1/\zeta(s)$ for $\sigma > 1$. If this approximation is also valid in the critical strip, then $M_N(s)$ should dampen large values of $\zeta(s)$.

The twisted second moment was calculated by Balasubramanian, Conrey and Heath-Brown [15] for mollifiers of length $N = T^{1/2-\varepsilon}$ and where $a(n) \ll n^{\varepsilon}$.

Bettin, Chandee and Radziwiłł [28] calculated the twisted second moment for mollifiers of length $N = T^{1/2+\delta}$, where $\delta = 0.01515\ldots$ and where $a(n) \ll n^{\varepsilon}$.

Setting $k = 1$ and $a(n) = \mu(n)P(\log(n/y)/\log y)$, where $P(x)$ is a polynomial satisfying $P(0) = 0$, $P(1) = 1$ that is optimised through the calculus of variations, we have a mollified second moment which was considered by Levinson [222] when he showed that one-third of the zeros of $\zeta(s)$ lie on the critical line. Conrey [56] increased this length to $N = T^{4/7-\varepsilon}$ and proved that 40% of the zeros of $\zeta(s)$ lie on the critical line, a fact we discuss further in Section 1.3.7.3.

Conrey, Ghosh and Gonek [74] considered the problem of twisted second moments in a more general setting. To describe their result, we set up some notation. Let T be a large positive real number and let

$$B(s,P) = \sum_{n \le y} \frac{\mu(n)P\left(\frac{\log y/n}{\log y}\right)}{n^s}$$

where $y = T^{\theta}$ for $\theta < 1/2$, $P(x)$ is an entire function with $P(0) = 0$, and $\mu(n)$ is the Möbius function (1.27). Let a, b be complex numbers and $Q_1(x)$ and $Q_2(x)$ be polynomials.

They claim that for fixed c with $1/2 \le c < 3/2 - \theta$, and $a, b \ll 1$, then as $T \to \infty$,

$$\frac{1}{i}\int_{c+i}^{c+iT} Q_1\left(-\frac{d}{da}\right)\zeta\left(s+\frac{a}{\log T}\right)Q_2\left(-\frac{d}{db}\right)\zeta\left(1-s+\frac{b}{\log T}\right)B(s,P_1)B(1-s,P_2)\,ds$$
$$\sim T\left\{Q_1(0)Q_2(0)P_1(1)P_2(1) + \frac{\partial}{\partial u}\frac{\partial}{\partial v}\frac{1}{\theta}\left(\int_0^1 T_aQ_1T_bQ_2\,dx\right)\left(\int_0^1 P_1P_2\,dx\right)\Bigg|_{u=v=0}\right\},$$

where $P_1 = P_1(x+u)$, $P_2 = P_2(x+v)$,

$$T_a Q_1 = e^{-a(x+\theta u)} Q_1(x+\theta u) \text{ and } T_b Q_2 = e^{-b(x+\theta v)} Q_2(x+\theta v).$$

Then several results follow easily from here. For example, it is easy to see that this reduces down to the twisted second moment, and that

$$\int_1^T \left|\zeta\left(\frac{1}{2}+it\right)\right|^2 \left|B\left(\frac{1}{2}+it,P\right)\right|^2 \, dt \sim T\left(P(1)^2 + \frac{1}{\theta}\int_0^1 P'(x)^2 \, dx\right).$$

Also, if we let $P_1(x) = P_2(x) = x$, $Q_1(x) = Q_2(x) = -1-x$, $c = 1/2$, $a = -b = -1.3$ and let $\theta \to 1/2^-$, then Levinson's [222] result that at least one-third of the zeros of the zeta function lie on the critical line. Various zero density results follow, for example those found in [276, 278, 204].

For the twisted fourth moment, Deshouillers and Iwaniec [101] were able to obtain upper bounds when the Dirichlet polynomial has length $N = T^{1/5-\varepsilon}$. This was later improved by Watt [307] for length $N = T^{1/4-\varepsilon}$. Gaggero Jara [203] was able to obtain a leading order result for the mollified fourth moment for length $N = T^{4/589-\varepsilon}$ but wasn't able to obtain lower order terms. Independently, Motohashi [248], and Hughes and Young [188] were able to obtain full asymptotics, with the later doing so for length $N = T^{1/11-\varepsilon}$. Finally, Bettin, Bui, Li and Radziwiłł [26] have extended this for length $N = T^{1/4-\varepsilon}$.

As hinted to above, these mollified moments have applications to proportions of zeros on the critical line, which we discuss further in Section 1.3.7.3, as well as to gaps between zeta zeros discussed in Section 1.4.3.3, and for lower bounds of moments discussed in Section 1.3.2.1.

1.3.7.3 Zeros on the critical line

As alluded to in Section 1.3.7.2, one use of these mollified moments is to calculate proportions of zeros on the critical line. We already gave a brief history of calculating proportions of zeros on the critical line when we discussed the Riemann Hypothesis in Section 1.1.3.1, but give a more detailed history here.

We write $N_0(T)$ for the number of zeros of $\zeta(s)$ on the critical line up to height T above the real axis, and let $N(T)$ be as in (1.4). We let

$$\kappa = \liminf_{T\to\infty} \frac{N_0(T)}{N(T)}$$

denote the proportion of non-trivial zeros of $\zeta(s)$ that lie on the critical line.

Selberg [276] first implicitly showed that a positive proportion of the non-trivial zeros of the zeta function are on the critical line. He did this by introducing a mollifier to a method of Hardy and Littlewood [165] for detecting zeros of $\zeta(s)$. Min [238] later made this proportion explicit.

Since first introducing the mollifier method, a great deal of progress has been made on the proportion of zeros on the critical line. They are based on a different approach to the one taken by Selberg, and started when Levinson [222] introduced the mollifier method to an approach of Siegel's [282] in detecting zeros of $\zeta(s)$. Levinson showed that $\kappa \geq 0.3474$, while Conrey [56] improved this to $\kappa \geq 0.4088$. Further improvements have since been made, for example by Bui, Conrey, and Young [42] who showed $\kappa \geq 0.4105$. Feng [115] gave a further improvement, although it has been suggested that there is an error in this work. The value that is claimed to follow from this work is $\kappa \geq 0.4107$. Bui [41] pushed this further to show $\kappa \geq 0.4109$. The current record is due to Pratt, Robles, Zaharescu and Zeindler [265], who showed that $\kappa \geq 0.4172$, or rather, more than over five-twelfths of the non-trivial zeros of the Riemann zeta function lie on the critical line. Wu [315] independently showed this same result for Dirichlet L-functions as a side calculation when calculating a twisted second moment of a Dirichlet L-function, and showed agreement with the result of Pratt, Robles, Zaharescu and Zeindler. Note that these methods give as a free corollary various improvements in the proportions of simple zeros, as discussed in Section 1.4.3.1.

A third method has been explored by Baluyot [17], where he combines the mollifier method with a zero detecting method of Atkinson's [11] to show in a new way that the proportion κ is positive. This relies on the twisted fourth moment of Hughes and Young [188], discussed in the previous section. He uses this method to show that $\kappa > 0.0001049$. While this is obviously a smaller proportion than what was previously known, it does open up a new way to find these proportions.

The method we focus on here is Levinson's method, as he was the first to exploit it to show that one-third of the zeros of $\zeta(s)$ lie on the critical line. Levinson's original proof runs for over fifty pages, with the main difficulty being a certain moments result. Knowing how to calculate mollifiers using the Ratios Conjecture, discussed in Section 6.1.3, Young [316] was able to shorten this argument down to just eight pages. We give a rough outline of the steps used by Young here.

The first result to note is known as Littlewood's Lemma [227], which is an analogous result to Jenson's formula, a result that relates the average size of a function to its zeros. Littlewood's Lemma is the result for rectangles which is generally more useful when working with Dirichlet series. We state a version that ignores some technicalities as we aren't giving full proofs when describing these applications.

Lemma 1.15 (Littlewood)**.** *Let f be analytic and non-zero on the rectangular positively oriented contour C with vertices $\sigma_1, \sigma_1 + iT, \sigma_0 + iT, \sigma_0$, where $\sigma_0 < \sigma_1$. Then*

$$\sum_{\rho \in C} \mathrm{Dist}(\rho) = \frac{1}{2\pi} \int_0^T \log |f(\sigma_0 + it)| \, dt + \mathcal{E}$$

where $\mathrm{Dist}(\rho)$ *is the distance of the zero* ρ *to the line* $\Re(s) = \sigma_0$ *and* $\mathcal{E}$ *is an error term that can be ignored and might be different on different occasions.*

The second result to note is Speiser's Theorem [292], which provides an equivalent form of the Riemann Hypothesis.

Theorem 1.16 (Speiser)**.** *The Riemann Hypothesis is equivalent to the assertion that the derivative of* $\zeta(s)$ *has no zeros to the left of the critical line inside the critical strip.*

We define $N_L(T)$ to be the number of zeros of $\zeta(s)$ to the left of the critical line inside the critical strip up to height T above the real axis and $N_L'(T)$ to be the number of zeros of $\zeta'(s)$ to the left of the critical line inside the critical strip up to height T above the real axis. Then Levinson and Montgomery [223] made Speiser's Theorem quantitative by showing that

$$N_L(T) = N_L'(T) + O(\log T).$$

Recall that $N_0(T)$ is the number of zeros of $\zeta(s)$ on the critical line up to height T above the real axis. Then we know from previous discussions that the number of zeros to the right of the critical line inside the critical strip is equal to the number of zeros to the left of the critical line inside the critical strip. Therefore,

$$\begin{aligned} N(T) &= N_0(T) + 2N_L(T) \\ &= N_0(T) + 2N_L'(T) + O(\log T). \end{aligned}$$

Rearranging,

$$N_0(T) = N(T) - 2N_L'(T) + O(\log T)$$

so if we can find a small upper bound for $N_L'(T)$, then we will have a lower bound for $N_0(T)$ as we know what $N(T)$ equals already by (1.5).

Due to technical reasons, we don't count zeros of $\zeta'(1-s)$, and instead count zeros of the function $V(s)$, where

$$V(s) = Q\left(-\frac{1}{L}\frac{d}{ds}\right)\zeta(s)$$

and $Q(x)$ is a real polynomial satisfying $Q(0) = 1$, with $L = \log T$. Levinson [222] originally takes $Q(x) = 1 - x$, but Conrey [56] showed that more general choices of $Q(x)$ can be used to improve results.

Set

$$\sigma_0 = \frac{1}{2} - \frac{R}{L}$$

where $R > 0$ is real number chosen later, and let $N = T^{\theta}$ where $0 < \theta < 1/2$.

Suppose $\psi(s)$ is a mollifier of the form

$$\psi(s) = \sum_{n \leq N} \frac{\mu(n)}{n^{s+1/2-\sigma_0}} P\left(\frac{\log N/n}{\log N}\right)$$

where $P(x)$ is a real polynomial with $P(0) = 0$ and $P(1) = 1$. Levinson originally takes $P(x) = x$ but again this can be optimised in more general cases.

Then one can show

$$N_L'(T) \leq \frac{T}{4\pi} \log\left(\frac{1}{T}\int_0^T |V\psi(\sigma_0 + it)|^2 \, dt\right) + \mathcal{E}$$

and evaluating this integral is where the main difficulty lies.

Young showed a simpler way to evaluate this moment, which we summarise as the following theorem.

Theorem 1.17 (Young)**.** *We have*

$$\frac{1}{T}\int_0^T |V\psi(\sigma_0 + it)|^2 \, dt = c(P, Q, R, \theta) + \mathcal{E}$$

as $T \to \infty$, where

$$c(P, Q, R, \theta) = 1 + \frac{1}{\theta}\int_0^1 \int_0^1 e^{2Rv}\left(\frac{d}{dx} e^{R\theta x} P(x+u) Q(v + \theta x)\Big|_{x=0}\right)^2 \, du dv.$$

With Levinson's original choices of $P(x) = x$, $Q(x) = 1 - x$, $R = 1.3$, $\theta = 1/2$, we have, $c(P, Q, R, \theta) \approx 2.35$. Then we have

$$\kappa \geq 1 - \frac{1}{R}\log\left(\frac{1}{T}\int_0^T |V\psi(\sigma_0 + it)|^2 \, dt\right) + o(1).$$

and using Levinson's original inputs gives $\kappa \geq 0.34$.

Farmer [112] conjectures that we can set $\theta = \infty$ for mollifiers. This means that the mollifier can be made arbirarily long, and so turns the mollifier into $1/\zeta(s)$. This prompted him to first consider what has become known as the Ratio's Conjecture, described in Chapter 6. This together with Theorem 1.17 implies that we have 100% of the zeros lie on the critical line. This conjecture is of particular interest as Bettin and Gonek [29] have shown that the $\theta = \infty$ conjecture implies the Riemann Hypothesis which is stronger than showing 100% of the zeros lie on the critical line. Farmer [112] also argues that a strong form of this conjecture implies Montgomery's Pair Correlation conjecture. Additionally, Radziwiłł [266] showed that as $\theta \to \infty$, $\psi(s)$ is essentially the best possible mollifier of length T^θ for $\zeta(s)$. In particular his work implies that Levinson's method can give $\kappa = 1$ only if it is used with mollifiers of length T^θ when θ is arbitrarily large.

1.3.7.4 Zero-density estimates

One can show that there are relatively few zeros in the region $1/2 < \sigma_0 < 1$ (and so few in the region $0 < \sigma_0 < 1/2$ by the functional equation).

These results are typically of the form

$$N(\sigma, T) \ll T^{A(\sigma)(1-\sigma)+\varepsilon}$$

as $T \to \infty$, where

$$N(\sigma, T) = \#\{\rho = \beta + i\gamma \;:\; \sigma \leq \beta \leq 1, 0 < \gamma < T\}$$

counts the number of zeros of $\zeta(s)$ with real part at least σ and imaginary part at most T. Note that the $\varepsilon > 0$ in the above equation for $N(\sigma, T)$ can be made (in theory) explicit in this section, replacing it with powers of logarithms.

The Density Hypothesis asserts that

$$N(\sigma, T) \ll T^{2(1-\sigma)+\varepsilon}$$

for all $\varepsilon > 0$, that is, $A(\sigma) = 2$.

Clearly the Riemann Hypothesis is equivalent to $N(\sigma, T) = 0$ for all $\sigma > 1/2$ and all $T > 0$. It is known [193] that the Lindelöf Hypothesis implies the Density Hypothesis. We also know thanks to the proof of the Prime Number Theorem and the fact there are no zeros on the line $\Re(s) = 1$ (see Section 1.1.4) that $N(1, T) = 0$, so $A(1) = 0$.

Ingham [194] proved the uniform bound for $N(\sigma, T)$ with

$$A(\sigma) = \frac{3}{2 - \sigma}$$

in the range $1/2 \leq \sigma \leq 3/4$, using the Montgomery–Vaughan Mean-Value Theorem [243]. Huxley [189] proved the uniform bound $N(\sigma, T)$ with

$$A(\sigma) = \frac{3}{3\sigma - 1}$$

in the range $3/4 \leq \sigma \leq 1$ using the Montgomery–Halász large value estimate [242] and [156].

Combined, these values of $A(\sigma)$ show

$$N(\sigma, T) \ll T^{\frac{12}{5}(1-\sigma)+\varepsilon}.$$

Together, these bounds show results on prime numbers, in particular,

$$p_{n+1} - p_n \ll p_n^{7/12+\varepsilon}$$

where p_n denotes the n^{th} prime number. Note that the Density Hypothesis implies

$$p_{n+1} - p_n \ll p_n^{1/2+\varepsilon}$$

while the Riemann Hypothesis implies

$$p_{n+1} - p_n \ll p_n^{1/2} \log p_n,$$

neither of which are strong enough to prove the conjecture that between any two square numbers there is always a prime number.

Guth and Maynaard [153] improved the Huxley bound above to show

$$N(\sigma, T) \ll T^{\frac{30}{13}(1-\sigma)+\varepsilon}$$

in the full range, showing

$$p_{n+1} - p_n \ll p_n^{17/30+\varepsilon}.$$

For the summary of the intervening history between the combined result of Montgomery and Huxley, and of Montgomery and Guth–Maynaard, see Table 2 in Trudgian and Yang [300].

To see the link between these results and continuous moments, we sketch the argument of the first zero-density estimate of Bohr and Landau [33], following the sketch given in Gonek [148].

Let C be a positively oriented rectangular contour enclosing the region $1/2 \le \Re(s) < 1$ with left side $\Re(s) = \sigma_0$ up to a height T. By Littlewood's Lemma 1.15 we have

$$\sum_{\rho \in C} \text{Dist}(\rho) = \frac{1}{2\pi} \int_0^T \log |f(\sigma_0 + it)| \, dt + \mathcal{E}$$

where $\text{Dist}(\rho)$ is the distance of the zero ρ to the line $\Re(s) = \sigma_0$.

Then for σ a fixed real number with $\sigma_0 < \sigma < 1$, for non-trivial zeros $\rho = \beta + i\gamma$ of $\zeta(s)$, we have

$$\sum_{\rho \in C} \text{Dist}(\rho) \ge \sum_{\substack{\rho \in C \\ \sigma \le \beta}} \text{Dist}(\rho) \ge (\sigma - \sigma_0) N(\sigma, T).$$

Typically it is difficult to calculate the integral of the logarithm directly, so instead use the arithmetic-geometric mean to write

$$\frac{1}{2\pi} \int_0^T \log |f(\sigma_0 + it)| \, dt = \frac{1}{4\pi} \int_0^T \log(|f(\sigma_0 + it)|^2) \, dt \le \frac{T}{4\pi} \log \left(\frac{1}{T} \int_0^T |f(\sigma_0 + it)|^2 \, dt \right).$$

It is known (Theorem 7.2 of [298]) that

$$\int_0^T |\zeta(\sigma_0 + it)|^2 \, dt \sim \zeta(2\sigma_0) T$$

so this last inequality is $O(T)$. Therefore,

$$N(\sigma, T) \ll \frac{T}{\sigma - \sigma_0}$$

and since $N(T) \sim T \log T$, we have

$$\frac{N(\sigma, T)}{N(T)} = O\left(\frac{1}{\log T}\right)$$

for any fixed $\sigma > 1/2$. This means that the proportion of zeros to the right of the critical line is infinitesimally small.

Note that if we had included mollifiers in this argument, then we would have obtained better zero-density estimates. As seen above, we now have much better zero-density estimates.

1.3.8 Joint Moments of the Riemann zeta function and Joint Moments of the Hardy Z-function

Hall [158] conjectured that the joint moments of the Riemann zeta function are of the form

$$\int_0^T \left|\zeta\left(\frac{1}{2} + it\right)\right|^{2s-2h} \left|\zeta'\left(\frac{1}{2} + it\right)\right|^{2h} \, dt \sim C(s, h) T (\log T)^{s^2+2h}.$$

These joint moments can also be written in terms of the Hardy Z-function (see Section 1.3.8.1) as

$$\int_0^T |Z(t)|^{2s-2h} |Z'(t)|^{2h} \, dt \sim \tilde{C}(s, h) T (\log T)^{s^2+2h},$$

where the coefficients $C(s, h)$ can be written in terms of $\tilde{C}(s, h)$ and vice versa, as shown in [181].

For the joint moments of the Riemann zeta function, we already know due to Hardy and Littlewood [164] that $C(1, 0) = 1$, and to Ingham [192] that $C(1, 1) = 1/3$. Also, Ingham [192] showed $C(2, 0) = 1/2\pi^2$ and Conrey [55] (and independently Hall [157]) showed that $C(2, 1) = 2/15\pi^2$ and $C(2, 2) = 61/1680\pi^2$. The analogous results for the Hardy Z-function joint moments can be deduced from these, with $\tilde{C}(1, 1) = 1/12$, $\tilde{C}(2, 1) = 1/120\pi^2$ and $\tilde{C}(2, 2) = 1/1120\pi^2$. Conrey and Ghosh [66, 67] have shown that $\tilde{C}(1, 1/2) = (e^2 - 5)/4\pi$ but $C(1, 1/2)$ is currently unproven. We come back to this result of Conrey and Ghosh in Section 1.3.8.3 and in Chapter 7. As with the usual continuous moments, RMT has since been used to predict higher moments, which we describe to in Section 1.3.8.2.

We now take this opportunity to discuss the Hardy Z-function, a function that acts like the Riemann zeta function on the critical line, as well as some of its properties and various related points of interest, before giving some background on the RMT approach to joint moments.

1.3.8.1 The Hardy Z-function

The Riemann—Siegel theta function is defined as

$$e^{-2i\theta(t)} = \chi\left(\frac{1}{2}+it\right), \tag{1.28}$$

where $\chi(s)$ is the factor from the functional equation of $\zeta(s)$ stated in (1.1). The Hardy Z-function can be defined in terms of the Riemann—Siegel theta function, where

$$Z(t) = e^{i\theta(t)}\zeta\left(\frac{1}{2}+it\right).$$

This means we can write

$$Z(t) = \chi\left(\frac{1}{2}+it\right)^{-1/2}\zeta\left(\frac{1}{2}+it\right).$$

Note that $Z(t)$ is real for real t, $Z(-t) = Z(t)$, and satisfies $|Z(t)| = |\zeta(1/2+it)|$.

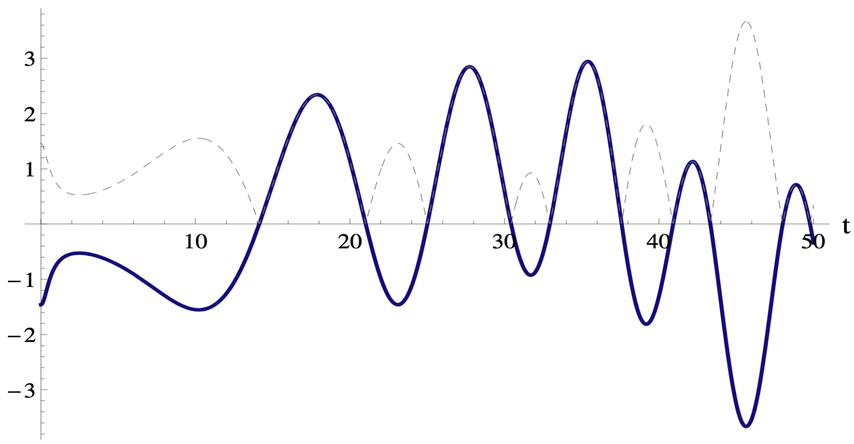

Figure 1.3: A plot of $Z(t)$ (dark blue) and $|\zeta(1/2+it)|$ (dashed) for $0 \leq t \leq 50$.

From these observations, we know that the zeros of $\zeta(s)$ on the critical line correspond to the real zeros of $Z(t)$ which makes $Z(t)$ an invaluable tool in the study of the zeros of the zeta function on the critical line. For example, Hardy used his Z-function to give the first proof that there are infinitely many zeros of the Riemann zeta function on the critical line [199].

The Riemann–Siegel formula allows us to write

$$Z(t) = 2\sum_{n=1}^{N} n^{-1/2}\cos(\theta(t) - t\log n) + R$$

where $N = \lfloor (t/2\pi)^{1/2} \rfloor$ and R is a certain error term. This is a highly efficient way of calculating values of the Riemann zeta function, with increasing accuracy as t increases.

The Riemann–Siegel formula was derived and used by Riemann, but never published by him. It was not until 1932 that Carl Siegel uncovered the formula following a study of Riemann's unpublished notes. The method of choice before the rediscovery of the Riemann–Siegel formula to calculate values of zeta was Euler–Maclaurin summation, which requires $O(t)$ steps to evaluate zeta on the half-line. The advantage to the Riemann–Siegel formula is that it requires only $O(t^{1/2})$ steps. This method has been used to verify the correctness of the Riemann Hypothesis up to very large values of t, with modern variations giving improvements to the calculations.

Turing [301] developed a method which allows one to calculate the number of zeros in the critical strip up to a height T. Once all zeros on the critical line up to height T have been counted using the Riemann–Siegel formula, Turing's method is then used to verify that the zeros found are indeed the only zeros in this part of the critical strip. In fact, Turing was trying to use this method to show that the Riemann Hypothesis is false.

We return to the observation that the zeros of $\zeta(s)$ on the critical line correspond to the real zeros of $Z(t)$. We note that for $\gamma \leq \gamma^+$ consecutive positive ordinates of non-trivial zeros of $\zeta(s)$, there is exactly one zero of $Z'(t)$ (under the Riemann Hypothesis), call it λ, with $\gamma \leq \lambda \leq \gamma^+$. A proof of this result can be found in [199]. These points λ will be essential in our results given in Chapter 7, where we sum over these points, and this notation provides an unambiguous way of writing the results discussed there. Note that there are two zeros of $Z'(t)$ between $t = 0$ and the first positive zero of $Z(t)$. These additional zeros typically only introduce small errors and are generally ignored.

1.3.8.2 Joint Moments through RMT

We note that the background in this section has appeared in a paper [183]. Notation and cross-references have been updated for this thesis.

Following the groundbreaking work of Keating and Snaith [211, 210], the problem of calculating joint moments of the Riemann zeta function and its derivative through RMT was taken up by Hughes [181] in his thesis. The approaches taken involved calculating analogous moments of characteristic polynomials of random unitary matrices.

Hughes [181] considered the joint moment for the Riemann zeta function and conjectured the coefficient $F_\zeta(s,h)$ for integer s, h in terms of combinatorial sums, where $F_\zeta(s,h)$ is given in

$$\int_0^T \left|\zeta\left(\frac{1}{2}+it\right)\right|^{2s-2h} \left|\zeta'\left(\frac{1}{2}+it\right)\right|^{2h} \, dt \sim a_s F_\zeta(s,h) T (\log T)^{s^2+2h}$$

as $T \to \infty$, where a_s is defined in (1.19).

Similarly, Hughes predicted that

$$\int_0^T |Z(t)|^{2s-2h} |Z'(t)|^{2h} \, dt \sim a_s F_Z(s,h) T (\log T)^{s^2+2h}$$

as $T \to \infty$, where a_s is defined in (1.19), together with a way of translating between $F_\zeta(s,h)$ and $F_Z(s,h)$.

The conjectures agreed with all values known at the time as described in Section 1.3.8. The expressions for $F_\zeta(s,h)$ and $F_Z(s,h)$ made sense for real s as well, but not general real h. We focus on the Hardy Z-function joint moment in this thesis, but note that many of the following results also hold for $F_\zeta(s,h)$.

Alternative approaches yielding different representations of the conjectured $F_Z(s,h)$ with $s,h \in \mathbb{N}$ were given by Conrey, Rubinstein and Snaith [85] (in the special case where $s=h$), by Dehaye [97, 98], by Basor et al. [20], and by Bailey et al. [12]. Links between $F(s,h)$ and Painlevé equations have been noted by Forrester and Witte [121], and Basor et al. [20].

However, the problem of non-integer s and h is much more difficult. Winn [312] was able to establish results for $s \in \mathbb{N}$ and $h \in \frac{1}{2}\mathbb{N}$ by finding connections with hypergeometric functions, giving an expression for $F_Z(s,h)$ in terms of a combinatorial sum. In particular, for $s=1$ and $h=1/2$ he obtained the $(e^2-5)/4\pi$ coefficient for the analogous RMT result to the Hardy Z-function joint moment considered by Conrey and Ghosh [66, 67].

Assiotis, Keating and Warren [9] proved results on the random matrix side for arbitrary real values of $s > -1/2$ and positive real values of h in the full range $0 < h < s + 1/2$. They also give a full history of these problems in their paper.

In addition to the work on the standard joint moment, Keating and Wei [212, 213] have considered the RMT analogue of joint moments for higher derivatives. The case of the joint moments of arbitrary numbers of higher order derivatives with arbitrary positive real exponents has been settled by Assiotis, Gunes, Keating and Wei [8].

Curran [92] unconditionally obtained upper bounds of the conjectured order for the joint moments in the range $1 \le s \le 2$ and $0 \le h \le 1$. Curran and Heycock [93] extend these upper bounds to all $0 \le h \le s \le 2$, and obtain lower bounds for all $0 \le h \le s + 1/2$. By assuming the Riemann Hypothesis, they give sharp bounds for all $0 \le h \le s$. They also prove upper bounds of the conjectured order for joint moments of the Riemann zeta function with its higher derivatives.

1.3.8.3 The Joint Moment of the Hardy Z-function and its derivative

For a long time, there was a problem that number theory could solve that RMT could not. We mentioned previously that Conrey and Ghosh [66, 67] showed $\tilde{C}(1/2,1) = (e^2-5)/4\pi$, which means that they showed

$$\int_0^T |Z(t)||Z'(t)|\ dt \sim \frac{e^2-5}{4\pi} T(\log T)^2.$$

However, while Hughes [181] predicted the general joint moments for even integer powers, his method didn't generalise to odd integer powers, nor did the work that followed on this problem. It would be over a decade before Winn [312] would develop the RMT tools to predict these results. We note that the corresponding problem with the Hardy Z-function replaced by the Riemann zeta function is still unproven from the number theory side.

To prove the joint moment result, Conrey and Ghosh [66] showed that under the Riemann Hypothesis,

$$\sum_{0<\gamma\leq T} \max_{\gamma\leq t\leq\gamma^+} \left|\zeta\left(\frac{1}{2}+it\right)\right|^2 \sim \frac{e^2-5}{4\pi} T(\log T)^2$$

as $T\to\infty$ where for each non-trivial zero $\rho = 1/2+i\gamma$, let γ^+ denote the ordinate of the successive non-trivial zero of $\zeta(s)$.

The relation between this sum and the joint moment follows by recalling that under the Riemann Hypothesis, there is a unique point $\gamma\leq\lambda\leq\gamma^+$ between successive zeros $\gamma\leq\gamma^+$ that satisfies $Z'(\lambda)=0$. In [67], they split the integral as

$$\int_0^T |Z(t)||Z'(t)|\,dt = \int_0^{\gamma_0} |Z(t)||Z'(t)|\,dt + \sum_{0<\lambda\leq T}\left(\int_\gamma^\lambda + \int_\lambda^{\gamma+}\right)|Z(t)||Z'(t)|\,dt + \int_{\gamma_T}^T |Z(t)||Z'(t)|\,dt,$$

where γ_0 denotes the least positive zero of $Z(t)$ and γ_T denotes the least zero of $Z(t)$ that is larger than T. Note that if $\gamma\leq t\leq\lambda$, $Z(t)Z'(t)\geq 0$ and if $\lambda\leq t\leq\gamma^+$, $Z(t)Z'(t)\leq 0$. Then the integral above becomes

$$\sum_{0<\lambda\leq T}\left(\frac{Z(t)^2}{2}\bigg|_\gamma^\lambda - \frac{Z(t)^2}{2}\bigg|_\lambda^{\gamma^+}\right) + O\left(T^\varepsilon\right) = \sum_{0<\lambda\leq T}|Z(\lambda)|^2 + O\left(T^\varepsilon\right)$$

since $Z(t)Z'(t)\ll t^\varepsilon$ and $|\gamma_T - T|\ll 1$.

For higher moments, Conrey [55] established under the Riemann Hypothesis that

$$\frac{\sqrt{21}}{90\pi^2}T(\log T)^5 \lesssim \sum_{0<\gamma\leq T}\max_{\gamma\leq t\leq\gamma^+}\left|\zeta\left(\frac{1}{2}+it\right)\right|^4 \lesssim \frac{1}{2\sqrt{15}\pi^2}T(\log T)^5,$$

where $A\lesssim B$ means $A\leq B(1+o(1))$, with some improvements on the upper bound due to Hall [159, 160]. By a similar argument to the above relating sums to integrals, this implies

$$\frac{\sqrt{21}}{180\pi^2}T(\log T)^5 \lesssim \int_0^T |Z(t)|^3|Z'(t)|\,dt \lesssim \frac{1}{4\sqrt{15}\pi^2}T(\log T)^5.$$

Although no other asymptotics for higher moments are known, Milinovich [235] established sharp (up to an epsilon) upper and lower bounds. He showed that for $k\in\mathbb{N}$ and for $\varepsilon>0$,

$$T(\log T)^{k^2+1-\varepsilon} \ll \sum_{0<\gamma\leq T}\max_{\gamma<t\leq\gamma^+}|Z(t)|^{2k} \ll T(\log T)^{k^2+1+\varepsilon}$$

for sufficiently large T. By a similar argument to that done by Conrey and Ghosh [67], Milinovich [235] shows

$$\sum_{0<\gamma\le T}\max_{\gamma<t\le\gamma^+}|Z(t)|^{2k} = k\int_0^T |Z(t)|^{2k-1}|Z'(t)|\ dt + O_{k,\varepsilon}(T^{\varepsilon}).$$

Finally, he conjectures for $k\in\mathbb{N}$ that

$$\sum_{0<\gamma\le T}\max_{\gamma<t\le\gamma^+}|Z(t)|^{2k}\sim C_kT(\log T)^{k^2+1}$$

as $T\to\infty$, but did not conjecture the value of the implied constant. As previously mentioned, this constant has since been conjectured from the RMT side by [312].

1.4 DISCRETE MOMENTS OF THE RIEMANN ZETA FUNCTION

Having seen all about continuous moments in Section 1.3, we now describe the history relating to discrete moments, which we recall are sums of the form

$$J_{2k,n}(T) = \sum_{0<\gamma\le T}\left|\zeta^{(n)}(\rho)\right|^{2k}$$

where the γ are the ordinates of the non-trivial zeros $\rho=\beta+i\gamma$ of $\zeta(s)$ and $\zeta^{(n)}(s)$ denotes the n^{th} derivative of $\zeta(s)$. This is defined for all $k\ge 0$ and if we assume all the zeros of $\zeta(s)$ are simple, for $k<0$. (When we just discuss the moments of the first derivative we will write $J_{2k}(T)$ for simplicity.)

We will assume the Riemann Hypothesis in this section for simplicity unless otherwise stated, although some results are unconditional. The reason we assume this is that we often consider sums of the form

$$\sum_{0<\gamma\le T}\zeta^{(n)}\left(\frac{1}{2}+i\gamma\right)^k\zeta^{(n)}\left(\frac{1}{2}-i\gamma\right)^k$$

which is exactly $J_{2k,n}(T)$ under the Riemann Hypothesis.

1.4.1 Discrete Moment Results

We have already seen a result on moments of derivatives of $\zeta(s)$, in Ingham's result (1.16) when proving the lower order terms for the second continuous moment. In the case $n=m$ he showed that

$$\int_0^T\left|\zeta^{(n)}\left(\frac{1}{2}+it\right)\right|^2\ dt\sim\frac{1}{2n+1}T(\log T)^{2n+1} \tag{1.29}$$

as $T\to\infty$.

Gonek initiated the study of the discrete moments in [143] by considering the analogous result for sums of the derivatives of $\zeta(s)$. In particular, he showed unconditionally for any real $|\alpha| \le L/2$, where $L = \frac{1}{2\pi}\log\frac{T}{2\pi}$, that

$$\sum_{0<\gamma\le T} \zeta^{(n)}\left(\rho + i\frac{\alpha}{L}\right)\zeta^{(m)}\left(1-\rho+i\frac{\alpha}{L}\right)$$
$$= (-1)^{n+m}\left(\frac{1}{n+m+1} - H(n,m,2\pi\alpha) - H(m,n,-2\pi\alpha)\right)\frac{T}{2\pi}(\log T)^{n+m+2}$$
$$+ O\left(T(\log T)^{n+m+1}\right) \quad (1.30)$$

where

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

Under the Riemann Hypothesis in the case where $n = m = 0$ and for T sufficient large with α as above, Gonek proved

$$\sum_{0<\gamma\le T}\left|\zeta\left(\frac{1}{2}+i(\gamma+\alpha L^{-1})\right)\right|^2 = \left(1-\left(\frac{\sin\pi\alpha}{\pi\alpha}\right)^2\right)\frac{T}{2\pi}(\log T)^2 + O(T\log T). \quad (1.31)$$

Setting $\alpha = 0$ and $n = m \ge 1$ gives the second moment of $\zeta(s)$ for all derivatives,

$$J_{2,n}(T) = \sum_{0<\gamma\le T}\left|\zeta^{(n)}\left(\frac{1}{2}+i\gamma\right)\right|^2 = \frac{n^2}{(2n+1)(n+1)^2}\frac{T}{2\pi}(\log T)^{2n+2} + O\left(T(\log T)^{2n+1}\right). \quad (1.32)$$

In addition, Milinovich [233] has obtained a full asymptotic for the second moment including all lower order terms and a power saving error term, showing

$$J_2(T) = \sum_{0<\gamma\le T}|\zeta'(\rho)|^2 = \sum_{n=0}^{4} a_n T\left(\log\frac{T}{2\pi}\right)^n + O\left(T^{1/2+\varepsilon}\right) \quad (1.33)$$

for some explicit constants a_n and for all $\varepsilon > 0$.

While no asymptotic was known for any moment other than the second, Gonek [145] and Hejhal [177] independently conjectured that

$$J_{2k}(T) \sim b_k T(\log T)^{(k+1)^2} \quad (1.34)$$

as $T \to \infty$ for any real k but with no suggestion for what the coefficient b_k should be. Just as Keating and Snaith [211] used RMT to calculate the unknown constant in the continuous moments case, Hughes, Keating and O'Connell [182] used similar methods to calculate the unknown constant for this conjecture. We will discuss this work in detail in Section 1.4.2.

The best known partial result in proving any moments higher than the second is due to Ng [253], who showed that there exists positive constants C_1, C_2 such that, for sufficiently large T,

$$C_1 T(\log T)^9 \leq J_4(T) \leq C_2 T(\log T)^9,$$

(and who states that the method extends easily to higher derivatives), obtaining the conjectured order for the fourth moment but not the coefficient for the leading order term. Under some additional assumptions, Garunkštis and Steuding [136] show that the upper bound in Ng's fourth moment result can be improved slightly.

There is also a partial result for the first moment, due to Garaev [135] where he restricts the sum to simple zeros of $\zeta(s)$ with real part $1/2$ (see also [220, 285]. He showed for a positive constant C that

$$J_1(T) = \sum_{0<\gamma\leq T} |\zeta'(\rho)| \leq CT(\log T)^{9/4},$$

a result that relies on a mean-value estimate for Dirichlet series due to Ramachandra [269]. Note that this result is of the conjectured order of magnitude given in (1.34).

Gonek [145] conjectured that

$$J_{-2}(T) \sim \frac{3}{\pi^3} T \tag{1.35}$$

as $T \to \infty$. Note that this result implies that all the zeros of $\zeta(s)$ are simple otherwise the sum would diverge for sufficiently large T. Gonek was able to prove that $J_{-2}(T) \ll T$ under the assumption that all the zeros are simple.

Milinovich and Ng [236] showed that for all $\varepsilon > 0$,

$$J_{-2}(T) \geq \left(\frac{3}{2\pi^3} - \varepsilon\right) T \tag{1.36}$$

as $T \to \infty$, which is the correct lower bound up to a factor of a half.

1.4.1.1 Upper and Lower Bounds

It can be deduced from (1.13) that for $\sigma \geq 1/2$ and $t \geq 10$

$$\left|\zeta'\left(\frac{1}{2} + it\right)\right| \ll \exp\left(\frac{c\log t}{\log\log t}\right)$$

for some $c > 0$. Then for $k > 0$ it follows that

$$J_{2k}(T) \ll \exp\left(\frac{2kc\log t}{\log\log t}\right)$$

for some $c > 0$.

However we can do much better. Milinovich and Ng [237] showed under the Generalised Riemann Hypothesis that the lower bound in the Gonek–Hejhal (1.34) conjecture is correct for all natural numbers k. Gao [132] improved this lower bound to all real $k > 0$. As a corollary, Ng [254] showed that for each $A > 0$, the inequality

$$|\zeta'(\rho)| \geq (\log|\gamma|)^A$$

is satisfied infinitely often when $\rho = \beta + i\gamma$ is a non-trivial zero of $\zeta(s)$.

For the upper bounds, Milinovich [234] showed that the upper bound it almost sharp for all natural numbers k, with an extra ε in the power, as in the upper bound for continuous moments by Soundararajan [291]. Additionally he showed that the upper bound for derivatives holds, that is, he showed for integer k, n and $\varepsilon > 0$, that

$$J_{2k,n}(T) \ll T(\log T)^{k^2+2kn+1+\varepsilon}.$$

Kirila [214] removed the ε in the upper bound and showed that it holds for all $k > 0$ and all derivatives.

In terms of the first derivative, we know that for $k > 0$,

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

Benli, Elma and Ng [22] have shown that the expected lower bound holds for all derivatives, and so under the Riemann Hypothesis, it is known for k, n integers that

$$T(\log T)^{k^2+2kn+1} \ll J_{2k,n}(T) = \sum_{0<\gamma\leq T} \left|\zeta^{(n)}\left(\frac{1}{2}+i\gamma\right)\right|^{2k} \ll T(\log T)^{k^2+2kn+1}.$$

It is reasonable to assume that the lower bound holds for all real $k > 0$ but this has yet to be shown for general $n > 1$.

For negative moments, under the assumption that all zeros are simple, Heap, Li and Zhao [168] proved that the lower bound of the Gonek–Hejhal conjecture is consistent for rational $k < 0$ and Gao and Zhao [133] show this lower bound is consistent for all $k < 0$. However we do not expect the lower bound to be sharp for $k < -3/2$. To see this, Gonek [147] defines

$$\Theta = \inf\{\theta \;:\; |\zeta'(\rho)|^{-1} \ll \gamma^{\theta}\}.$$

Then under the Riemann Hypothesis, we expect $|\zeta'(\rho)| \ll |\rho|^{\varepsilon}$ and so we expect $\Theta \geq 0$. As we have discussed, we expect to be able to model statistical behaviour of zeta zeros through statistics of eigenvalues of random unitary matrices. This suggests $\Theta = 1/3$ (see [182], for example), and so it is possible that

$$|\zeta'(\rho)| \ll |\gamma|^{-1/3+\varepsilon}$$

occurs infinitely often.

Additionally, we do not expect to get a good upper bound for negative moments. This is explained by Hiary and Odlyzko [179] who note that extreme values of negative moments are caused by very few zeros. Small values of $|\zeta(1/2 + i\gamma)|$ typically occur at pairs of consecutive zeros that are close to each other, called Lehmer pairs, discussed further in Chapter 2. For example, they show that for 15 sets of $\approx 10^9$ zeros near the 10^{23}-rd zero, 87% of the value of the moment for these zeros comes from just 4 zeta zeros. Understanding this very rare behaviour with a good bound is tough in part due to the rarity of these zeros. There are very few upper bounds in the negative moment case. Bui, Florea, and Milinovich [45] obtained an upper bound for a related sum but the sum is not over all zeros. Zeros that are close in some sense to other zeros are removed from this sum, so while they include what is expected to be arbitrarily close to the full density inside the set of all zeros, they are still excluding zeros that are expected to contribute a large amount to the total sum.

1.4.2 Random Matrix Theory meets Number Theory: Act III

In a similar manner to the approach taken by Keating and Snaith in modelling continuous moments of $\zeta(s)$, Hughes, Keating and O'Connell [182] calculated the analogous result for discrete moments of $\zeta'(\rho)$. Recall that to model continuous moments of $\zeta(s)$ we calculated moments of characteristic polynomials of random unitary matrices. In this instance, they calculated moments of derivatives of characteristic polynomials of random unitary matrices. Differentiating the characteristic polynomial with respect to θ gives

$$Z_N'(\theta) = i \sum_{j=1}^{N} e^{i(\theta_j - \theta)} \prod_{\substack{m=1 \\ m \neq j}}^{N} (1 - e^{i(\theta_m - \theta)}),$$

so

$$|Z_N'(\theta_j)| = \prod_{\substack{m=1 \\ m \neq j}}^{N} \left|1 - e^{i(\theta_m - \theta_j)}\right|.$$

To model moments of $J_{2k}(T)$, they calculated the expectation of

$$\frac{1}{N} \sum_{j=1}^{N} |Z_N'(\theta_j)|^{2k}.$$

By the rotational invariance of Haar measure,

$$\mathbb{E}_N \left\{ \frac{1}{N} \sum_{j=1}^{N} |Z_N'(\theta_j)|^{2k} \right\} = \mathbb{E}_N \left\{ |Z_N'(\theta_N)|^{2k} \right\} = \mathbb{E}_N \left\{ \prod_{n=1}^{N-1} \left|1 - e^{i(\theta_n - \theta_N)}\right|^{2k} \right\}. \tag{1.37}$$

The following lemma transforms expectation with respect to Haar measure over $U(N)$ to expectation with respect to Haar measure over $U(N-1)$. A proof can be found in [181].

Lemma 1.18 (Hughes)**.** *Writing $\mathbb{E}_N$ to denote expectation with respect to Haar measure over $U(N)$, if f is a 2π-periodic function, then*

$$\mathbb{E}_N\left\{\prod_{n=1}^{N-1} f(\theta_n-\theta_N)\right\} = \frac{1}{N}\mathbb{E}_{N-1}\left\{\prod_{n=1}^{N-1}\left|1-e^{i\theta_n}\right|^2 f(\theta_n)\right\}.$$

Applying Lemma 1.18 to (1.37) gives

$$\frac{1}{N}\mathbb{E}_{N-1}\left\{|Z_{N-1,\hat{U}}(0)|^{2k+2}\right\} = \frac{1}{N}\frac{G^2(k+2)}{G(2k+3)}\frac{G(N+2k+2)G(N)}{G^2(N+k+1)}$$

where $\hat{U}\in U(N-1)$. The evaluation of this expectation is essentially (1.21). This result holds for $\Re(k)>-3/2$. Clearly it can be continued meromorphically to the whole complex plane.

For k bounded and as $N\to\infty$,

$$\mathbb{E}_N\left\{|Z_N'(\theta_N)|^{2k}\right\} = \frac{G^2(k+2)}{G(2k+3)}N^{k(k+2)} + O\left(N^{k(k+2)-1}\right).$$

This calculation has modelled $J_{2k}(T)/N(T)$. Hughes, Keating and O'Connell then made the following conjecture.

Conjecture 1.19 (Hughes–Keating–O'Connell)**.** *For k fixed with $\Re(k)>-3/2$,*

$$J_{2k}(T) = \sum_{0<\gamma\le T}\left|\zeta'\left(\frac{1}{2}+i\gamma\right)\right|^{2k} \sim a_k\frac{G^2(k+2)}{G(2k+3)}\frac{T}{2\pi}(\log T)^{(k+1)^2}$$

as $T\to\infty$, with a_k defined in (1.19) *and G is the Barnes G-function defined in* (1.23).

Note that this conjecture is consistent with all known results and conjectures. Indeed, it also predicts what the true coefficient should be in Ng's fourth moment result, that is, it predicts

$$J_4(T)\sim\frac{1}{2880\pi^3}T(\log T)^9$$

as $T\to\infty$. This coefficient was conjectured from a purely number theoretical argument by Hughes [181], pushing a result of Conrey, Ghosh and Gonek [70] beyond its range of applicability. It also agrees with the Gonek–Hejhal conjecture (1.34), conjecturing the unknown coefficient b_k for $k=2$.

As in the continuous moment case, part of the motivation for studying the discrete moments is to establish the value distribution of the real part of the logarithm of $Z_N'(\theta)$. Hughes, Keating and O'Connell [182] showed that as $N\to\infty$, that the real part tends to a Gaussian random variable.

Theorem 1.20 (Hughes–Keating–O'Connell)**.** *For $a < b$,*

$$\lim_{N\to\infty} \mathrm{Haar}\left\{ \frac{\log\left|\frac{Z_N'(\theta_N)}{Ne^{\gamma_0-1}}\right|}{\sqrt{\frac{1}{2}(\log N + 3 + \gamma_0 - \frac{\pi^2}{2})}} \right\} = \frac{1}{\sqrt{2\pi}}\int_a^b e^{-\frac{x^2}{2}}\ dx$$

where the measure of the set is taken to be the usual Haar measure on $U(N)$ and where γ_0 is Euler's constant.

This should be compared with Hejhal's Central Limit Theorem [177] for $\zeta'(s)$, which shows that the real part of the logarithm of $\zeta'(s)$ tends to a Gaussian random variable.

Theorem 1.21 (Hejhal)**.** *If we assume the Riemann Hypothesis and the existence of an α such that*

$$\limsup_{T\to\infty} \frac{1}{N(2T)-N(T)}\left|\left\{n\ :\ T \le \gamma_n \le 2T,\ 0 \le \gamma_{n+1}-\gamma_n \le \frac{c}{\log T}\right\}\right| \le Mc^{\alpha}$$

holds uniformly for $0 < c < 1$, with M a suitable constant, then for $a < b$,

$$\lim_{T\to\infty} \frac{1}{N(2T)-N(T)}\left|\left\{n\ :\ T \le \gamma_n \le 2T,\ \frac{\log\left|\frac{\zeta'(\frac{1}{2}+i\gamma_n)}{\frac{1}{2\pi}\log\frac{\gamma_n}{2\pi}}\right|}{\sqrt{\frac{1}{2}\log\log T}} \in (a,b)\right\}\right| = \frac{1}{\sqrt{2\pi}}\int_a^b e^{-\frac{x^2}{2}}\ dx.$$

Recall that $N = \log T/2\pi$. Comparing the two Central Limit Theorems above, we see that the two results agree (up to errors of $O(1)$ which are subdominant in the large N, T limit). Çiçek [48] gives an alternative proof of Hejhal's result and improves it by providing a rate of convergence to the distribution. A similar result in this paper is proved which shows the imaginary part of the logarithm of $\zeta'(s)$ tends to a Gaussian random variable.

As in the continuous moments case, two obvious questions arise from Conjecture 1.19. The first, that of lower order terms, is addressed in Section 6.1.5. The second question, a more subtle one, concerns the arithmetic factor. As in the Keating–Snaith conjecture, Hughes, Keating and O'Connell were forced to insert the arithmetic factor after obtaining the RMT moments result. Why should the same arithmetic factor a_k occur in both the continuous and discrete moments conjectures?

This question was again settled by the hybrid model, this time for discrete moments, of Bui, Gonek and Milinovich [47]. Recall that we write

$$\zeta(s) = P_X(s)Z_X(s)(1+\mathcal{E}).$$

with an error term $\mathcal{E}$ which is not the same throughout and that we ignore here. Differentiating with respect to s we obtain

$$\zeta'(s) = \left(P_X'(s)Z_X(s) + P_X(s)Z_X'(s)\right)(1+\mathcal{E})$$

and on setting $s = \rho$ a non-trivial zero of $\zeta(s)$, we have

$$\zeta'(\rho) = P_X(\rho) Z'_X(\rho)(1 + \mathcal{E}).$$

Then they have the same prime part, $P_X(s)$, as in the continuous hybrid model of Gonek, Hughes and Keating, explaining why we should expect the same arithmetic factor in both moment conjectures. By assuming the splitting conjecture for discrete moments, Bui, Gonek and Milinovich re-established the Hughes, Keating and O'Connell conjecture, with the arithmetic term appearing naturally this time. They also showed that splitting holds to leading order for $k = 1$ in this case, corresponding to Gonek's second discrete moment result (1.32).

Returning to our questions, we now consider that of lower order terms for the discrete moments conjecture. In the continuous moments case, we have the recipe of Conrey, Farmer, Keating, Rubinstein and Snaith to predict the lower order terms for integer k. To calculate the lower order terms for the discrete moments we need a generalisation of the recipe, known as the Ratios Conjecture of Conrey, Farmer and Zirnbauer [63], discussed in detail in Section 6.1.

1.4.3 Applications of Discrete Moments

1.4.3.1 Simple Zeros of $\zeta(s)$

When calculating the number of zeros $N(T)$ of $\zeta(s)$, as given in (1.4), we count each zero with multiplicity, denoted $m(\rho)$. It is conjectured that $m(\rho) = 1$ for all zeros, that is, that all the non-trivial zeros of $\zeta(s)$ are simple. We review the evidence for this conjecture below, before discussing (potentially hypothetical) multiple zeros in the next section.

Let $N^*(T)$ be the number of simple non-trivial zeros of $\zeta(s)$ with $0 < \gamma \leq T$. Then

$$\kappa^* = \liminf_{T \to \infty} \frac{N^*(T)}{N(T)}$$

is the proportion of simple zeros of $\zeta(s)$.

All zeros that have been found numerically are known to be simple. Unconditionally Heath-Brown [173] (and independently, Selberg) showed that Levinson's [222] result that one-third of the non-trivial zeros lie on the critical line implies

$$\kappa^* \geq 0.3474.$$

Through Conrey's [56] result that two-fifths of the non-trivial zeros lie on the critical line, he improved the above proportion to

$$\kappa^* \geq 0.4058.$$

Various small improvements were made following this method of Levinson's, and they were due to Bui, Conrey, and Young [42], Feng [115], and Bui [41], with the latest improvement using this method due to Pratt, Robles, Zaharescu and Zeindler [265]. They showed that the proportion of zeros on the critical line is $\kappa^* \geq 0.407$. In proving an unconditional form of Montgomery's Pair Correlation Conjecture 1.3, Baluyot, Goldston, Suriajaya and Turnage-Butterbaugh [18] showed that $\kappa^* \geq 0.617$.

Montgomery observed that

$$N^*(T) \geq \sum_{0<\gamma\leq T} (2 - m(\rho)).$$

Assuming the Riemann Hypothesis, Montgomery's Theorem 1.2 implies

$$\sum_{0<\gamma\leq T} m(\rho) \leq \left(\frac{4}{3} + o(1)\right) N(T)$$

where the zeros are repeated according to multiplicity. Combining these two inequalities imply that

$$\kappa^* \geq 0.666...,$$

with incremental progress using this method due to Montgomery and Taylor [240] who showed $\kappa^* \geq 0.6725$, by Cheer and Goldston [52] who showed $\kappa^* \geq 0.6727$, and by Chirre, Gonçalves and de Laat [53] who showed $\kappa^* \geq 0.679$. Montgomery's Pair Correlation Conjecture 1.3 implies that 100% are simple [239].

By a mollifier method described below, Conrey, Ghosh, and Gonek [75] showed assuming the Riemann Hypothesis and the Generalised Lindelöf Hypothesis that

$$\kappa^* \geq 0.70307...,$$

with Bui and Heath-Brown [39] removing the assumption of the Generalised Lindelöf Hypothesis.

To obtain a lower bound for κ^* using this method, we need to know the mollified first and second moments of $\zeta'(s)$. Note that ρ is a simple zero of $\zeta(s)$ if and only if $\zeta'(\rho) \neq 0$. Hence by the Cauchy–Schwarz inequality,

$$\left| \sum_{0<\gamma\leq T} B\zeta'(\rho) \right|^2 \leq N^*(T) \sum_{0<\gamma\leq T} \left|B\zeta'(\rho)\right|^2$$

for a mollifier $B(s)$. We note that mollifiers are necessary to get a proportion of simple zeros, a theme we have already come across in this thesis in Sections 1.3.7.3 and 1.3.7.4. Conrey, Ghosh and Gonek [73] initially used this method without mollifiers to give a more straightforward proof that there are infinitely many simple zeros of $\zeta(s)$, as described in Chapter 2, equation (2.2).

We mention one further result in the theme of the above work. In 1986, Conrey, Ghosh and Gonek [71] considered the problem of showing that there are infinitely many zeros of the Dedekind zeta function $\zeta_K(s)$ of a quadratic number field $K = \mathbb{Q}(\sqrt{d})$. Unlike in the case of the Riemann zeta function where this was already known (albeit with complicated proofs), it was not known before this work that there were infinitely many simple zeros of $\zeta_K(s)$. Their proof is based on the fact that for a quadratic number field, we have the factorisation

$$\zeta_K(s) = \zeta(s)L(s,\chi),$$

where $\chi \bmod |d|$ is a real primitive character. In particular, a zero of the Riemann zeta function is also a zero of $\zeta_K(s)$.

Clearly a zero of $\zeta(s)$ is a simple zero of $\zeta_K(s)$ if and only if $\zeta'(\rho)L(1-\rho,\chi) \neq 0$. As before, they used the Cauchy–Schwarz inequality to write

$$\left|\sum_{0<\gamma\leq T} \zeta'(\rho)L(1-\rho,\chi)\right|^2 \leq \sum_{0<\gamma\leq T}{}^{*} 1 \sum_{0<\gamma\leq T} \left|\zeta'(\rho)L(1-\rho,\chi)\right|^2$$

where the star on the middle sum denotes counting only the simple zeros of $\zeta_K(s)$. The main difficulty lies in calculating the sum on the left-hand side. They showed

$$\sum_{0<\gamma\leq T} \zeta'(\rho)L(1-\rho,\chi) = L(1,\chi)\frac{T}{4\pi}(\log T)^2 + O(T\log T)$$

and as they also showed that

$$\sum_{0<\gamma\leq T} \left|\zeta'(\rho)L(1-\rho,\chi)\right|^2 \ll T^{2-\delta}$$

where $\delta > 0$, this implies that there are infinitely many simple zeros of $\zeta_K(s)$. Improving on this in [72], they obtained a positive proportion of simple zeros, showing that under the Riemann Hypothesis, the proportion of simple zeros of $\zeta_K(s)$ is at least $1/54$. By assuming the Riemann Hypothesis for $\zeta_K(s)$, this is improved to at least $1/27$. This relatively low (albeit positive) proportion is due to the fact that $\zeta(s)$ and $L(s,\chi)$ can share zeros. They note that the approach that they take in [75] does not work in this instance to improve the proportion, and doing so in any way would pose an interesting problem.

1.4.3.2 Multiple zeros of $\zeta(s)$

While we have only focused on simple zeros of the Riemann zeta function, the possibility remains that there could be multiple zeros. We consider this possibility in this section and discuss the results that are known for these zeros.

Before rigorously proving that at least 70% of the zeros are simple (see [75]), Conrey, Ghosh and Gonek [74] provided a sketch of some more general results, including how to calculate proportions of multiple zeros through some discrete moments. To describe their results we set up some notation.

Let T be a large positive real number and let

$$B(s,P)=\sum_{n\le y}\frac{\mu(n)P\left(\frac{\log y/n}{\log y}\right)}{n^s}$$

where $y=T^\theta$ for $\theta<1/2$, $P(x)$ is an entire function with $P(0)=0$, and $\mu(n)$ is the Möbius function given in (1.27). Let a,b be complex numbers and $Q_1(x)$ and $Q_2(x)$ be polynomials.

We consider a twisted discrete second moment, defined by

$$I_1(a,b,P_1,P_2,Q_1,Q_2)=\\ \sum_{0<\gamma\le T}Q_1\left(-\frac{d}{da}\right)\zeta\left(\rho+\frac{a}{\log T}\right)Q_2\left(-\frac{d}{db}\right)\zeta\left(1-\rho+\frac{b}{\log T}\right)B(\rho,P_1)B(1-\rho,P_2).$$

Theorem 1.22 (Conrey–Ghosh–Gonek). *If $0<\theta<1/2$ and $a,b\ll 1$, then as $T\to\infty$,*

$$\begin{aligned}I_1(a,b,P_1,P_2,Q_1,Q_2)\sim&\\ \frac{T}{2\pi}\log T\frac{\partial}{\partial u}\frac{\partial}{\partial v}\Bigg\{&\left(\frac{1}{\theta}\int_0^1 P_1P_2\,dx+\int_0^1 P_1\,dx\int_0^1 P_2\,dx\right)\\ &\times\left(\int_0^1 T_aQ_1T_bQ_2\,dx-\int_0^1 T_aQ_1\,dx\int_0^1 T_bQ_2\,dx\right)\\ +\int_0^1 P_1\,dx\int_0^1 P_2\,dx&\left(Q_1(0)-\int_0^1 T_aQ_1\,dx\right)\left(Q_2(0)-\int_0^1 T_bQ_2\,dx\right)\Bigg\}\Bigg|_{u=v=0},\end{aligned}$$

where $P_1=P_1(x+u)$, $P_2=P_2(x+v)$,

$$T_aQ_1=e^{-a(x+\theta u)}Q_1(x+\theta u)\quad\text{and}\quad T_bQ_2=e^{-b(x+\theta v)}Q_2(x+\theta v).$$

It should be possible to deduce this result from the more general result of Heap, Li, and Zhao [168] (as claimed in [46] but details should be written down), which builds on the work in [75] and [39].

Similarly, we consider a twisted discrete first moment, defined by

$$I_2(a,P,Q)=\sum_{0<\gamma\le T}Q\left(-\frac{d}{da}\right)\zeta\left(\rho+\frac{a}{\log T}\right)B(\rho,P).$$

Theorem 1.23 (Conrey–Ghosh–Gonek). *If $0<\theta<1/2$ and $a\ll 1$, then as $T\to\infty$,*

$$I_2(a,P,Q)\sim-\frac{T}{2\pi}\log T\frac{d}{du}\left\{\left(Q(0)-\int_0^1 T_aQ\,dx\right)\int_0^1 P\,dx\right\}\Bigg|_{u=0},$$

where $P=P(x+u)$and $T_aQ=e^{-a(x+\theta u)}Q(x+\theta u)$.

Likewise, it should be possible to deduce this result from the more general result of Benli, Elma and Ng [22] (but details should be written down).

To begin, Conrey, Ghosh and Gonek consider the proportion of simple zeros which we have already discussed in Section 1.4.3.1, but repeat here for completeness. Recall that $N(T)$ is the number of non-trivial zeros with $0 < \gamma \leq T$, given in (1.4), and $N^*(T)$ is the number of simple non-trivial zeros of $\zeta(s)$ with $0 < \gamma \leq T$. Then we set

$$\kappa^* = \liminf_{T\to\infty} \frac{N^*(T)}{N(T)}$$

to be the proportion of simple zeros of $\zeta(s)$. By the Cauchy–Schwarz inequality,

$$N^*(T) \geq \frac{\left|\sum_{0<\gamma\leq T} \zeta'(\rho)B(\rho,P)\right|^2}{\sum_{0<\gamma\leq T} |\zeta'(\rho)B(\rho,P)|^2}.$$

Clearly the right-hand side can be evaluated using Theorems 1.22 and 1.23, with the denominator requiring the assumption of the Riemann Hypothesis. The optimal choice of $P(x)$ can be calculated via the calculus of variations, giving

$$P(x) = -\theta x^2 + (1+\theta)x$$

so

$$\kappa^* \geq 1 - \frac{1}{(1+\theta)^3}.$$

As $\theta \to 1/2^-$, we obtain

$$\kappa^* \geq \frac{19}{27}$$

as before.

If we were to push Theorems 1.22 and 1.23 beyond their range of applicability in θ, we conjecture (assuming these two theorems still hold) that

$$\kappa^* \geq \begin{cases} \frac{988}{1331} \approx 0.7423\ldots & \text{as } \theta \to 4/7^- \\ \frac{7}{8} = 0.875 & \text{as } \theta \to 1^- \\ 1 & \text{as } \theta \to \infty. \end{cases}$$

We choose the values of $4/7$ to compare with the result of Conrey [56] on zeros on the critical line, 1 as we expect mollifiers to hold true to length T, and ∞ for Farmer's [112] $\theta = \infty$ conjecture.

The purpose of this section is to consider multiple zeros, however. We let $N^{(2)}(T)$ denote the number of simple and double non-trivial zeros with $0 < \gamma \leq T$ and let

$$\kappa^{(2)} = \liminf_{T\to\infty} \frac{N^{(2)}(T)}{N(T)}$$

be the proportion of simple and double zeros of $\zeta(s)$. Again by the Cauchy—Schwarz inequality,

$$N^{(2)}(T) \geq \frac{\left|\sum_{0<\gamma\leq T} \zeta'(\rho)B(\rho, P_1) + \zeta''(\rho)B(\rho, P_2)\right|^2}{\sum_{0<\gamma\leq T} |\zeta'(\rho)B(\rho, P_1) + \zeta''(\rho)B(\rho, P_2)|^2}.$$

Again, the right-hand side can be evaluated using Theorems 1.22 and 1.23, with the denominator requiring the assumption of the Riemann Hypothesis. Then optimising the polynomials (with a slightly more optimal choice than that given in [74]), we have

$$P_1(x) = -\left(\frac{7\theta + 3\theta^2 + 3\theta^3}{7}\right)x^3 + \left(\frac{-77 - 35\theta + 65\theta^2 + 30\theta^3 + 45\theta^4}{70\theta}\right)x^2 + \left(\frac{42 + 182\theta + 158\theta^2 + 85\theta^3 + 45\theta^4}{70\theta^2}\right)x$$

$$P_2(x) = x^3 - 3\left(\frac{7 + 14\theta + 3\theta^2 + 3\theta^3}{14\theta}\right)x^2 + \left(\frac{7 + 35\theta + 31\theta^2 + 15\theta^3 + 9\theta^4}{14\theta^2}\right)x$$

and so

$$\kappa^{(2)} \geq 1 - \frac{7 + 3\theta^2}{7 + 56\theta + 199\theta^2 + 416\theta^3 + 434\theta^4 + 280\theta^5 + 150\theta^6 + 45\theta^7}.$$

Then similarly to the simple zeros case above, if we were to push Theorems 1.22 and 1.23 beyond their range of applicability in θ, we conjecture (assuming these two theorems still hold) that

$$\kappa^{(2)} \geq \begin{cases} \frac{173}{181} \approx 0.9556\ldots & \text{as } \theta \to 1/2^- \\ \frac{512096}{528903} \approx 0.9682\ldots & \text{as } \theta \to 4/7^- \\ \frac{200180384}{206751921} \approx 0.9682\ldots & \text{as } \theta \to 1^- \\ 1 & \text{as } \theta \to \infty. \end{cases}$$

This means that under the Riemann Hypothesis, fewer than 4.44% of the non-trivial zeros of $\zeta(s)$ have multiplicity 3 or greater, with this percentage decreasing as the length of the mollifier increases.

In an entirely analogous way, we let $N^{(3)}(T)$ denote the number of simple, double, and triple non-trivial zeros with $0 < \gamma \leq T$ and let $N^{(4)}(T)$ denote the number of simple, double, triple, and quadruple non-trivial zeros with $0 < \gamma \leq T$. Similarly, let

$$\kappa^{(3)} = \liminf_{T\to\infty} \frac{N^{(3)}(T)}{N(T)} \quad \text{and} \quad \kappa^{(4)} = \liminf_{T\to\infty} \frac{N^{(4)}(T)}{N(T)}$$

be the proportion of simple, double, and triple (and quadruple) zeros of $\zeta(s)$. Again by the Cauchy—Schwarz inequality,

$$N^{(3)}(T) \geq \frac{\left|\sum_{0<\gamma\leq T} \zeta'(\rho)B(\rho, P_1) + \zeta''(\rho)B(\rho, P_2) + \zeta'''(\rho)B(\rho, P_3)\right|^2}{\sum_{0<\gamma\leq T} |\zeta'(\rho)B(\rho, P_1) + \zeta''(\rho)B(\rho, P_2) + \zeta'''(\rho)B(\rho, P_3)|^2}$$

and similarly

$$N^{(4)}(T) \geq \frac{\left|\sum_{0<\gamma\leq T}\zeta'(\rho)B(\rho,P_1)+\zeta''(\rho)B(\rho,P_2)+\zeta'''(\rho)B(\rho,P_3)+\zeta^{(IV)}(\rho)B(\rho,P_4)\right|^2}{\sum_{0<\gamma\leq T}\left|\zeta'(\rho)B(\rho,P_1)+\zeta''(\rho)B(\rho,P_2)+\zeta'''(\rho)B(\rho,P_3)+\zeta^{(IV)}(\rho)B(\rho,P_4)\right|^2}.$$

Again, we can evaluate the right-hand side of both of these inequalities using Theorems 1.22 and 1.23, with the denominators requiring the assumption of the Riemann Hypothesis. Next we optimise the polynomials P_1, P_2, P_3 for $N^{(3)}(T)$ and P_1, P_2, P_3, P_4 for $N^{(4)}(T)$. We don't state any of these polynomials for brevity as the coefficients are fairly complicated. In the optimisation that we have found for the $N^{(3)}(T)$ case, P_1 is of degree 6, P_2 is of degree 5 and P_3 is of degree 4, while for the $N^{(4)}(T)$ case, P_1 is of degree 8, P_2 is of degree 7, P_3 is of degree 6, and P_4 is of degree 5. We then have

$$\kappa^{(3)} \geq 1 - \frac{1}{1+15\theta+105\theta^2+455\theta^3+1065\theta^4+1353\theta^5+875\theta^6+255\theta^7}$$

and

$$\kappa^{(4)} \geq 1 - \frac{1}{1+24\theta+276\theta^2+2024\theta^3+8526\theta^4+21504\theta^5+32984\theta^6+30096\theta^7+14994\theta^8+3136\theta^9}.$$

Then similarly to the cases above, if we were to push Theorems 1.22 and 1.23 beyond their range of applicability in θ, we conjecture (assuming these two theorems still hold) that

$$\kappa^{(3)} \geq \begin{cases} \frac{27507}{27635} \approx 0.9954\ldots & \text{as } \theta \to 1/2^- \\ \frac{295389868}{296213411} \approx 0.9972\ldots & \text{as } \theta \to 4/7^- \\ \frac{4093}{4094} \approx 0.9998\ldots & \text{as } \theta \to 1^- \\ 1 & \text{as } \theta \to \infty \end{cases}$$

and

$$\kappa^{(4)} \geq \begin{cases} \frac{301321}{301449} \approx 0.9996\ldots & \text{as } \theta \to 1/2^- \\ \frac{3820131104}{3820954647} \approx 0.9998\ldots & \text{as } \theta \to 4/7^- \\ \frac{113564}{113565} \approx 0.999991\ldots & \text{as } \theta \to 1^- \\ 1 & \text{as } \theta \to \infty. \end{cases}$$

Clearly the proportion of multiple zeros is decreasing quickly as n increases. It would be a good exercise to extend this method to show that the proportion of simple, double, ..., n-tuple zeros tends to zero at $n \to \infty$. It would also be interesting to see if Theorems 1.22 and 1.23 could be proved with longer mollifiers as this also increases each of the proportions of simple and multiple zeros. Deducing full proofs of these two theorems from [168] and [22] should also be written formally. Finally, it would be interesting to see if the $\theta = \infty$ conjecture from [112] implies all the zeros of the Riemann zeta function are simple, not just 100%, in the same way that Bettin and Gonek [29] showed that the $\theta = \infty$ conjecture implies all the zeros of the Riemann zeta function are on the critical line, not just 100%.

1.4.3.3 Gaps between zeros of $\zeta(s)$

While questions have already been considered regarding the horizontal and vertical distribution of the zeros of $\zeta(s)$, further questions can be asked. Consider the sequence $0 < \gamma_1 \leq \gamma_2 \leq ...$ of consecutive ordinates of the non-trivial zeros of $\zeta(s)$ and note that the average size of $\gamma_{n+1} - \gamma_n$ is $2\pi/\log\gamma_n$. Normalising, we set

$$\lambda = \limsup_{n\to\infty} \frac{(\gamma_{n+1} - \gamma_n)\log\gamma_n}{2\pi}$$

and

$$\mu = \liminf_{n\to\infty} \frac{(\gamma_{n+1} - \gamma_n)\log\gamma_n}{2\pi}.$$

By definition, $\mu \leq 1 \leq \lambda$ but it is conjectured that $\mu = 0$ and $\lambda = \infty$. This means that there are infinitely many pairs of zeros arbitrarily close, and arbitrarily far apart relative to the average spacing. The idea of looking at gaps between zeros started with Montgomery and his Pair Correlation Conjecture 1.3. This conjecture implies that $\mu = 0$, as for any $c > 0$, where the sum is over normalised zeros w_n,

$$0 < \lim_{T\to\infty} \frac{1}{N(T)} \sum_{\substack{\gamma,\gamma'\in[0,T] \\ 0\leq w_m - w_n \leq c}} 1 = \int_0^c \left(1 - \left(\frac{\sin \pi x}{\pi x}\right)^2\right) dx < c$$

so take c arbitrarily small and this quantity will still be positive, giving us a pair of zeros arbitrarily close. For large gaps, recall that we believe that we can model zeta zeros through random unitary matrices thanks to Montgomery's Pair Correlation Conjecture 1.3 and the link noted by Dyson. Together with the conjecture that n-level correlations of zeros of $\zeta(s)$ also follow these random matrix statistics due to Rudnick and Sarnak [275], this implies that $\lambda = \infty$.

Selberg (unpublished but announced in [279]) and Fujii [122, 123] showed that $\mu < 1 < \lambda$. For references to these results and corrections to some misprints that have occurred, see [90]. There is a vast literature of results, both unconditional and conditional, about the sizes of μ and λ. For a selection and summary of this literature, see Page 15 of [302].

There are relations between the class number problem, gaps between zeros, and exceptional zeros of L-functions. We let $h(K)$ denote the class number of $K = \mathbb{Q}(\sqrt{d})$, where d is a fundamental discriminant. In Article 303 of *Disquisitiones Arithmeticae* [138], Gauss conjectured that $k(K) \to \infty$ as d runs through negative discriminants. For a full history of this problem and its solutions, see Section 6 in Chapter 20 of Ireland and Rosen

[196]. This implies that there are only finitely many imaginary quadratic fields K with $h(K) = n$ for any fixed positive integer n. The Class Number Problem for imaginary quadratic fields is to give a complete list of fundamental discriminants for each fixed positive integer n.

For $n = 1$, this is a resolved conjecture of Gauss, who conjectured the only d are

$$d = -3, -4, -7, -8, -11, -19, -43, -67, -163$$

which was proved independently by Heegner [176], Stark [293] and Baker [14]. What happens for $n \geq 2$?

The Class Number Formula (for $d < -4$) states

$$h(K) = \frac{1}{\pi}\sqrt{|d|}L(1, \chi_d)$$

where $L(s, \chi_d)$ is the Dirichlet L-function with coefficients $\chi_d = \left(\frac{d}{n}\right)$ where $\left(\frac{\cdot}{\cdot}\right)$ denotes the Kronecker symbol.

We want a bound on $h(K)$. Under the Generalised Riemann Hypothesis, we have $(\log\log|d|)^{-1} \ll L(1, \chi_d) \ll (\log\log|d|)$, so

$$\sqrt{|d|}(\log\log|d|)^{-1} \ll h(K) \ll \sqrt{|d|}(\log\log|d|).$$

The problem with finding a stronger, unconditional bound on $L(1, \chi_d)$ is that we may have an Riemann–Siegel zero of $L(s, \chi_d)$, a real zero which is close to 1. Siegel [281] gave an unconditional bound, but the implied constant is not computable. Goldfeld [140] and Gross–Zagier [152] showed a better unconditional bound with computable constant, and Watkins [306] used this to give a complete list of fundamental discriminants with $h(K) = 2, 3, \ldots, 100$.

The connection of gaps to the class number problem comes from a result of Conrey and Iwaniec [77] which states as a corollary that if for all large T there are $\gg T(\log T)^{4/5}$ non-trivial zeros of $\zeta(s)$ up to height T where the average spacing between pairs of these consecutive zeros is less than $1/2$, then

$$L(1, \chi_d) \gg \frac{1}{(\log|d|)^{90}}$$

with computable implied constant.

Therefore if we can find better values of μ, and in particular $\mu < 1/2$, then we get stronger lower bounds on $L(1, \chi_d)$ (and so better bounds on $h(K)$), and in turn will imply that there are no Riemann–Siegel zeros.

How can we compute small and large gaps? We begin by returning to Gonek's second discrete moment result (1.30). For any real $|\alpha| \leq L/2$, setting $n = m = 0$ and assuming the Riemann Hypothesis gives

$$\sum_{0<\gamma\le T}\left|\zeta\left(\frac{1}{2}+i\left(\gamma+\frac{\alpha}{L}\right)\right)\right|^2=\left(1-\left(\frac{\sin\pi\alpha}{\pi\alpha}\right)^2\right)\frac{T}{2\pi}(\log T)^2+O(T\log T), \tag{1.38}$$

Notice that the coefficient of the leading order term is exactly that from the integrand in Montgomery's Pair Correlation 1.3.

Under the Riemann Hypothesis, Mueller [249, 250] then exploited this connection to prove results for large gaps, and Conrey, Ghosh and Gonek [69] used this method to also calculate small gaps between zeros.

As an example, we sketch how to calculate large gaps. Integrate both sides of (1.38) over $[-\beta/2,\beta/2]$ for some $\beta>\lambda$, giving

$$\sum_{0<\gamma\le T}\int_{-\beta/2}^{\beta/2}\left|\zeta\left(\frac{1}{2}+i\gamma+it\right)\right|^2\;dt\sim F(\beta)T\log T,$$

using (1.14), where

$$F(\beta)=\int_{-\beta/2}^{\beta/2}\left(1-\left(\frac{\sin\pi\alpha}{\pi\alpha}\right)^2\right)\;d\alpha.$$

Now if $\beta>\lambda$ then $F(\beta)\ge 1$. Using a computer package we can show $F(1.9)=0.997$ so

$$\lambda>1.9.$$

Hughes [181] showed that if we assume results on the fourth discrete moment, using Conjecture 1.19, then we have $\lambda>2.7$. Steuding and Steuding [294] then assumed the whole discrete moments Conjecture 1.19 to show that $\lambda=\infty$.

We noted above that if we can show that $\mu<1/2$ then we have no Riemann–Siegel zeros. However, in their paper on small gaps between zeros of $\zeta(s)$, Conrey, Ghosh and Gonek [69] showed that this method cannot break through this barrier, and so we would need a different approach to this problem.

1.4.3.4 Behaviour of $M(x)$

The summatory function of the Möbius function $\mu(n)$ is given by

$$M(x)=\sum_{n\le x}\mu(n).$$

Based on numerical evidence, some number theorists used to believe Merten's conjecture, that

$$M(x)=O(\sqrt{x})$$

holds for $x\ge 2$. This was an attractive belief as it implies the Riemann Hypothesis. However, Ingham [195] showed that Merten's conjecture implied that the ordinates of the zeros of $\zeta(s)$ satisfy some rational linear relations. This would contradict what we call the Linear Independence Hypothesis, which states that there are no rational linear relations between zeros of any L-functions. This hypothesis seemed to first appear in the work of Wintner [313] to study the error term in the Prime Number Theorem, which we come back to at the end of this section.

It was believed that it was more likely that the Linear Independence Hypothesis was true, and in 1985, Odlyzko and te Reile [260] showed that Merten's conjecture is false by showing

$$\liminf_{x\to\infty} \frac{M(x)}{\sqrt{x}} < -1.009 \text{ and } \limsup_{x\to\infty} \frac{M(x)}{\sqrt{x}} > 1.06.$$

For a full history of Merten's conjecture, see Odlyzko and te Reile's paper [260]. We note that their method doesn't give an x such that these inequalities hold, and we still do not know one such that $M(x) > \sqrt{x}$. In fact, Ingham went further and showed that the Linear Independence Hypothesis implies

$$\liminf_{x\to\infty} \frac{M(x)}{\sqrt{x}} = -\infty \text{ and } \limsup_{x\to\infty} \frac{M(x)}{\sqrt{x}} = +\infty.$$

The Linear Independence Hypothesis, together with the Riemann Hypothesis, has some fascinating consequences. Chebyshev, in 1853, in a letter to Fuss [50], asked questions about whether there are more primes congruent to $1 \bmod 4$ or $3 \bmod 4$ to some real number x, denoted $\pi(x;4,1)$ and $\pi(x;4,3)$ respectively. Littlewood [225] proved that $\pi(x;4,3) - \pi(x;4,1)$ changes sign infinitely often, and unlike the $\pi(x) - \mathrm{Li}(x)$ case (as discussed in Section 1.1.4), it is easier to find when these sign changes occur - the first is at $x = 26861$. The notion of comparing primes in different arithmetic progressions is called a prime number race, and many results are reliant on both the Linear Independence Hypothesis and the Riemann Hypothesis, as shown by Rubinstein and Sarnak [273]. We note that prime number races can be generalized to an arbitrary modulus and to more than two residue classes. For a summary of this area, see [151] for a friendly introduction in the topic of prime number races and see [229] for the annotated bibliography that lists and summarises every publication in the field of comparative prime number theory.

Returning to $M(x)$, it is still possible that the weak Merten's conjecture is true. This states that

$$\int_1^X \left(\frac{M(x)}{x}\right) dx \ll \log X.$$

This conjecture implies that the Riemann Hypothesis is true, that all the zeros are simple, and that

$$\sum_{\gamma>0} \frac{1}{|\rho\zeta'(\rho)|^2}$$

converges, showing a clear link between $M(x)$ and discrete moments of $\zeta(s)$. We can obtain this last sum through partial summation of $J_{-2}(T)$.

In fact, it can be shown that the Riemann Hypothesis and the Gonek–Hejhal conjecture (1.34) implies the weak Merten's conjecture. Moreover, it seems likely that

$$\int_1^X \left(\frac{M(x)}{x}\right) \, dx \sim \sum_{\gamma>0} \frac{2}{|\rho\zeta'(\rho)|^2} \log X.$$

In showing this, Ng [252] argues that

$$M(x) = O\left(\sqrt{x}(\log\log x)^{3/2}\right)$$

except on a set of finite logarithmic measure.

While we know that Merten's conjecture is false, thankfully this does not disprove the Riemann Hypothesis. The Riemann Hypothesis is equivalent to

$$M(x) = O\left(x^{1/2+\varepsilon}\right)$$

for every $\varepsilon > 0$.

The best known unconditional upper bound is

$$M(x) = O\left(x \exp\left(-c(\log x)^{3/5}(\log\log x)^{-1/5}\right)\right)$$

for some constant $c > 0$ while the Riemann Hypothesis implies

$$M(x) = O\left(\sqrt{x} \exp\left(A\frac{\log x}{\log\log x}\right)\right)$$

for some constant $A > 0$. For Omega results, the best unconditional result is

$$M(x) = \Omega\left(x^{1/2}\right)$$

while if the Riemann Hypothesis is false,

$$M(x) = \Omega\left(x^{\theta}\right)$$

for some $\theta > 1/2$. Note the similarities between the error terms here and those in the Prime Number Theorem. For a summary of these results, see [251].

The question still remains about the true size of $M(x)$. We first note that Ng [252] showed that a limiting distribution exists for

$$\phi(y) = e^{-y/2}M(e^{-y/2}),$$

assuming the Riemann Hypothesis and that $J_{-2}(T) \ll T$. Assuming results for $J_{-1}(T)$ and $J_{-2}(T)$, Ng conjectured

$$M(x) = \Omega_{\pm}\left(\sqrt{x}(\log\log\log x)^{5/4}\right).$$

Note that this power of 5/4 comes from the Gonek–Hejhal conjecture for $k = -1/2$. This conjecture was proved under the same assumptions on $J_{-1}(T)$ and $J_{-2}(T)$ and an effective version of the Linear Independence Hypothesis by Lamzouri [218].

Gonek (unpublished, with no specified value of the constant) and Ng [251] conjectured that

$$\liminf_{x\to\infty} \frac{M(x)}{\sqrt{x}(\log\log\log x)^{5/4}} = -\frac{8a}{5}, \text{ and } \limsup_{x\to\infty} \frac{M(x)}{\sqrt{x}(\log\log\log x)^{5/4}} = \frac{8a}{5},$$

where Ng (unpublished) conjectures that

$$a = \frac{1}{\sqrt{\pi}} e^{3\zeta'(-1)-\frac{11}{12}\log 2} \prod_p \left(1-\frac{1}{p}\right)^{\frac{1}{4}} \sum_{m=0}^{\infty} \left(\frac{\Gamma(m-1/2)}{m!\Gamma(-1/2)}\right)^2 p^{-m} \approx 0.16712\ldots,$$

based on that coefficient from the discrete moment Conjecture 1.19 of Hughes, Keating and O'Connell with $k = -1/2$. Additionally, assuming this effective version of the Linear Independent Hypothesis, together the bounds on negative discrete moment for $J_{-1}(T)$ and $J_{-2}(T)$, Ng (upcoming paper) proved

$$\liminf_{x\to\infty} \frac{M(x)}{\sqrt{x}(\log\log\log x)^{5/4}} \le -\frac{8a}{5}, \text{ and } \limsup_{x\to\infty} \frac{M(x)}{\sqrt{x}(\log\log\log x)^{5/4}} \ge \frac{8a}{5}.$$

1.4.3.5 The Error in the Prime Number Theorem

We now return to the Prime Number Theorem, specifically to the error term in the Prime Number Theorem and come full circle with the initial motivation for this chapter. Define

$$E(x) = \frac{\psi(x)-x}{\sqrt{x}}$$

where $\psi(x)$ is defined in (1.6). Assuming the Riemann Hypothesis and the Linear Independence Hypothesis, Wintner [314] showed that there exists an absolutely continuous probability measure ν such that

$$\lim_{X\to\infty} \int_2^X f(E(x))\ \frac{dx}{x} = \int_{-\infty}^{\infty} f(x)\ d\nu(x)$$

for all bounded continuous functions f on $\mathbb{R}$. By studying the tail of the limiting distribution ν, Montgomery [241] conjectured in 1980 that

$$\liminf_{x\to\infty} \frac{\psi(x)-x}{\sqrt{x}(\log\log\log x)^2} = -\frac{1}{2\pi}, \text{ and } \limsup_{x\to\infty} \frac{\psi(x)-x}{\sqrt{x}(\log\log\log x)^2} = \frac{1}{2\pi}.$$

Lamzouri [218], assuming an effective version of the Linear Independence Hypothesis, proved

$$\liminf_{x\to\infty} \frac{\psi(x)-x}{\sqrt{x}(\log\log\log x)^2} \le -\frac{1}{2\pi}, \text{ and } \limsup_{x\to\infty} \frac{\psi(x)-x}{\sqrt{x}(\log\log\log x)^2} \ge \frac{1}{2\pi}.$$

— 2 —

Shanks' Conjecture

2.1 OVERVIEW OF CHAPTER

Shanks' conjecture [280], now a theorem, dates from 1961 and states that

$$\zeta'(\rho) \text{ is real and positive in the mean}$$

as $\rho = \beta + i\gamma$ ranges over non-trivial zeros of the Riemann zeta function. This simple assertion is the basis for the thesis, including various proofs and generalisations of this problem.

More recently this assertion, again now a theorem proved in Chapter 3 and in [207, 186], has been generalised to higher derivatives, which we call the Generalised Shanks' Conjecture and states that

$$\text{on average, } \zeta^{(n)}(\rho) \text{ is positive if } n \text{ is odd, and negative if } n \text{ is even.}$$

Note that Shanks' conjecture was first conjectured, and later proved, in the usual order of events, but that we still call the established assertion Shanks' "conjecture". This nomenclature leads to an unusual situation where the extension is reasonably labelled the "Generalised Shanks' Conjecture" even though its first appearance in the literature was as a proven result!

In this first viewing of Shanks' conjecture and its generalisation, we begin by presenting a historical overview of the topic. Furthermore we will also give a simple heuristic that provides the leading term, including the sign, of the asymptotic formula for the average value of $\zeta^{(n)}(\rho)$. This heuristic follows almost immediately from an explicit formula known as the Landau–Gonek Theorem which we also discuss further.

Additionally, we will also use this heuristic to find the behaviour of the averages of other L-functions, including $1/\zeta'(s)$ over the non-trivial zeros of the Riemann zeta function, and our method applies directly to derivatives of Dirichlet L-functions over the non-trivial zeros of the associated Dirichlet L-function in an identical proof (up to those obvious changes between the Riemann zeta function and Dirichlet L-functions).

Much of the work presented in this chapter has already appeared in print in [184], written jointly with Chris Hughes and Greg Martin. Notation and cross-references have been updated for this thesis.

2.2 HISTORICAL BACKGROUND OF SHANKS' CONJECTURE

Shanks first made his conjecture [280] when he was reviewing Haselgrove's tables [167] of numerical values of the Riemann zeta function. He plotted the graph of $t \mapsto \zeta(1/2+it)$, copied below, and noticed that the way this curve approaches the origin, mainly through the third and fourth quadrants. This suggests the phase of $\zeta'(1/2+i\gamma)$ is close to zero in the mean and thus $\zeta'(1/2+i\gamma)$ is positive and real in the mean. This observation stands in contrast to the general behaviour of the function $\zeta'(1/2+it)$, whose mean value tends quickly to 0.

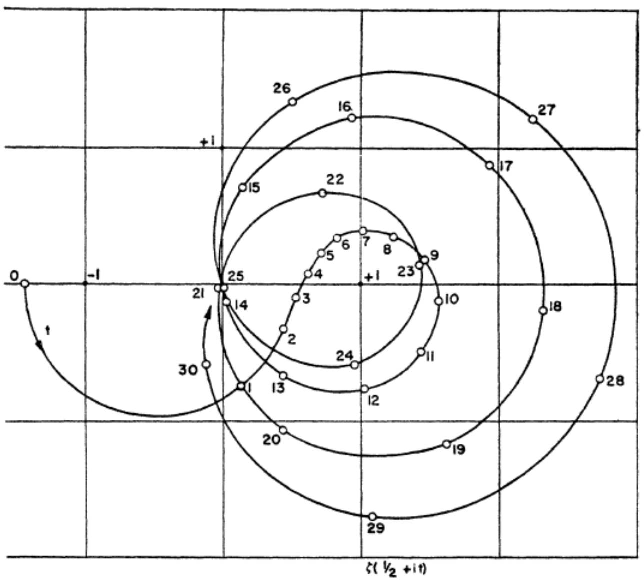

FIG. 1.—$\zeta\ (\frac{1}{2} + it)$ in the complex plane, for $0 \leqq t \leqq 30$.

This suggests the conjecture* that $\mathrm{Lim}_{N\to\infty}\ (1/N) \sum_1^N \phi_n\ =\ 0$, that is, that

$$\zeta'(\tfrac{1}{2} + i\gamma_n)$$

is positive real in the mean. Since violations against the "Law" are associated with exceptionally close zeros or exceptionally large values of $Z(t)$, some extremes discovered by D. H. Lehmer are of interest, and are listed in Table IV:

Figure 2.1: Plot of $t \mapsto \zeta(1/2+it)$, with the original conjecture below the graph.

We note that in Shanks' comments below his graph in Figure 2.1, he refers to violations of some 'Law'. This refers to Gram's Law, which states that given two consecutive Gram points g_n and g_{n+1}, we say that Gram's Law holds true for $[g_n, g_{n+1})$ if this Gram interval contains exactly one zero of $\zeta(\frac{1}{2}+it)$. A Gram point is one on the critical line where where $\zeta(\frac{1}{2}+ig_n)$ takes real, non-zero values. The Riemann–Siegel function $\theta(t)$, defined in (1.28), allows us to give another, equivalent definition of Gram points. These are precisely the points g_n for $n \geq -1$ with $t > 7$ such that

$$\theta(g_n) = n\pi.$$

This technique was initially used by Danish mathematician Gram [150] in 1903 to find the first 15 zeros of zeta.

Gram's Law is a bit of a misnomer - Gram himself didn't believe that there would always be exactly one zero in a Gram interval. The first time Gram's Law fails is the interval $[g_{125}, g_{126})$, which doesn't contain any zeros, while the next interval $[g_{126}, g_{127})$ contains two zeros. Titchmarsh [297] proved that Gram's Law fails infinitely many times. In the case of the original Gram's Law, it is still unknown whether it is true a positive proportion of the time, let alone infinitely many times. While this is an interesting topic of discussion in its own right, it takes us too far away from the theme of this thesis. We refer the interested reader to [162] for further information, as well as a probabilistic model of Gram's Law.

The other tibit of information that Shanks alluded to in his comments below Figure 2.1 are about exceptionally close zeros of the Riemann zeta function, called Lehmer pairs. Lehmer first found a close pair of zeros with imaginary parts 7005.06266... and 7005.10056... (the 6709$^{\text{th}}$ and 6710$^{\text{th}}$ zeros). More precisely, Csordas, Smith and Varga [91] define a Lehmer pair as having the property that their ordinates γ_n and γ_{n+1} obey the inequality

$$\frac{1}{(\gamma_n - \gamma_{n+1})^2} \geq C \sum_{m \notin \{n,n+1\}} \left(\frac{1}{(\gamma_m - \gamma_n)^2} + \frac{1}{(\gamma_m - \gamma_{n+1})^2} \right)$$

for some constant $C > 5/4$.

For each $t \in \mathbb{R}$, define the entire function

$$H_t(z) := \int_0^\infty e^{tu^2} \Phi(u) \cos(uz) \; du$$

where $\Phi(u)$ is a certain super-exponentially decaying function. Newman [38] showed there is a finite constant Λ, the De Bruijn–Newman constant, such that the zeros of $H_t(z)$ are all real precisely when $t \geq \Lambda$. The Riemann Hypothesis is equivalent to the fact that $\Lambda \leq 0$ and Newman conjectured $\Lambda \geq 0$. If there are infinitely many Lehmer pairs, then it would follow that $\Lambda \geq 0$. This has been shown unconditionally by Rodgers and Tao

[272]. Newman is known to have said "This new conjecture is a quantitative version of the dictum that the Riemann hypothesis, if true, is only barely so."

We now return to Shanks' conjecture and the generalisation to higher derivatives. We present a different graph to the one Shanks created: Figure 2.2 shows a scatter plot of $\zeta'(\rho)$ at the first 100,000 non-trivial zeros of $\zeta(s)$. This new graph clearly displays symmetry along the real axis and a bias towards the positive side of the complex plane. Interestingly the graph appears to be a cardioid in shape, although we have set aside the search for a proof of why this should be the case for now.

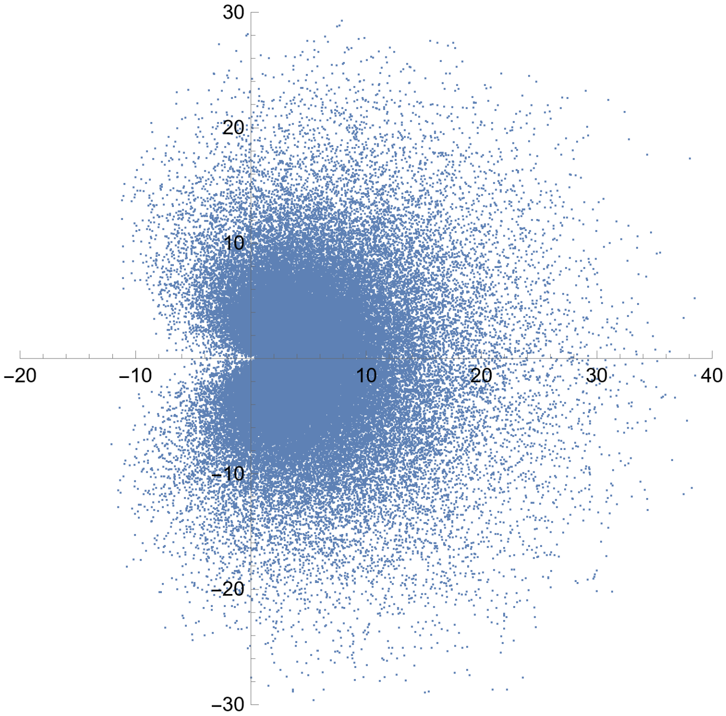

Figure 2.2: Scatterplot of $\zeta'(\rho)$ for the first 100,000 zeros of the zeta function.

As mentioned in Section 1.4.3.1, in 1985 Conrey, Ghosh and Gonek [73] were looking for a straightforward proof of the fact that there are infinitely many simple zeros of $\zeta(s)$. To this end, they used the Cauchy–Schwarz inequality to write

$$\left|\sum_{0<\gamma\leq T}\zeta'(\rho)\right|^2 \leq \sum_{0<\gamma\leq T}^{*} 1 \sum_{0<\gamma\leq T}|\zeta'(\rho)|^2$$

where the star on the middle sum denotes counting only the simple zeros. We denoted this sum as $N^*(T)$ previously. This sum only counts simple zeros as if there were any zeros of higher degree, the sum on the left-hand side would be zero and so wouldn't contribute to the answer.

To complete the proof they used the asymptotic for the discrete second moment on the right-hand side, given in (1.32) and so only needed to find the leading order behaviour of the sum on the left-hand side. They showed

$$\sum_{0<\gamma\leq T} \zeta'(\rho) = \frac{T}{4\pi}(\log T)^2 + O(T\log T) \tag{2.1}$$

which coincidently proved Shanks' conjecture. Combining these two asymptotics with the Cauchy–Schwarz inequality above shows

$$N^*(T) \gg T \tag{2.2}$$

as $T \to \infty$, which completes their proof that there are infinitely many simple zeros of the Riemann zeta function.

The downside of the method to prove that infinitely many of the zeros of the Riemann zeta function are simple is that it is not strong enough to show that a positive proportion of the non-trivial zeros of $\zeta(s)$ are simple, whereas other methods are, as we have already discussed in Section 1.4.3.1.

It is now clear what the third type of moment is that we alluded to earlier when we first discussed continuous and discrete moments. Moments of the form found in (2.1) are the key point of interest in this thesis. Specifically, we will study moments of the form

$$\sum_{0<\gamma\leq T} \zeta^{(n)}(\rho)^k$$

as $T \to \infty$, for integer k, n, or more generally,

$$\sum_{0<\gamma\leq T} \zeta^{(n_1)}(\rho)\ldots\zeta^{(n_k)}(\rho)$$

as $T \to \infty$, for integer $n_1, \ldots n_k$, where $\rho = \beta + i\gamma$ denotes a non-trivial zero of the Riemann zeta function. The specific questions we ask have been given in the Preface to this thesis, with full details given in each chapter from this one onwards.

Before we describe the generalisation of Shanks' conjecture to higher derivatives, it is worth describing the ongoing research progress on the distribution of $\zeta'(\rho)$. In 1994 Fujii [126] found explicit lower order terms for the asymptotic formula (2.1) (he later corrected a slight error in the lowest-order coefficient in [128], when writing a paper where he combined $\zeta'(\rho)$ with Landau's Theorem, as seen in Chapter 4). The full correct asymptotic is given by

$$\sum_{0<\gamma\leq T} \zeta'(\rho) = \frac{T}{4\pi}\left(\log\frac{T}{2\pi}\right)^2 + (-1+\gamma_0)\frac{T}{2\pi}\log\frac{T}{2\pi} + (1-\gamma_0-\gamma_0^2-3\gamma_1)\frac{T}{2\pi} + E(T) \tag{2.3}$$

where γ_0 and γ_1 are coefficients in the Laurent expansion of $\zeta(s)$ about $s = 1$, given by

$$\zeta(s) = \frac{1}{s-1} + \sum_{j=0}^{\infty} \frac{(-1)^j}{j!} \gamma_j (s-1)^j,$$

where the γ_j are the Stieltjes constants and γ_0 is Euler's constant.

Unconditional bounds for $E(T)$ were given by Fujii, where

$$E(T) = O\left(Te^{-C\sqrt{\log T}}\right),$$

with C a positive constant. Under the Riemann Hypothesis, he showed

$$E(T) = O\left(T^{1/2}(\log T)^{7/2}\right).$$

The best known conditional error term is shown in Section 3.1.6 and can be found in [186], to be

$$E(T) = O\left(T^{1/2}(\log T)^{13/4}\right).$$

In 2021 Kobayashi [215] gave a similar result for Dirichlet L-functions, with the same leading order asymptotic term.

In 2010 Trudgian [299] gave an alternative proof of Shanks' conjecture, based on Shanks' observation of the connection between $\arg \zeta'(\rho)$ and Gram's Law. Although care needs to be taken in the definition of the argument (*a priori* it is only defined up to a multiple of 2π), Trudgian was able to show that

$$\sum_{0<\gamma\leq T} \arg \zeta'(\rho) \ll_{\varepsilon} T^{\varepsilon}$$

for every $\varepsilon > 0$.

We are now ready to explore the generalisation of Shanks' Conjecture to $\zeta^{(n)}(s)$, the n^{th} derivative of $\zeta(s)$, for every positive integer n. This extension, which we call the Generalised Shanks' Conjecture, states that $\zeta^{(n)}(\rho)$ is real and positive in the mean if n is even, while $\zeta^{(n)}(\rho)$ is real and negative in the mean if n is odd.

In 2011, using ideas similar to those in Conrey, Ghosh and Gonek's proof of Shanks' original conjecture, Kaptan, Karabulut and Yıldırım [207] found the main term for the summatory function of $\zeta^{(n)}(\rho)$. Specifically, they showed that

$$\sum_{0<\gamma\leq T} \zeta^{(n)}(\rho) = \frac{(-1)^{n+1}}{n+1} \frac{T}{2\pi} (\log T)^{n+1} + O\big(T(\log T)^n\big) \tag{2.4}$$

which clearly implies the Generalised Shanks' Conjecture as stated above. They have also proved a similar result for derivatives of Dirichlet L-functions, with the same leading order asymptotic term.

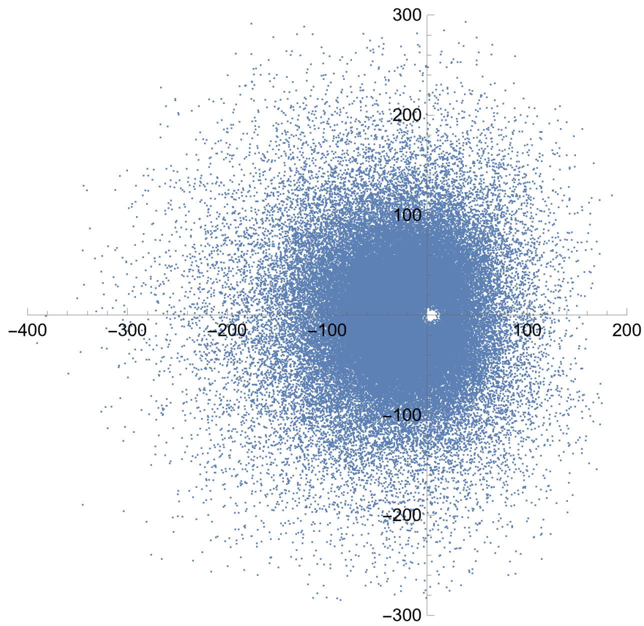

Figure 2.3: Scatterplot of $\zeta''(\rho)$ for the first 100,000 zeros of the zeta function.

In 2022, together with Hughes [186], we investigated the Generalised Shanks' Conjecture and found lower order terms for the asymptotic formula (2.4), the proof of which will be given in Chapter 3. The result can be stated in the form

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

$$+ (-1)^{n+1}\sum_{k=0}^{n}\binom{n}{k}(-1)^k k!\left(-1+\sum_{j=0}^{k}\frac{1}{j!}\gamma_j\right)\frac{T}{2\pi}\left(\log\frac{T}{2\pi}\right)^{n-k} + n!A_n\frac{T}{2\pi} + E_n(T) \tag{2.6}$$

where the γ_j are the coefficients in the Laurent expansion of $\zeta(s)$ about $s=1$, and where the A_j are the coefficients in the Laurent expansion of $\zeta'(s)/\zeta(s)$ about $s=1$.

The unconditional error term is the same as given by Fujii in the first derivative case. If we assume the Riemann hypothesis, then we can improve his error term in the first derivative case, and in general, we have

$$E_n(T) = O\left(T^{1/2}(\log T)^{n+9/4}\right).$$

In Chapter 3 we are able to give an equivalent version of this result derived from a

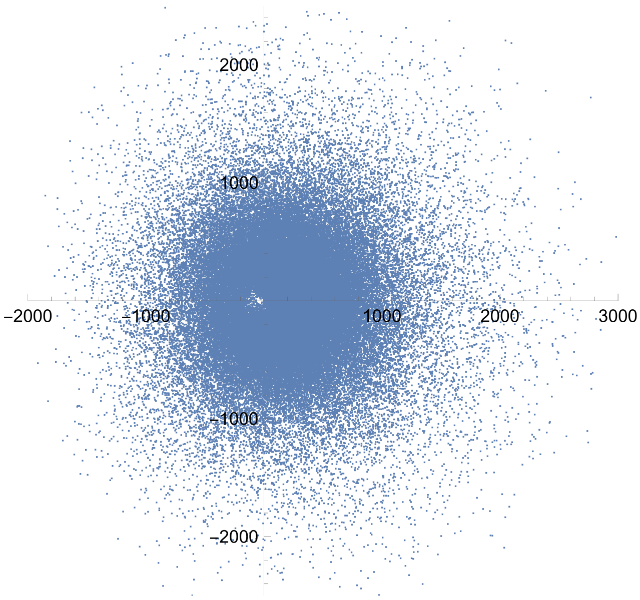

Figure 2.4: Scatterplot of $\zeta'''(\rho)$ for the first 100,000 zeros of the zeta function.

result of Fujii's [126], which can be written unconditionally, for T sufficiently large, as

$$\sum_{0<\gamma\le T} \zeta^{(n)}(\rho) = n! \sum_{\ell=0}^{n+1} \frac{(-1)^{n-\ell+1}}{(n-\ell+1)!} \frac{T}{2\pi} \left(\log \frac{T}{2\pi}\right)^{n-\ell+1} + n! \sum_{m=0}^{n} \sum_{\ell=0}^{n-m} \frac{(-1)^{n-m-\ell+1}\gamma_m}{(n-m-\ell)!m!} \frac{T}{2\pi} \left(\log \frac{T}{2\pi}\right)^{n-m-\ell} + n! A_n \frac{T}{2\pi} + O\left(Te^{-C\sqrt{\log T}}\right),$$

where the coefficients γ_j and A_n are from the Laurent expansions of $\zeta(s)$ and $\zeta'(s)/\zeta(s)$ about $s=1$, respectively.

In Chapter 6 we are able to give an integral form of this result, using the Ratios Conjecture. This can be written (under the Riemann Hypothesis) as

$$\sum_{0<\gamma\le T} \zeta^{(n)}\left(\frac{1}{2}+i\gamma\right) = \frac{n!}{2\pi} \int_1^T \left(A_n + \frac{(-1)^{n+1}L^{n+1}}{(n+1)!} + \sum_{m=0}^{n} \frac{(-1)^{m+1}L^m \gamma_{n-m}}{m!(n-m)!}\right) dt + O\left(T^{1/2+\varepsilon}\right),$$

where $L = \log t/2\pi$ and again the γ_j are the coefficients in the Laurent expansion of $\zeta(s)$ about $s=1$, and where the A_j are the coefficients in the Laurent expansion of $\zeta'(s)/\zeta(s)$ about $s=1$.

Furthermore, we have also extended Fujii's combination (mentioned earlier) of $\zeta'(s)$ and Landau's Theorem to all derivatives of $\zeta(s)$, as will be shown in Chapter 4 and has appeared in [262] .

In a recent paper, Benli, Elma and Ng [22] have generalised (2.5), giving a full asymptotic for sums of the form

$$\sum_{0<\gamma\leq T} \zeta(\rho+\alpha)X(\rho)Y(1-\rho)$$

where α is a small complex number and $X(s), Y(s)$ are Dirichlet polynomials. As an application of this result, they set $X(s) \equiv Y(s) \equiv 1$ and differentiate with respect to α n-times and set $\alpha = 0$ to reobtain (2.5).

All of the results we have described have relatively complicated proofs, and it is unclear that any of them provide an intuitive explanation for the alternating signs in the Generalised Shanks' Conjecture, or indeed of the positive sign in Shanks' original conjecture. We now present a simple heuristic that explains these signs, and indeed recovers the leading order term in the asymptotic formula (2.1) and (2.4).

2.3 HEURISTIC FOR THE GENERALISED SHANKS' CONJECTURE

2.3.1 Preliminary Lemmas

2.3.1.1 Dirichlet Series Approximations

We begin with some preliminaries concerning the Riemann zeta function, which we recall for $\Re(s) > 1$ can be written as the convergent Dirichlet series

$$\zeta(s) = \sum_{m=1}^{\infty} \frac{1}{m^s}.$$

Since Dirichlet series converge locally uniformly we may differentiate term by term; and since the derivative of $\frac{1}{m^s} = e^{-s\log m}$ is $(-\log m)m^{-s}$, we see that

$$\zeta^{(n)}(s) = (-1)^n \sum_{m=1}^{\infty} \frac{(\log m)^n}{m^s}$$

for $\Re(s) > 1$. This can be extended beyond the range of absolute convergence in a myriad of ways. We sketch the proof of one such method in the following lemma.

Lemma 2.1. *For $s = \sigma + it$,*

$$\zeta^{(n)}(s) = (-1)^n \sum_{m\leq x} \frac{(\log m)^n}{m^s} - \frac{d^n}{ds^n}\left[\frac{x^{1-s}}{1-s}\right] + O\left(\frac{(\log x)^n}{x^\sigma}\right)$$

uniformly for $\sigma \geq \sigma_0 > 0$ and $|t| < Cx$ where C is a positive constant less than 2π. Restricting ourselves to $t > 2$ and setting $x = t$ we have

$$\zeta^{(n)}(s) = (-1)^n \sum_{m \leq t} \frac{(\log m)^n}{m^s} + O(t^{-\sigma}(\log t)^n). \tag{2.7}$$

Proof. We sketch the proof for (2.7), using an adaptation of the method found in Titchmarsh [298, pages 74–77]. Equation (4.11.2) from that book shows that for $\sigma > 0$ and $N \in \mathbb{N}$,

$$\zeta(s) = \sum_{m=1}^{N} \frac{1}{m^s} - \frac{N^{1-s}}{1-s} + s\int_N^\infty \frac{[u] - u + 1/2}{u^{s+1}}\, du - \frac{1}{2}N^{-s}.$$

If we differentiate this equality n times with respect to s, we get

$$\begin{aligned}\zeta^{(n)}(s) = (-1)^n \sum_{m=1}^{N} \frac{(\log m)^n}{m^s} - \frac{d^n}{ds^n}\left[\frac{N^{1-s}}{1-s}\right] - \frac{1}{2}(-\log N)^n N^{-s} \\ + n\int_N^\infty \frac{([u] - u + 1/2)(-\log u)^{n-1}}{u^{s+1}}\, du + s\int_N^\infty \frac{([u] - u + 1/2)(-\log u)^{n}}{u^{s+1}}\, du. \end{aligned} \tag{2.8}$$

When $\sigma > \sigma_0$ for a fixed $\sigma_0 > 0$, the last three terms can be uniformly estimated as

$$\begin{aligned} -\frac{1}{2}(-\log N)^n N^{-s} &\ll \frac{(\log N)^n}{N^{\sigma_0}} \\ \int_N^\infty \frac{([u] - u + 1/2)(-\log u)^{n-1}}{u^{s+1}} du &\ll \frac{(\log N)^{n-1}}{N^{\sigma_0}} \\ s\int_N^\infty \frac{([u] - u + 1/2)(-\log u)^{n}}{u^{s+1}} du &\ll |s|\frac{(\log N)^n}{N^{\sigma_0}}. \end{aligned}$$

Moreover, if we define $g(m) = \frac{(\log m)^n}{m^\sigma}$ and $f(m) = -\frac{t \log m}{2\pi}$, we may apply [298, Lemma 4.10] to get

$$\begin{aligned} (-1)^n \sum_{t<m\leq N} \frac{(\log m)^n}{m^s} &= (-1)^n \sum_{t<m\leq N} g(m) e^{2\pi i f(m)} \\ &= (-1)^n \int_t^N g(u) e^{2\pi i f(u)} du + O\left(\frac{(\log t)^n}{t^\sigma}\right) \\ &= \int_t^N \frac{(-\log u)^n}{u^s} du + O\left(\frac{(\log t)^n}{t^\sigma}\right). \end{aligned}$$

On the other hand,

$$\int_t^N \frac{(-\log u)^n}{u^s} du = \frac{d^n}{ds^n}\left[\frac{N^{1-s}}{1-s}\right] - \frac{d^n}{ds^n}\left[\frac{t^{1-s}}{1-s}\right]$$

(to see this, note that for $n = 0$ the integral is directly calculable, and for $n > 1$ simply differentiate both sides with respect to s the appropriate number of times). If we restrict ourselves to $t > 2$, we obtain

$$\frac{d^n}{ds^n}\left[\frac{t^{1-s}}{1-s}\right] \ll \frac{t^{1-\sigma}(\log t)^n}{|1 - \sigma + it|} \ll t^{-\sigma}(\log t)^n.$$

Therefore, plugging all this back into (2.8), we have shown that when $\sigma > \sigma_0$ for a fixed $\sigma_0 > 0$,

$$\zeta^{(n)}(s) = (-1)^n \sum_{m\leq t} \frac{(\log m)^n}{m^s} + O\left(|s|\frac{(\log N)^n}{N^{\sigma_0}}\right) + O\left(\frac{(\log t)^n}{t^\sigma}\right).$$

Letting $N \to \infty$ completes the derivation of (2.7). □

2.3.1.2 The Landau–Gonek Theorem

We begin this section by stating the Landau–Gonek Theorem, found in [146] which concerns sums of the form X^ρ over the non-trivial zeros of the Riemann zeta function. This is in essence an exponential sum. It was proved by Landau [219] for fixed X and made uniform by Gonek [144, 146]. This formula has a great many applications. For example, Gonek [146] reproved the leading order behaviour for the second discrete moment of the Riemann zeta function given in (1.31) using the Landau–Gonek Theorem, as well as a result of Montgomery's on simple zeros. Other applications will be seen throughout this thesis.

Theorem (Landau–Gonek)**.** *For $X, T > 1$,*

$$\sum_{0<\gamma\leq T} X^\rho = -\frac{T}{2\pi}\Lambda(X) + O(X\log(2XT)\log\log(3X)) + O\left(\log X \min\left(T, \frac{X}{\langle X\rangle}\right)\right) + O\left(\log T \min\left(T, \frac{1}{\log X}\right)\right) \tag{2.9}$$

where $\rho = \beta + i\gamma$ a non-trivial zero of $\zeta(s)$, $\Lambda(X)$ denotes the von Mangoldt function, and where $\langle X\rangle$ denotes the distance from X to the nearest prime power other than X itself.

The large number of error terms are explained by Gonek [144]. They are due to the different behaviour of the sum in different ranges of X. He also notes that when $X = m \in \mathbb{N}$ and $T \gg m$, the last two error terms of (2.9) are absorbed by the first error term and so (2.9) becomes

$$\sum_{0<\gamma\leq T} m^\rho = -\frac{T}{2\pi}\Lambda(m) + O(m\log(2mT)\log\log(3m)). \tag{2.10}$$

The difference in formula (2.9) and formula (2.10) highlights the differences in behaviour of sums of this form when X is no longer an arbitrary positive real number but is instead a positive integer.

Fujii has generalised Gonek's result (assuming the Riemann Hypothesis) in [124] and [125] to find the subleading and subsubleading behaviour. This is given by

$$\sum_{0<\gamma\leq T} X^{1/2+i\gamma} = -\frac{T}{2\pi}\Lambda(X) + X^{1/2+iT}\left(\frac{\log\frac{T}{2\pi}}{2\pi i\log X} + \frac{1}{\pi}\arg\zeta\left(\frac{1}{2}+iT\right)\right) + O\left(\frac{\log T}{(\log\log T)^2}\right). \tag{2.11}$$

We state a corollary of the Landau–Gonek Theorem, found in [146]. Note that under the Riemann Hypothesis, for a non-trivial zero ρ of $\zeta(s)$, we have $\overline{\rho} = 1 - \rho$. Then

$$\sum_{0<\gamma\leq T} m^{1-\rho} = \sum_{0<\gamma\leq T} \overline{m^{\rho}} = \overline{\sum_{0<\gamma\leq T} m^{\rho}} = -\frac{T}{2\pi}\Lambda(m) + O(m\log(2mT)\log\log(3m))$$

since the right-hand side of (2.10) is real. Dividing through by m gives the following result.

Corollary 2.2 (Gonek). *Under the Riemann Hypothesis, for $T > 1, m \in \mathbb{N}$ with $m \geq 2$ and $\rho = 1/2 + i\gamma$ a non-trivial zero of the Riemann zeta function $\zeta(s)$,*

$$\sum_{0<\gamma\leq T} m^{-\rho} = -\frac{T}{2\pi}\frac{\Lambda(m)}{m} + O(\log(2mT)\log\log(3m)), \tag{2.12}$$

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

We now sketch where the main term in the Landau–Gonek Theorem comes from. By Cauchy's Theorem, we can write

$$\sum_{0<\gamma\leq T} X^{\rho} = \frac{1}{2\pi i}\int_{\mathcal{C}} \frac{\zeta'}{\zeta}(s)X^s \, ds$$

where $\mathcal{C}$ is a certain contour that encloses the non-trivial zeros of $\zeta(s)$ that goes past the 1-line, say $c + i$ to $c + iT$, where $c = 1 + 1/\log T$. The other sides of the contour aren't relevant to our sketch, as it can be shown that the integrals along them only contribute to the error term.

The integral along this line gives

$$\begin{aligned}\frac{1}{2\pi}\int_{c+i}^{c+iT} \frac{\zeta'}{\zeta}(s)X^s \, ds &= \frac{1}{2\pi}\int_1^T \left(-\sum_{n=2}^{\infty}\frac{\Lambda(n)}{n^{c+it}}\right) X^{c+it} \, ds \\ &= -\sum_{n=2}^{\infty}\Lambda(n)\left(\frac{X}{n}\right)^c \frac{1}{2\pi}\int_1^T \left(\frac{X}{n}\right)^{it} \, dt\end{aligned}$$

since we can expand the logarithmic derivative of $\zeta(s)$ as a Dirichlet series as $c > 1$. The diagonal terms (those where $X = n$) contribute to the main term, again with the rest of the terms contributing to the error terms. The right-hand side contributes

$$-\sum_{n=2}^{\infty}\Lambda(n)\left(\frac{X}{n}\right)^c \frac{1}{2\pi}\int_1^T \left(\frac{X}{n}\right)^{it} \, dt = -\frac{T}{2\pi}\Lambda(X) + \mathcal{E},$$

where $\mathcal{E}$ is some error term, and so we can see where the Landau–Gonek Theorem should reasonably come from. That is, we have sketched that

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

where $\mathcal{E}$ is some error term that Landau and Gonek considered and found explicitly.

Other generalisations of the Landau–Gonek Theorem can be found. For example, in the case of a Dirichlet L-function, we could follow the above method to show

$$\sum_{0<\gamma_\chi\le T} X^{\rho_\chi} = -\frac{T}{2\pi}\Lambda(X)\chi(X) + \mathcal{E}$$

where the sum is over the non-trivial zeros $\rho_\chi = \beta_\chi + \gamma_\chi$ of a Dirichlet L-function, and where we can derive a similar error term to that in the Landau–Gonek Theorem, rather than leaving it implicit by just writing $\mathcal{E}$. Similarly, under the Generalised Riemann Hypothesis, we could show for an integer $m \ge 2$ that

$$\sum_{0<\gamma_\chi\le T} m^{-\rho_\chi} = -\frac{T}{2\pi}\frac{\Lambda(m)\overline{\chi}(m)}{m} + \mathcal{E}.$$

2.3.2 The Heuristic

We now state the short heuristic argument which yields the Generalised Shanks' Conjecture as stated in Section 2.1. We ignore error terms on the whole so the equal signs are not 'true' equalities but show the general argument. (See Chapter 3 on how to derive the rigorous result.)

We note that while the heuristic requires the assumption of the Riemann Hypothesis (as we will use Corollary 2.2), the general results with a full, rigorous proof of (2.1) and (2.4) do not, except for improvements in the error term.

Using the approximate formula (2.7) for $\zeta(s)$ and Corollary 2.2, we may write for $n \ge 1$,

$$\begin{aligned}\sum_{0<\gamma\le T} \zeta^{(n)}(\rho) &\approx (-1)^n \sum_{0<\gamma\le T}\sum_{m\le\gamma} (\log m)^n m^{-\rho} \\ &= (-1)^n \sum_{m\le T} (\log m)^n \sum_{m<\gamma\le T} m^{-\rho} \\ &\approx (-1)^{n+1}\frac{T}{2\pi}\sum_{m\le T}\frac{(\log m)^n\Lambda(m)}{m} - (-1)^{n+1}\frac{1}{2\pi}\sum_{m\le T}(\log m)^n\Lambda(m).\end{aligned} \tag{2.13}$$

To finish the heuristic, we need to sum the two series in the last line. By Chebyshev's Theorem [5],

$$C(x) = \sum_{m\le x}\frac{\Lambda(m)}{m} = \log x + O(1)$$

so by partial summation, we have

$$\begin{aligned}\sum_{m\le T}\frac{(\log m)^n\Lambda(m)}{m} &= C(T)(\log T)^n - n\int_1^T \frac{C(x)(\log x)^{n-1}}{x}\,dx \\ &= \frac{1}{n+1}(\log T)^{n+1} + O\big((\log T)^n\big).\end{aligned}$$

and similarly

$$\sum_{m \leq T} (\log m)^n \Lambda(m) = O\big(T(\log T)^n\big).$$

Combining this with our argument above, we have

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

as $T \to \infty$, which is the leading order the asymptotic result for the Generalised Shanks' Conjecture, as given in (2.4).

Remark. Note that this result assumes $n \geq 1$. When $n = 0$ the left-hand side is trivially zero, whilst the right-hand side, as written, is not. This is explained by noticing that when $n \geq 1$ the term when $m = 1$ in the sum (2.13) is not present, since $(\log 1)^n = 0$. However, if $n = 0$ this term is present and is not accounted for in the Landau–Gonek Theorem, which holds for $m \geq 2$ only. The $m = 1$ term in that case clearly contributes $N(T)$, which perfectly cancels the $-\frac{T}{2\pi} \log T + O(T)$ term coming from the calculation given above.

Remark. This argument can be applied *mutatis mutandis* for Dirichlet L-functions, yielding exactly the same leading order behaviour as for the Riemann zeta function. This result was already known [207, 215].

2.3.2.1 *The Error Terms*

In the previous section in the last part of equation (2.13), we ignored the error terms coming from Corollary 2.2. Including them one can see that they contribute

$$\ll \sum_{m \leq T} (\log m)^n \log\log(3m) \log T \ll T(\log T)^{n+1} \log\log T$$

which dominates the main term! However, these are worst-case point-wise estimates and take no account of any potential cancellation when averaged, so it is likely that when summed over m the true error is smaller and the main term is correct. (Indeed that is what is proved, by different methods, in [73, 207] for $n = 1$ and $n \geq 2$ respectively.)

The point is that whilst this method must remain a heuristic, it is a much quicker approach to find the main term in the overage of $\zeta^{(n)}(\rho)$ and gives some sense of why the Generalised Shanks' Conjecture holds true, that is, why the mean of $\zeta^{(n)}(\rho)$ is real and positive/negative.

Remark. In Chapter 3 we prove that the true value of the mean of $\zeta^{(n)}(\rho)$ (that is, the main term and all the lower order terms up to a power saving) is given by

$$\sum_{\substack{m,r \\ m,r \leq \frac{T}{2\pi}}} \Lambda(r)(\log r)^n$$

which shows that the heuristic in the previous section can only yield the main term since the last line of equation (2.13) differs from the true value by $O(T(\log T)^n)$. This result is found with full details in Chapter 3 and in [186].

2.4 SHANKS' CONJECTURE FOR THE RECIPROCAL

As we have seen in Sections 1.3.6 and 1.4.1, negative moments are also of interest. It is natural to ask if there is an analogue to Shanks' conjecture for negative moments of the derivatives of $\zeta(s)$. Garaev and Sankaranarayanan in [134] have proved a negative moment of $\zeta'(\rho)$ (under the assumption of simple zeros) which we can rederive with the heuristic. Note that if we could find a proof that didn't assume the simple zeros hypothesis, then proving the following asymptotic would imply that all zeros of the Riemann zeta function are simple (else the right-hand side of the asymptotic would blow up as $T \to \infty$). We also note that the following result can be found [195, 244, 236] in under the additional assumption of the Riemann Hypothesis.

Theorem 2.3 (Garaev–Sankaranarayanan)**.** *Assume all the non-trivial zeros of $\zeta(s)$ are simple. Then*

$$\sum_{0<\gamma\leq T} \frac{1}{\zeta'(\rho)} \sim \frac{T}{2\pi} \tag{2.14}$$

as $T \to \infty$.

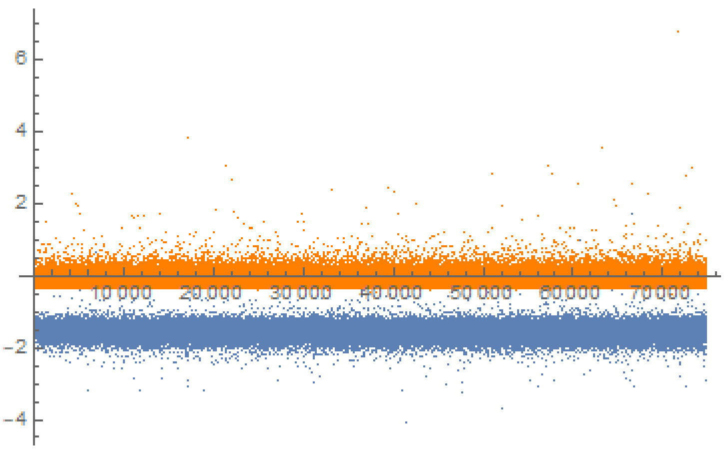

Figure 2.5: The real (blue) and imaginary (orange) part of $\sum_{0<\gamma\leq T} \frac{1}{\zeta'(\rho)} - \frac{T}{2\pi}$ plotted over the first 100,000 zeros.

Consider Theorem 2.3 above, together with the Figure 2.5. Clearly if we were to state a Shanks' style conjecture (although again, it is already a theorem), we would claim

$$1/\zeta'(\rho) \text{ is real and positive in the mean.}$$

However it is also clear that there is some constant, subleading real term from the graph. We make the following conjecture (although believe we could remove the assumptions of simple zeros and the Riemann Hypothesis). As before, a proof without assuming the simple zeros hypothesis would imply that all the non-trivial zeros of the Riemann zeta function are simple.

Conjecture. *Assume all the non-trivial zeros of $\zeta(s)$ are simple and the Riemann Hypothesis is true. Then*

$$\sum_{0<\gamma\leq T} \frac{1}{\zeta'(\rho)} = \frac{T}{2\pi} + C + O\left(T^{1/2+\varepsilon}\right) \tag{2.15}$$

as $T \to \infty$.

We have suggested an error term of $O\left(T^{1/2+\varepsilon}\right)$ to be consistent with other zeta function conjectures, but the numerics suggest the true size of the error term should be far smaller. The constant C however, is a different story. Typically, the lower order terms of a moments problem involves some arithmetic information, so a safe bet would be to say that $C = f(\gamma_0)$. At a numerical value of roughly -1.6, we suggest that $C = -1 - \gamma_0$ but this guess is based solely on a numerical approximation. Clearly the constant should be contained within the error term, but we can see a clear systematic negative bias from Figure 2.5 and so we include the constant explicitly in this conjecture. Investigating this error term and the value of the missing constant would be of interest.

We can also compare this result with a conjecture of Gonek's [145], stated in (1.35). He conjectured the following result.

Conjecture 2.4 (Gonek)**.** *Assume all the non-trivial zeros of $\zeta(s)$ are simple and the Riemann Hypothesis is true. Then*

$$J_{-2}(T) = \sum_{0<\gamma\leq T} \frac{1}{|\zeta'(\rho)|^2} \sim \frac{3}{\pi^3} T$$

as $T \to \infty$.

Again, we note that if we could find a proof that didn't assume the simple zeros hypothesis, then proving the following asymptotic would imply that all zeros of the Riemann zeta function are simple.

Recall also that Milinovich and Ng [236] have shown a lower bound for this result, correct up to a factor of a half, stated in (1.36).

Interestingly, as a final comment before we use the heuristic to derive Theorem 2.3, we note that both Theorem 2.3 and Conjecture 2.4 are of the same order of magnitude.

2.4.1 Negative Shanks' Conjecture via the Heuristic

Given

$$\zeta'(\rho) = \lim_{x\to 0} \frac{\zeta(\rho+x)-\zeta(\rho)}{x} = \lim_{x\to 0} \frac{\zeta(\rho+x)}{x},$$

it is plausible (but certainly not rigorously proven, since we have ignored all issues with rearranging the, at best, conditionally convergent sums) that

$$\begin{aligned} \sum_{0<\gamma\le T} \frac{1}{\zeta'(\rho)} &= \sum_{0<\gamma\le T} \lim_{x\to 0} \frac{x}{\zeta(\rho+x)} \\ &= \lim_{x\to 0+} x \sum_{0<\gamma\le T} \sum_{m=1}^{\infty} \frac{\mu(m)}{m^{\rho+x}} \\ &= \lim_{x\to 0^+} x \left(N(T) + \sum_{m=2}^{\infty} \frac{\mu(m)}{m^x} \sum_{0<\gamma\le T} m^{-\rho} \right) \end{aligned}$$

where the second line is conditionally convergent for $\Re(x) > 0$ if the Riemann Hypothesis holds, and the $N(T)$ term comes from the $m = 1$ term in that sum. Then applying the Landau–Gonek Theorem (again ignoring the error terms) to the second sum in the previous equation, this equals

$$\begin{aligned} &\lim_{x\to 0^+} x \left(\sum_{m=2}^{\infty} \frac{\mu(m)}{m^x} \sum_{0<\gamma\le T} m^{-\rho} \right) \approx -\frac{T}{2\pi} \lim_{x\to 0^+} x \sum_{n=1}^{\infty} \frac{\mu(n)\Lambda(n)}{n^{1+x}} \\ &= \frac{T}{2\pi} \lim_{x\to 0^+} x \sum_{p \text{ prime}} \frac{\log p}{p^{1+x}} \end{aligned}$$

where last line follows since $\mu(n)\Lambda(n) = -\log(p)$ if $n = p$ a prime, and zero otherwise.

By the Prime Number Theorem we have

$$\lim_{x\to 0^+} x \sum_{p} \frac{\log p}{p^{1+x}} = \lim_{x\to 0^+} x \int_2^{\infty} \frac{\log y}{y^{1+x}} \frac{dy}{\log y} = 1$$

giving us the heuristic derivation of Theorem 2.3.

Remark. This argument can be applied *mutatis mutandis* for Dirichlet L-functions, yielding exactly the same leading order behaviour as for the Riemann zeta function. This result doesn't seem to already be known, but a similar proof to that of Garaev and Sankaranarayanan should follow (under the assumptions of simple zeros and the Generalised Riemann Hypothesis). We state this result in full for future interest.

Conjecture 2.5. *Assume the Generalised Riemann Hypothesis, and that all the zeros of a Dirichlet L-function* $L(s,\chi)$ *are simple. Then for* $\rho_\chi = \beta_\chi + i\gamma_\chi$ *a non-trivial zero of* $L(s,\chi)$*, we have*

$$\sum_{0<\gamma_\chi\le T} \frac{1}{L'(\rho_\chi,\chi)} \sim \frac{T}{2\pi}.$$

— 3 —

The Generalised Shanks' Conjecture

In Chapter 2 we introduced Shanks' conjecture, which states for $\rho = \beta + i\gamma$ a non-trivial zero of $\zeta(s)$, that

$$\zeta'(\rho) \text{ is real and positive in the mean.}$$

While Conrey, Ghosh and Gonek [75] established the truth of this conjecture to leading order, Fujii [126, 128] extended their result by showing for sufficiently large T that

$$\sum_{0<\gamma\leq T} \zeta'(\rho) = \frac{T}{4\pi}\left(\log\frac{T}{2\pi}\right)^2 + (-1+\gamma_0)\frac{T}{2\pi}\log\frac{T}{2\pi} + (1-\gamma_0-\gamma_0^2-3\gamma_1)\frac{T}{2\pi} + E(T) \quad (3.1)$$

where γ_0 and γ_1 are coefficients in the Laurent expansion of $\zeta(s)$ about $s = 1$ and $E(T)$ is a particular error term, depending on whether we assume the Riemann hypothesis or not. The unconditional error term is the same as that in the Prime Number Theorem (1.7) and the conditional error term given when assuming the Riemann hypothesis is given by

$$E(T) = O\left(T^{1/2}(\log T)^{7/2}\right).$$

The aim of Section 3.1 is to do the same for the Kaptan, Karabulut and Yıldırım [207] result for sums of $\zeta^{(n)}(\rho)$, that is to find lower order terms for

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

This comes in the form of a polynomial in $\log T$ of degree $n+1$, with a similar error term to that of Fujii's. Their proof verifies the Generalised Shanks' Conjecture, which states for $\rho = \beta + i\gamma$ a non-trivial zero of $\zeta(s)$, that

$$\zeta^{(n)}(\rho) \text{ is real and positive/negative in the mean if } n \text{ is odd/even.}$$

In Section 3.1.6 we show how we can improve the error term in Fujii's result, as well as how to improve the initial error term that we gave Hughes and Pearce-Crump [186]. This improvement comes in the form of a saving of a fourth-root of a logarithm in T.

In Section 3.2 we show how we can derive an equivalent asymptotic to the one given in Theorem 3.1 using a shifted asymptotic formula of Fujii's.

We end this chapter by briefly discussing the Generalised Shanks' Conjecture over short intervals. This means that we instead sum over the ordinates of zeros of size between T and $T+H$, where $T^{1/2+\varepsilon} \ll H \ll T$. This result to leading order is as expected, and shows for such H, for sufficiently large T,

$$\sum_{T<\gamma\leq T+H} \zeta^{(n)}(\rho) = (-1)^{n+1}\frac{1}{n+1}\frac{H}{2\pi}(\log T)^{n+1} + O\left(H(\log T)^n\right) + O\left(T^{1/2+\varepsilon}\right).$$

The work presented in Section 3.1 has already appeared in print in [186]. Notation and cross-references have been updated for this thesis, as well as an improved error term as previously mentioned. This improved error term written in this chapter takes the place of what was given in the original paper.

3.1 THE GENERALISED SHANKS' CONJECTURE

In this section we prove the following result.

Theorem 3.1. *For $\rho = \beta + i\gamma$ a non-trivial zero of $\zeta(s)$, and where $\zeta^{(n)}(s)$ denotes the n^{th} derivative of $\zeta(s)$, we have for T sufficiently large,*

$$\sum_{0<\gamma\leq T} \zeta^{(n)}(\rho) = (-1)^{n+1}\frac{1}{n+1}\frac{T}{2\pi}\left(\log\frac{T}{2\pi}\right)^{n+1} + (-1)^{n+1}\sum_{k=0}^{n}\binom{n}{k}(-1)^k k!\left(-1+\sum_{j=0}^{k}\frac{1}{j!}\gamma_j\right)\frac{T}{2\pi}\left(\log\frac{T}{2\pi}\right)^{n-k} + n!A_n\frac{T}{2\pi} + E_n(T) \tag{3.2}$$

where the γ_j are the coefficients in the Laurent expansion of $\zeta(s)$ about $s=1$, given by

$$\zeta(s) = \frac{1}{s-1} + \sum_{j=0}^{\infty}\frac{(-1)^j}{j!}\gamma_j(s-1)^j,$$

and where the A_j are the coefficients in the Laurent expansion of $\zeta'(s)/\zeta(s)$ about $s=1$, given by

$$A_n = \begin{cases} \gamma_0 & \text{if } n=0 \\ \frac{(-1)^n(n+1)}{n!}\gamma_n - \sum_{j=0}^{n-1} A_j \frac{(-1)^{n-1-j}}{(n-1-j)!}\gamma_{n-1-j} & \text{otherwise.} \end{cases} \tag{3.3}$$

The error term is given by

$$E_n(T) = O\left(T\mathrm{e}^{-C\sqrt{\log T}}\right)$$

with C is a positive constant. If we assume the Riemann hypothesis, then

$$E_n(T) = O\left(T^{1/2}(\log T)^{n+9/4}\right).$$

The expression for A_n given in (3.3) is found in [197] with equivalent forms in [230, 35].

Remark. Two simpler but equivalent representations of this theorem can be found in Theorem 3.17 and in Section 6.2.4.1, both of which are derived in different ways.

3.1.1 Overview of the Proof

In this section we give a brief outline of the proof, explaining the method we will follow to prove Theorem 3.1.

In Subsection 3.1.2, we state some preliminary lemmas that we will use throughout this section.

In Subsection 3.1.3, we begin by considering the integral S given by

$$S = \frac{1}{2\pi i}\int_R \frac{\zeta'}{\zeta}(s)\zeta^{(n)}(s)\ ds$$

where R is the positively oriented rectangular contour with vertices $c+i, c+iT, 1-c+iT, 1-c+i$ with $c = 1+\frac{1}{\log T}$. The non-trivial zeros of $\zeta(s)$ up to a height T are contained within R and so by Cauchy's Theorem the integral represents the summation

$$S = \sum_{0<\gamma\leq T} \zeta^{(n)}(\rho)$$

in question. We then show that the contribution to the integral from the bottom, top and right-hand side of the contour is contained within the error term of the theorem, so the main contribution comes from the integral along the left-hand side of the integral.

In Subsection 3.1.4, we evaluate this part of the contour integral. Through this, by Lemma 3.11 we link the integral to a summation

$$(-1)^n \sum_{mr\leq \frac{T}{2\pi}} \Lambda(r)(\log r)^n$$

which is then the main object in question.

In Subsection 3.1.5, Lemma 3.12 we use Perron's formula to evaluate this sum as a complex integral up a vertical line just to the right of the critical strip.

In Subsection 3.1.6, we will evaluate that complex integral and show that

$$\frac{1}{2\pi i}\int_{c-iV}^{c+iV} \left(\frac{\zeta'}{\zeta}(s)\right)^{(n)} \zeta(s)\frac{Y^s}{s}\ ds = \operatorname*{Res}_{s=1}\left(\frac{\zeta'}{\zeta}(s)\right)^{(n)} \zeta(s)\frac{Y^s}{s} + E_n(Y)$$

where $Y = \frac{T}{2\pi}$ and V is given explicitly to optimise the error term $E_n(Y)$, which we can describe both unconditionally and under the assumption of the Riemann hypothesis.

Finally, in Subsection 3.1.7, we will evaluate the residue at $s = 1$ to find the asymptotic expansion described in Theorem 3.1 by considering the Laurent expansions around the pole $s = 1$ of the terms in the above integrand.

Combining all of these steps together gives the result.

We finish the section by giving some examples in Subsection 3.1.8. Firstly, we can recover the asymptotic in (3.1) by specialising to the case $n = 1$, and in particular recover Shanks' Conjecture. We then give the first new case where $n = 2$, as well as providing some good numerical evidence for the strength of the result.

3.1.2 Preliminary Lemmas

We start by stating the strong form of the convexity bound for the zeta function and the n^{th} derivatives of the zeta function. The case $n = 0$ can be found in Ivić [198, Ch. I, Sect. 1.5], while the cases for all other n can be derived from this using Cauchy's theorem on derivatives of analytic functions on $\zeta(s)$ in a small disc of radius $\frac{1}{\log t}$ centred at $s = \sigma + it$.

Lemma 3.2. *For $t \geq t_0 > 0$ uniformly in σ,*

$$\zeta^{(n)}(\sigma + it) \ll \begin{cases} t^{1/2-\sigma}(\log t)^{n+1} & \text{if } \sigma \leq 0 \\ t^{(1-\sigma)/2}(\log t)^{n+1} & \text{if } 0 \leq \sigma \leq 1 \\ (\log t)^{n+1} & \text{if } \sigma \geq 1. \end{cases}$$

The following result follows from Gonek [143, Sect. 2, p. 126].

Lemma 3.3. *If T is such that $|T - \gamma| \gg \frac{1}{\log T}$ for any ordinate γ, uniformly for $-1 \leq \sigma \leq 2$ we have*

$$\left(\frac{\zeta'}{\zeta}(s)\right)^{(n)} \ll (\log T)^{n+2}. \tag{3.4}$$

To obtain the form of the functional equation for $\zeta^{(n)}(1 - s)$ that we will need, we will use the following result from Gonek [143], which is his Lemma 6.

Lemma 3.4. *For σ fixed, $n \geq 0$ and $t \geq 1$ we have*

$$\chi^{(n)}(1 - s) = (-1)^n \chi(1 - s) \left(\log \frac{t}{2\pi}\right)^n + O(t^{\sigma-3/2}(\log t)^{n-1}).$$

Lemma 3.5. *For $\sigma \geq 1$ and $t \geq 1$*

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

Proof. By the functional equation (1.1), and using the Leibniz product rule

$$(-1)^n \zeta^{(n)}(1 - s) = \sum_{k=0}^{n} \binom{n}{k} (-1)^{n-k} \chi^{(n-k)}(1 - s) \zeta^{(k)}(s).$$

Using Lemma 3.4 and Lemma 3.2 to bound $\zeta^{(k)}(s)$ for $\sigma \geq 1$, this equals

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

Dividing through by the factor of $(-1)^n$ gives the result. □

As another application of Lemma 6 from [143] we can rewrite the logarithmic derivative of the functional equation for $\zeta(s)$ as

$$\frac{\zeta'}{\zeta}(1-s) = -\log \frac{t}{2\pi} - \frac{\zeta'}{\zeta}(s) + O\left(t^{\sigma-3/2}\right) \tag{3.5}$$

valid for any fixed σ, which we will also need later.

3.1.3 Beginning the proof

Throughout we assume T is sufficiently large and satisfies $|T-\gamma| \gg \frac{1}{\log T}$, where γ is the imaginary part of any zero ρ. (This constraint simplifies the arguments, but has no effect on the resulting expressions or final theorem.) Consider the integral

$$S = \frac{1}{2\pi i} \int_R \frac{\zeta'}{\zeta}(s) \zeta^{(n)}(s)\ ds \tag{3.6}$$

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

By Cauchy's Residue Theorem,

$$S = \sum_{0<\gamma\leq T} \zeta^{(n)}(\rho).$$

We need to evaluate S in another way to determine the behaviour of $\sum_{0<\gamma\leq T} \zeta^{(n)}(\rho)$. To do this, we begin by splitting the integral S along each part of the contour, so

$$S = \frac{1}{2\pi i} \left(\int_{c+i}^{c+iT} + \int_{c+iT}^{1-c+iT} + \int_{1-c+iT}^{1-c+i} + \int_{1-c+i}^{c+i} \right) \frac{\zeta'}{\zeta}(s) \zeta^{(n)}(s)\ ds$$
$$= S^R + S^T + S^L + S^B,$$

say. We will first bound S^B, S^T, S^R trivially within error terms as follows. Our main aim will then be to evaluate S^L which we will do in the next section.

Lemma 3.6. *The integral along the bottom of the contour is $S^B = O(1)$.*

Proof. This follows as the integral is of finite length with a bounded integrand. □

Lemma 3.7. *The integral along the top of the contour is* $S^T = O\left(T^{1/2}(\log T)^{n+2}\right)$.

Proof. By the convexity result from Lemma 3.2 and using Lemma 3.3 to bound the logarithmic derivative, we may write

$$\begin{aligned}
S^T &\ll \int_{1-c}^{c} \left|\frac{\zeta'}{\zeta}(\sigma+iT)\zeta^{(n)}(\sigma+iT)\right| \, d\sigma \\
&\ll (\log T)^2 \left\{\int_{1-c}^{0} + \int_0^1 + \int_1^c\right\} \left|\zeta^{(n)}(\sigma+iT)\right| \, d\sigma \\
&\ll (\log T)^2 \left\{\int_{1-c}^{0} T^{1/2-\sigma}(\log T)^{n+1} \, d\sigma + \int_0^1 T^{(1-\sigma)/2}(\log T)^{n+1} \, d\sigma + \int_1^c (\log T)^{n+1} \, d\sigma\right\} \\
&\ll T^{1/2}(\log T)^{n+2}
\end{aligned}$$

since $c = 1 + \frac{1}{\log T}$. □

Lemma 3.8. *The integral along the right-hand side of the contour is* $S^R = O\left((\log T)^{n+3}\right)$.

Proof. Along the right-hand side of the contour we need to evaluate

$$S^R = \frac{1}{2\pi i}\int_{c+i}^{c+iT} \frac{\zeta'}{\zeta}(s)\zeta^{(n)}(s) \, ds.$$

Writing $\frac{\zeta'}{\zeta}(s)$ and $\zeta^{(n)}(s)$ in terms of their Dirichlet series, we have

$$\frac{\zeta'}{\zeta}(s) = -\sum_{r=1}^{\infty}\frac{\Lambda(r)}{r^s} \quad \text{and} \quad \zeta^{(n)}(s) = (-1)^n\sum_{m=1}^{\infty}\frac{(\log m)^n}{m^s} \tag{3.7}$$

where $\Lambda(r)$ is the von Mangoldt function given by

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

Substituting into S^R we have

$$\begin{aligned}
S^R &= \frac{1}{2\pi i}\int_1^T \left(-\sum_{r=1}^{\infty}\frac{\Lambda(r)}{r^{c+it}}\right)\left((-1)^n\sum_{m=1}^{\infty}\frac{(\log m)^n}{m^{c+it}}\right) \, idt \\
&\ll \sum_{r=1}^{\infty}\sum_{m=1}^{\infty}\frac{\Lambda(r)(\log m)^n}{r^c m^c}\int_1^T (rm)^{-it} \, dt \\
&\ll \sum_{r=1}^{\infty}\sum_{m=1}^{\infty}\frac{\Lambda(r)(\log m)^n}{r^c m^c \log rm} \\
&\ll \frac{\zeta'}{\zeta}(c)\zeta^{(n)}(c) \\
&\ll (\log T)^{n+3}.
\end{aligned}$$

where the final line follows from Lemmas 3.2 and 3.3. □

Since S^B, S^T, S^R are all within an error term of $O\left(T^{1/2}(\log T)^{n+2}\right)$, only the integral over the left-hand side of the contour will contribute in any meaningful way. Observe that

$$S^L = \frac{1}{2\pi i}\int_{1-c+iT}^{1-c+i}\frac{\zeta'}{\zeta}(s)\zeta^{(n)}(s)\ ds = -\frac{1}{2\pi i}\int_{c-iT}^{c-i}\frac{\zeta'}{\zeta}(1-s)\zeta^{(n)}(1-s)\ ds = -\overline{I},$$

where

$$I = \frac{1}{2\pi i}\int_{c+i}^{c+iT}\frac{\zeta'}{\zeta}(1-s)\zeta^{(n)}(1-s)\ ds. \tag{3.8}$$

3.1.4 EVALUATING I

Our main aim then for this section is to evaluate I. To do this we want to write I in such a way that we can apply Gonek's Lemma 5 from [143] which we will state below when we use it later in this section.

Lemma 3.9. *We can write the integral I given in* (3.8) *as*

$$I = \frac{(-1)^{n+1}}{2\pi}\int_1^T \chi(1-c-it)\left[\sum_{k=0}^{n}\binom{n}{k}\left(\log\frac{t}{2\pi}\right)^{n-k+1}\sum_{m=1}^{\infty}\frac{(-1)^k(\log m)^k}{m^{c+it}}\right.$$
$$\left.+\sum_{k=0}^{n}\binom{n}{k}\left(\log\frac{t}{2\pi}\right)^{n-k}\sum_{m=1}^{\infty}\frac{(-1)^{k+1}(\log m)^k}{m^{c+it}}\sum_{r=1}^{\infty}\frac{\Lambda(r)}{r^{c+it}}\right]\ dt + O\left(T^{1/2}(\log T)^{n+2}\right).$$

Proof. Substituting the results from Lemma 3.5 and (3.5) into I gives

$$I = \frac{1}{2\pi i}\int_{c+i}^{c+iT}\left(-\log\frac{t}{2\pi}+\frac{\zeta'}{\zeta}(s)+O(t^{c-3/2})\right)$$
$$\times\left((-1)^n\chi(1-s)\sum_{k=0}^{n}\binom{n}{k}\left(\log\frac{t}{2\pi}\right)^{n-k}\zeta^{(k)}(s)+O\left(t^{c-3/2}(\log t)^n\right)\right)\ ds.$$

Writing $s = c+it$, expanding the bracket in the integral and simplifying the error term gives

$$I = \frac{(-1)^{n+1}}{2\pi}\int_1^T \chi(1-c-it)\left[\sum_{k=0}^{n}\binom{n}{k}\left(\log\frac{t}{2\pi}\right)^{n-k+1}\zeta^{(k)}(c+it)\right.$$
$$\left.+\sum_{k=0}^{n}\binom{n}{k}\left(\log\frac{t}{2\pi}\right)^{n-k}\zeta^{(k)}(c+it)\frac{\zeta'}{\zeta}(c+it)\right]\ dt + O\left(T^{1/2}(\log T)^{n+2}\right). \tag{3.9}$$

where we have used $\chi(1-c-it) \ll t^{1/2-c}$, and $\zeta^{(k)}(c+it) \ll (\log t)^{k+1}$, and $\frac{\zeta'}{\zeta}(c+it) \ll (\log t)^2$. Writing $\zeta^{(k)}(s)$ and $\frac{\zeta'}{\zeta}(s)$ as their Dirichlet series (3.7) and substituting into I gives the result. □

We will now require the use of Lemma 5 from Gonek [143, Sect. 4, p. 131]. As it is such an important result for our proof, we state it here, with the phrasing adapted to suit our needs.

Lemma 3.10 (Gonek)**.** *Let $\{b_m\}_{m=1}^{\infty}$ be a sequence of complex numbers such that for any $\varepsilon > 0$, $b_m \ll m^{\varepsilon}$. Let $c > 1$ be as before and let k be a non-negative integer. Then for T sufficiently large,*

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

We can finally simplify I to get a single sum that we will work on evaluating in the next section.

Lemma 3.11. *The integral I can be written as*

$$I = (-1)^n \sum_{mr\le\frac{T}{2\pi}} \Lambda(r)(\log r)^n + O(T^{1/2}(\log T)^{n+2})$$

where the sum is taken over all integers m and r such that $mr \le T/2\pi$.

Proof. Before we apply Lemma 3.10, we will split the integral I given in (3.9) substituting the Dirichlet series to simplify the argument slightly. To do this, we write

$$\begin{aligned}
I &= \frac{(-1)^{n+1}}{2\pi}\int_1^T \chi(1-c-it)\sum_{k=0}^{n}\binom{n}{k}\left(\log\frac{t}{2\pi}\right)^{n-k+1}\sum_{m=1}^{\infty}\frac{(-1)^k(\log m)^k}{m^{c+it}}\,dt \\
&\quad + \frac{(-1)^{n+1}}{2\pi}\int_1^T \chi(1-c-it)\sum_{k=0}^{n}\binom{n}{k}\left(\log\frac{t}{2\pi}\right)^{n-k}\sum_{m=1}^{\infty}\frac{(-1)^{k+1}(\log m)^k}{m^{c+it}}\sum_{r=1}^{\infty}\frac{\Lambda(r)}{r^{c+it}}\,dt \\
&\quad + O\left(T^{1/2}(\log T)^{n+2}\right) \\
&= J_1 + J_2 + O\left(T^{1/2}(\log T)^{n+2}\right),
\end{aligned}$$

say.

For J_1, we have

$$\begin{aligned}
J_1 &= (-1)^{n+1}\sum_{k=0}^{n}\binom{n}{k}(-1)^k\frac{1}{2\pi}\int_1^T \chi(1-c-it)\left(\log\frac{t}{2\pi}\right)^{n-k+1}\sum_{m=1}^{\infty}\frac{(\log m)^k}{m^{c+it}}\,dt \\
&= (-1)^{n+1}\sum_{k=0}^{n}\binom{n}{k}(-1)^k\left(\sum_{m\le\frac{T}{2\pi}}(\log m)^k(\log m)^{n-k+1} + O\left(T^{1/2}(\log T)^{n-k+1}\right)\right) \\
&= (-1)^{n+1}\sum_{k=0}^{n}\binom{n}{k}(-1)^k\sum_{m\le\frac{T}{2\pi}}(\log m)^{n+1} + O\left(T^{1/2}(\log T)^{n+1}\right) \\
&= 0 + O\left(T^{1/2}(\log T)^{n+1}\right)
\end{aligned}$$

since by the Binomial Theorem,

$$\sum_{k=0}^{n}\binom{n}{k}(-1)^k = (1+(-1))^n = 0.$$

For J_2, we have

$$\begin{aligned}
J_2 &= (-1)^{n+1}\sum_{k=0}^{n}\binom{n}{k}(-1)^{k+1}\frac{1}{2\pi}\int_1^T \chi(1-c-it)\left(\log\frac{t}{2\pi}\right)^{n-k}\sum_{m=1}^{\infty}\frac{(\log m)^k}{m^{\sigma+it}}\sum_{r=1}^{\infty}\frac{\Lambda(r)}{r^{c+it}}\,dt\\
&= (-1)^{n+1}\sum_{k=0}^{n}\binom{n}{k}(-1)^{k+1}\frac{1}{2\pi}\int_1^T \chi(1-c-it)\left(\log\frac{t}{2\pi}\right)^{n-k}\sum_{mr=1}^{\infty}\frac{\Lambda(r)(\log m)^k}{(mr)^{c+it}}\,dt\\
&= (-1)^{n+1}\sum_{k=0}^{n}\binom{n}{k}(-1)^{k+1}\left(\sum_{mr\le\frac{T}{2\pi}}\Lambda(r)(\log m)^k(\log mr)^{n-k}+O\left(T^{1/2}(\log T)^{n-k}\right)\right)\\
&= (-1)^{n}\sum_{mr\le\frac{T}{2\pi}}\Lambda(r)\sum_{k=0}^{n}\binom{n}{k}(-\log m)^k(\log mr)^{n-k}+O\left(T^{1/2}(\log T)^{n}\right)\\
&= (-1)^{n}\sum_{mr\le\frac{T}{2\pi}}\Lambda(r)(\log mr-\log m)^n+O\left(T^{1/2}(\log T)^{n}\right)\\
&= (-1)^{n}\sum_{mr\le\frac{T}{2\pi}}\Lambda(r)(\log r)^n+O\left(T^{1/2}(\log T)^{n}\right).
\end{aligned}$$

where the last three sums are over all integers m and r such that $mr \le T/2\pi$. Our results follow from combining J_1 and J_2. □

Therefore

$$\begin{aligned}
S^L &= -\overline{I}\\
&= (-1)^{n+1}\sum_{mr\le\frac{T}{2\pi}}\Lambda(r)(\log r)^n+O\left(T^{1/2}(\log T)^{n+2}\right).
\end{aligned}$$

Since we have shown that the terms from S^B, S^T, S^R are harmless within the error term of $O\left(T^{1/2}(\log T)^{n+2}\right)$, we have that the integral given in equation (3.6) is equal to the sum

$$S = (-1)^{n+1}\sum_{mr\le\frac{T}{2\pi}}\Lambda(r)(\log r)^n+O\left(T^{1/2}(\log T)^{n+2}\right). \tag{3.10}$$

3.1.5 Evaluating the sum S

As we have discussed above, all that remains to do is to evaluate the sum in (3.10). To do this, we first note that by Perron's formula, we have

$$(-1)^{n+1}\sum_{mr\le\frac{T}{2\pi}}\Lambda(r)(\log r)^n = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty}\left(\frac{\zeta'}{\zeta}(s)\right)^{(n)}\zeta(s)\frac{Y^s}{s}\,ds$$

where we set $Y=\frac{T}{2\pi}$ and $c = 1+\frac{1}{\log T}$ as before.

Since we want to be able to evaluate the integral on the right-hand side, we will modify this slightly and instead use a truncated Perron formula.

Lemma 3.12. *For $2 \le V \le Y$, as $Y \to \infty$,*

$$(-1)^{n+1} \sum_{mr \le Y} \Lambda(r)(\log r)^n = \frac{1}{2\pi i} \int_{c-iV}^{c+iV} \left(\frac{\zeta'}{\zeta}(s)\right)^{(n)} \zeta(s) \frac{Y^s}{s} \, ds + R(Y,V),$$

where

$$R(Y,V) \ll \frac{Y}{V}(\log Y)^{n+2}.$$

We will use a specific V later in this section. The choice of V will depend on whether we assume the Riemann hypothesis or not.

Proof. If we let $a(k)$ denote the coefficients in Dirichlet series for $\left(\frac{\zeta'}{\zeta}(s)\right)^{(n)} \zeta(s)$, namely

$$a(k) = (-1)^{n+1} \sum_{r|k} \Lambda(r)(\log r)^n$$

then by the truncated Perron formula we have that the integral in the lemma equals

$$\sum_{k \le Y} a(k) + R(Y,V)$$

with

$$\begin{aligned} R(Y,V) &\ll \sum_{\frac{Y}{2}<k<2Y} |a(k)| \min\left(1, \frac{Y}{V|Y-k|}\right) + \frac{4^c + Y^c}{V} \sum_{k=1}^{\infty} \frac{|a(k)|}{k^c} \\ &= A + B. \end{aligned}$$

Writing $k = mr$ we see $\sum_{k \le Y} a(k)$ equals the sum in the lemma. To evaluate the error, note that $|a(k)| \le (\log k)^{n+1}$ (with equality only if k is prime). Therefore

$$\begin{aligned} A &\ll (\log Y)^{n+1} \sum_{\frac{Y}{2}<k<2Y} \min\left(1, \frac{Y}{V|Y-k|}\right) \\ &\ll (\log Y)^{n+1} \sum_{\ell \le Y} \frac{Y}{V} \frac{1}{\ell} \\ &\ll \frac{Y}{V}(\log Y)^{n+2}. \end{aligned}$$

For B, since $c = 1 + \frac{1}{\log T}$, the Dirichlet series converges, and so

$$B = \frac{4^c + Y^c}{V} \left| \left(\frac{\zeta'}{\zeta}(c)\right)^{(n)} \zeta(c) \right| \ll \frac{Y}{V}(\log Y)^{n+2}$$

where we use the fact that $Y \asymp T$.

Combining A and B gives the required bound on $R(Y,V)$. □

3.1.6 The Error Term

We will show that the error term can be described explicitly as follows, depending on whether we assume the Riemann hypothesis or not.

Lemma 3.13. *For $Y = \frac{T}{2\pi}$, as $Y \to \infty$, we have*

$$\frac{1}{2\pi i}\int_{c-iV}^{c+iV}\left(\frac{\zeta'}{\zeta}(s)\right)^{(n)}\zeta(s)\frac{Y^s}{s}\,ds = \operatorname*{Res}_{s=1}\left(\frac{\zeta'}{\zeta}(s)\right)^{(n)}\zeta(s)\frac{Y^s}{s} + E_n(Y)$$

where $E_n(Y)$ is an error term given by one of the following three cases:

1. *Unconditionally, by setting $V = \mathrm{e}^{C\sqrt{\log Y}}$, we obtain*

$$E_n(Y) = O\left(Y\mathrm{e}^{-C\sqrt{\log Y}}\right)$$

   where C a positive constant that is not necessarily the same in each instance.

2. *Assuming the Riemann hypothesis, setting $V = 2\pi Y$, we obtain*

$$E_n(Y) = O\left(Y^{1/2+\varepsilon}\right)$$

   for $\varepsilon > 0$.

3. *Assuming the Riemann hypothesis, setting $V = Y/(\log Y)^{3/2}$, we obtain*

$$E_n(Y) = O\left(Y^{1/2}(\log Y)^{n+9/4}\right).$$

We will calculate the residue in Section 3.1.7. First, we will show how we can obtain the different expressions for $E_n(Y)$ in the following subsections. We will also show in the final subsection that we are able to obtain a slightly better error term than that given in Fujii [126]. This argument first appeared in [186] for the $n = 1$ case and beats what is given in [186] for $n \geq 2$. We call the error term $E_n(T)$ here for consistency with our later comments on the error term as it grows with n, even though the first two error terms given in Lemma 3.13 don't have any explicit n-dependence.

3.1.6.1 The Unconditional Case

From Titchmarsh [298, Sect. 3.8, p. 54], we know there is a positive constant C such that for $c' = 1 - \frac{C}{\log V}$, all the zeros of $\zeta(s)$ are $\gg \frac{1}{\log T}$ away from the line running from $c' - iV$ to $c' + iV$. By Cauchy's Residue Theorem, the integral is

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

By Lemmas 3.2 and 3.3, if $V \ll T$, the integral on the horizontal lines can be estimated as

$$\frac{1}{2\pi i}\int_{c'\pm iV}^{c\pm iV}\left(\frac{\zeta'}{\zeta}(s)\right)^{(n)}\zeta(s)\frac{Y^s}{s}\,ds \ll (\log V)^{n+3}\frac{Y^c}{V}(c-c') \ll \frac{Y}{V}(\log V)^{n+2}$$

where we use the fact that $c-c' \ll \frac{1}{\log V}$ and $Y^c \ll Y$ since $c = 1+\frac{1}{\log(2\pi Y)}$.

For the integral on the vertical line, we have

$$\frac{1}{2\pi i}\int_{c'-iV}^{c'+iV}\left(\frac{\zeta'}{\zeta}(s)\right)^{(n)}\zeta(s)\frac{Y^s}{s}\,ds \ll Y^{c'}(\log V)^{n+3}\int_{-V}^{V}\frac{1}{1+|t|}\,dt \ll Y^{c'}(\log V)^{n+4}.$$

Since $c' = 1-\frac{C}{\log V}$, balancing the two errors comes from taking $V = \exp(C\sqrt{\log Y})$ for some positive constant C, and so we have

$$\frac{1}{2\pi i}\int_{c-iV}^{c+iV}\left(\frac{\zeta'}{\zeta}(s)\right)^{(n)}\zeta(s)\frac{Y^s}{s}\,ds = \operatorname*{Res}_{s=1}\left(\frac{\zeta'}{\zeta}(s)\right)^{(n)}\zeta(s)\frac{Y^s}{s} + O\left(Y\mathrm{e}^{-C\sqrt{\log Y}}\right).$$

3.1.6.2 The Conditional Case: No dependence on n

We assume the Riemann Hypothesis. One approach would be to choose $c' = \frac{1}{2}+\frac{1}{\log T}$ to guarantee a zero-free region, and set $V = T = 2\pi Y$. In that case, an application of Cauchy's Residue Theorem yields

$$\frac{1}{2\pi i}\int_{c-iV}^{c+iV}\left(\frac{\zeta'}{\zeta}(s)\right)^{(n)}\zeta(s)\frac{Y^s}{s}\,ds = \operatorname*{Res}_{s=1}\left(\frac{\zeta'}{\zeta}(s)\right)^{(n)}\zeta(s)\frac{Y^s}{s} + O\left(T^{1/2+\varepsilon}\right)$$

for $\varepsilon > 0$, where the horizontal pieces of the contour are estimated in a manner similar to that in the previous section, and the vertical piece of the contour uses the bound $\zeta(s) \ll t^{\varepsilon}$ for $\sigma \geq 1/2$.

As we have previously noted, we can get a better bound, one that depends explicitly upon n as we show in the next section. This error term originally appeared in our paper [186] for the case $n = 1$ but we give a general proof in this thesis for all n, and so we have combined the proofs and omitted the special case.

3.1.6.3 The Conditional Case: Dependence on n

We again assume the Riemann Hypothesis in this section. We can get a better bound, one that depends explicitly upon n, by choosing $c' = 1-c = -\frac{1}{\log T}$ (that is, just to the left of the critical strip) and $V \ll T$. By Cauchy's Residue Theorem,

$$\frac{1}{2\pi i}\int_{c-iV}^{c+iV}\left(\frac{\zeta'}{\zeta}(s)\right)^{(n)}\zeta(s)\frac{Y^s}{s}\,ds = \operatorname*{Res}_{s=1}\left(\frac{\zeta'}{\zeta}(s)\right)^{(n)}\zeta(s)\frac{Y^s}{s}$$
$$+\sum_{|\gamma|<V}\operatorname*{Res}_{s=\rho}\left(\frac{\zeta'}{\zeta}(s)\right)^{(n)}\zeta(s)\frac{Y^s}{s} + \frac{1}{2\pi i}\left(\int_{c'+iV}^{c+iV}+\int_{c'-iV}^{c'+iV}-\int_{c'-iV}^{c-iV}\right)\left(\frac{\zeta'}{\zeta}(s)\right)^{(n)}\zeta(s)\frac{Y^s}{s}\,ds,$$

where the sum runs through the non-trivial zeros $\rho = \beta + i\gamma$ of $\zeta(s)$, lying inside the contour.

To estimate the integral on the horizontal lines, choose V so that all the zeros of zeta are bounded by $\gg \frac{1}{\log V}$ away from the horizontal line. Therefore we may use Lemma 3.3 to bound the logarithmic derivative by $(\log V)^{n+2}$ along the line. Using the convexity result from Lemma 3.2, we obtain, unconditionally,

$$\begin{aligned}\frac{1}{2\pi i}\int_{c'\pm iV}^{c\pm iV}\left(\frac{\zeta'}{\zeta}(s)\right)^{(n)}\zeta(s)\frac{Y^s}{s}ds \ll &(\log V)^{n+2}\int_{-\frac{1}{\log V}}^{0} V^{1/2-\sigma}\log V\frac{Y^\sigma}{V}\,d\sigma\\ &+(\log V)^{n+2}\int_0^1 V^{(1-\sigma)/2}\log V\frac{Y^\sigma}{V}\,d\sigma\\ &+(\log V)^{n+2}\int_1^{1+\frac{1}{\log V}}\log V\frac{Y^\sigma}{V}\,d\sigma\\ \ll &\frac{Y}{V}(\log V)^{n+2}.\end{aligned}$$

For the integral on the vertical line, since $V \le T$ and $c' = -\frac{1}{\log T}$ we may again use Lemma 3.3 as the vertical line is bounded away from any zeros of zeta. Using Lemma 3.2 to bound zeta just to the left of the critical strip, we obtain (again unconditionally),

$$\frac{1}{2\pi i}\int_{c'-iV}^{c'+iV}\left(\frac{\zeta'}{\zeta}(s)\right)^{(n)}\zeta(s)\frac{Y^s}{s}\,ds \ll \int_1^V(\log t)^{n+2}\times t^{1/2}\times\log t\times\frac{1}{t}\,dt \ll V^{1/2}(\log V)^{n+3}.$$

We now consider the poles at $s=\rho$ for each ρ with $|\gamma|<V$, where ρ is a non-trivial zero of $\zeta(s)$.

First we note that for $-1\le\sigma\le 2$ and $0<t_0\le t\le V$, we have

$$\frac{\zeta'}{\zeta}(\sigma+it) = \sum_{|\gamma-t|<1}\frac{1}{s-\rho} + O(\log V).$$

Being careful with the error term, we may differentiate this n times to give

$$\left(\frac{\zeta'}{\zeta}(\sigma+it)\right)^{(n)} = \sum_{|\gamma-t|<1}\frac{(-1)^n n!}{(s-\rho)^{n+1}} + O(\log V).$$

For each ρ, we need to consider the coefficient of $(s-\rho)^n$ in the expansion of $\zeta(s)\frac{Y^s}{s}$ to find the residue at $s=\rho$. For this, note that by the triple product rule, we may write

$$\left(\zeta(s)\frac{Y^s}{s}\right)^{(n)} = \sum_{\substack{k_1+k_2+k_3=n\\ k_1,k_2,k_3\ge 0}}\binom{n}{k_1,k_2,k_3}\zeta^{(k_1)}(s)(Y^s)^{(k_2)}\left(\frac{1}{s}\right)^{(k_3)}$$

where $\binom{n}{k_1,k_2,k_3}$ is the multinomial coefficent given by

$$\binom{n}{k_1,k_2,k_3} = \frac{n!}{k_1!k_2!k_3!}.$$

Therefore, at each zero ρ,

$$\left(\zeta(s)\frac{Y^s}{s}\right)^{(n)}\Bigg|_{s=\rho} = \sum_{\substack{k_1+k_2+k_3=n\\k_1,k_2,k_3\geq 0}} (-1)^{k_3} k_3! \binom{n}{k_1,k_2,k_3} \frac{\zeta^{(k_1)}(\rho)Y^\rho(\log Y)^{k_2}}{\rho^{k_3+1}}.$$

As we are just bounding these terms, we do not worry about the coefficient such as the $n!$, $(-1)^n$ and the multinomial coefficients. Assuming RH, so $\rho = \frac{1}{2} + i\gamma$ and summing over all zeros with $|\gamma| < V$, we have

$$\sum_{|\gamma|<V} \operatorname*{Res}_{s=\rho} \left(\frac{\zeta'}{\zeta}(s)\right)^{(n)} \zeta(s)\frac{Y^s}{s} \ll Y^{1/2} \sum_{\substack{k_1+k_2+k_3=n\\k_1,k_2,k_3\geq 0}} (\log Y)^{k_2} \sum_{\gamma<V} \frac{\left|\zeta^{(k_1)}(\frac{1}{2}+i\gamma)\right|}{\left|\frac{1}{2}+i\gamma\right|^{k_3+1}}. \tag{3.11}$$

Under the Riemann Hypothesis, Garaev [135] showed that

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

To prove this result, he uses two key facts. The first is the following lemma.

Lemma 3.14. *Let $f(t)$ be a real-valued function that is continuously differentiable on the interval $[t_0, t_k]$. Let $t_0 < t_1 < ... < t_k$, and assume that $f(t)$ has at least one zero in each interval $[t_j, t_{j+1}], 0 \leq j \leq j-1$. Then*

$$\sum_{1\leq j\leq k} |f(t_j)| \leq \int_{t_0}^{t_k} |f'(t)|\, dt.$$

The other result Garaev uses is the following inequality from Ramachandra [270].

Lemma 3.15 (Ramachandra). *The inequality*

$$\frac{1}{T}\int_1^T \zeta^{(n)}\left(\frac{1}{2}+it\right)\, dt \ll (\log T)^{n+1/4}$$

holds.

To obtain a bound for the n^{th} derivative, we begin by proving the following corollary of Lemma 3.14.

Corollary 3.16. *Let $S(t)$ be a complex-valued function that is $(n+1)$-times differentiable on the interval $[t_0, t_k]$ with $t_0 < t_1 < ... < t_k$ and $S(t_j) = 0$ for all $0 \leq j \leq k$. Then*

$$\sum_{1\leq j\leq k} |S^{(n)}(t_j)| \leq \sqrt{2}\int_{t_0}^{t_k} |S^{(n+1)}(t)|\, dt.$$

Proof. We write $S(t) = A_1(t)+iA_2(t)$ where the $A_m(t)$ for $m = 1, 2$ are $(n+1)$-differentiable functions on the interval $[t_0, t_k]$. Then $A_m(t_j) = 0$ for $0 \le j \le k$. By the generalised form of Rolle's theorem, the $A_m^{(n)}(t)$ have zeros in each interval (t_j, t_{j+n}) for $0 \le j \le k - n$. Applying Lemma 3.14 to $f(t) = A_m^{(n)}(t)$ gives

$$\sum_{1\le j\le k} |A_m^{(n)}(t_j)| \le \int_{t_0}^{t_k} |A_m^{(n+1)}(t)|\ dt.$$

Combining these,

$$\sum_{1\le j\le k} |S^{(n)}(t_j)| \le \sqrt{2}\int_{t_0}^{t_k} |A_1^{(n+1)}(t)| + |A_2^{(n+1)}(t)|\ dt \le \sqrt{2}\int_{t_0}^{t_k} |S^{(n+1)}(t)|\ dt.$$

□

Applying Lemma 3.15 to Corollary 3.16 with $S(t) = \zeta(\frac{1}{2} + it)$ and $t_j = \gamma_j$ gives the following bound for all zeros with $1 \le \gamma_k \le T$. Under the Riemann Hypothesis, we have shown that

$$\sum_{0<\gamma\le T} \left|\zeta^{(n)}\left(\frac{1}{2} + i\gamma\right)\right| \ll T(\log T)^{n+5/4}.$$

Now by partial summation,

$$\begin{aligned}(\log Y)^{k_2} \sum_{\gamma<V} \frac{\left|\zeta^{(k_1)}(\frac{1}{2} + i\gamma)\right|}{\left|\frac{1}{2} + i\gamma\right|^{k_3+1}} &\ll \int_1^V \frac{(\log t)^{k_1+5/4}}{t^{k_3+1}}\ dt \\ &\ll \begin{cases} \log^{k_2} Y\,(\log V)^{k_1+9/4} & \text{if } k_3 = 0 \\ \log^{k_2} Y & \text{if } k_3 \ge 1. \end{cases}\end{aligned}$$

Clearly the dominant error term is when $k_3 = 0$ (which forces $k_2 = n - k_1$), and so the sum over the residues at the zeros in (3.11) is bounded by

$$\begin{aligned}\sum_{|\gamma|<V} \operatorname*{Res}_{s=\rho} \left(\frac{\zeta'}{\zeta}(s)\right)^{(n)} \zeta(s)\frac{Y^s}{s} &\ll \sum_{k_1=0}^{n} Y^{1/2}(\log Y)^{n-k_1}(\log V)^{k_1+9/4} \\ &\ll Y^{1/2}(\log Y)^{n+9/4}.\end{aligned}$$

Balancing this error term with the error term from the vertical line comes from taking $V = Y/(\log Y)^{3/2}$, and so we have

$$\frac{1}{2\pi i}\int_{c-iV}^{c+iV} \left(\frac{\zeta'}{\zeta}(s)\right)^{(n)} \zeta(s)\frac{Y^s}{s}\ ds = \operatorname*{Res}_{s=1} \left(\frac{\zeta'}{\zeta}(s)\right)^{(n)} \zeta(s)\frac{Y^s}{s} + O\left(Y^{1/2}(\log Y)^{n+9/4}\right).$$

3.1.7 Finding the Leading Asymptotic Terms

We now evaluate

$$\operatorname*{Res}_{s=1}\left(\frac{\zeta'}{\zeta}(s)\right)^{(n)}\zeta(s)\frac{Y^s}{s}$$

from Lemma 3.13. We expand each of the terms in this residue calculation in their Laurent expansions about $s=1$. Since

$$\frac{\zeta'(s)}{\zeta(s)}=-\frac{1}{s-1}+A_0+A_1(s-1)+...+A_k(s-1)^k+...+A_n(s-1)^n+O\left((s-1)^{n+1}\right),$$

where the A_n are defined in (3.3), we have

1. The Laurent expansion for $\left(\frac{\zeta'}{\zeta}(s)\right)^{(n)}$ about $s=1$:

$$\left(\frac{\zeta'}{\zeta}(s)\right)^{(n)}=\frac{(-1)^{n+1}n!}{(s-1)^{n+1}}+n!A_n+O((s-1)).$$

2. The Laurent expansion for $\zeta(s)$ about $s=1$:

$$\zeta(s)=\frac{1}{s-1}+\gamma_0-\gamma_1(s-1)+...+\frac{(-1)^k}{k!}(s-1)^k+...+\frac{(-1)^n}{n!}(s-1)^n+O\left((s-1)^{n+1}\right).$$

3. The Laurent expansion for Y^s about $s=1$:

$$\begin{aligned}Y^s=&Y\Bigg(1+(s-1)\log Y+...+\frac{(s-1)^k}{k!}(\log Y)^k+...+\frac{(s-1)^n}{n!}(\log Y)^n\\&+\frac{(s-1)^{n+1}}{(n+1)!}(\log Y)^{n+1}+O\left((s-1)^{n+2}\right)\Bigg).\end{aligned}$$

4. The Laurent expansion for $\frac{1}{s}$ about $s=1$:

$$\frac{1}{s}=1-(s-1)+(s-1)^2+...+(-1)^k(s-1)^k+...+(-1)^n(s-1)^n+O\left((s-1)^{n+1}\right).$$

We now work out the residue at $s=1$ by considering the terms in powers of $(\log Y)^k$, as k runs from $k=n+1$ down to $k=0$. We consider a combinatorial style argument to make sure we consider all possible terms. The following table shows this for various powers of $(\log Y)^k$.

To calculate the resulting contribution to the residue for the leading order behaviour, that is, the coefficient of $Y(\log Y)^{n+1}$, there is only one way to obtain a factor of $\frac{1}{s-1}$ for the residue calculation. We have to have the $\frac{(-1)^{n+1}n!}{(s-1)^{n+1}}$ term from $\left(\frac{\zeta'}{\zeta}(s)\right)^{(n)}$, the $\frac{1}{s-1}$ term from $\zeta(s)$, the $\frac{(s-1)^{n+1}}{(n+1)!}$ term from Y^s and the 1 term from $\frac{1}{s}$. Combined, the coefficient for $Y(\log Y)^{n+1}$ is $\frac{(-1)^{n+1}}{n+1}$.

To calculate the subleading term there are two distinct possibilities.

1. The first possibility is to have the $\frac{(-1)^{n+1}n!}{(s-1)^{n+1}}$ term from $\left(\frac{\zeta'}{\zeta}(s)\right)^{(n)}$, the γ_0 term from $\zeta(s)$, the $\frac{(s-1)^n}{n!}$ term from Y^s and the 1 term from $\frac{1}{s}$. The resulting contribution to the residue for this term is $(-1)^{n+1}\gamma_0$.
2. The other possibility is to have the $\frac{(-1)^{n+1}n!}{(s-1)^{n+1}}$ term from $\left(\frac{\zeta'}{\zeta}(s)\right)^{(n)}$, the $\frac{1}{s-1}$ term from $\zeta(s)$, the $\frac{(s-1)^n}{n!}$ term from Y^s and the $-(s-1)$ term from $\frac{1}{s}$. The resulting contribution to the residue for this term is $(-1)^{n+2}$.

Combined, the coefficient for the $Y(\log Y)^n$ term is $(-1)^{n+1}(\gamma_0 - 1)$.

The other terms in all lower order cases follow in a similar manner - Table 3.1 shows all possibilities, with one extra caveat for the lowest order term which has an additional term.

In the lowest-leading order case, the coefficient of the Y term, there are all the usual terms for the subleading behaviour, with one additional term. The additional term comes from the $n!A_n$ term from $\left(\frac{\zeta'}{\zeta}(s)\right)^{(n)}$, the $\frac{1}{s-1}$ term from $\zeta(s)$, the 1 term from Y^s, and the 1 term from $\frac{1}{s}$. Combined, the extra term for Y has coefficient $n!A_n$.

Combining all of the terms in the above table, and putting $Y = \frac{T}{2\pi}$ we have shown that

$$\operatorname*{Res}_{s=1}\left(\frac{\zeta'}{\zeta}(s)\right)^{(n)}\zeta(s)\frac{\left(\frac{T}{2\pi}\right)^s}{s} = (-1)^{n+1}\frac{1}{n+1}\frac{T}{2\pi}\left(\log\frac{T}{2\pi}\right)^{n+1}$$
$$+ (-1)^{n+1}\sum_{k=0}^{n}\binom{n}{k}(-1)^k k!\left(-1+\sum_{j=0}^{k}\frac{1}{j!}\gamma_j\right)\frac{T}{2\pi}\left(\log\frac{T}{2\pi}\right)^{n-k} + n!A_n\frac{T}{2\pi}.$$

Combining this with the results from Lemma 3.13 and using the appropriate choices for V in Lemma 3.12 we see that

$$(-1)^{n+1}\sum_{mr\le\frac{T}{2\pi}}\Lambda(r)(\log r)^n = \operatorname*{Res}_{s=1}\left(\frac{\zeta'}{\zeta}(s)\right)^{(n)}\zeta(s)\frac{\left(\frac{T}{2\pi}\right)^s}{s} + E_n(T).$$

Finally, (3.10) shows that sum is equal to $S = \sum_{0<\gamma\le T}\zeta^{(n)}(\rho)$ (plus an error that is smaller than $E_n(T)$), and the result follows.

3.1.8 Examples of the first moment of specific n^{th} derivatives of the Riemann zeta function $\zeta(s)$

The first test of a good theorem is if it can recover any previously known results. We begin this section by doing exactly that in the $n = 1$ case where we recover Shanks' Conjecture and Fujii's asymptotics, given in (3.1). After that we give another example, as well as showing some numerical data showing that our result is in excellent agreement with the true values. We have chosen $n = 2$ to show the most simple new case in full detail. The calculations for higher level derivatives become unwieldy to do by hand so we could employ a computer package to manage this for us to obtain any specific n^{th} order derivative that we choose.

$\left(\frac{\zeta'}{\zeta}(s)\right)^{(n)}$	$\zeta(s)$	Y^s	$\frac{1}{s}$	Contribution to the residue
$\frac{(-1)^{n+1}n!}{(s-1)^{n+1}}$	$\frac{(-1)^k}{k!}\gamma_k(s-1)^k$	$\frac{(s-1)^{n-k}Y(\log Y)^{n-k}}{(n-k)!}$	1	$(-1)^{n+1}\frac{n!}{(n-k)!}\frac{(-1)^k}{k!}\gamma_k Y(\log Y)^{n-k}$
$\frac{(-1)^{n+1}n!}{(s-1)^{n+1}}$	$\frac{(-1)^{k-1}}{(k-1)!}\gamma_{k-1}(s-1)^{k-1}$	$\frac{(s-1)^{n-k}Y(\log Y)^{n-k}}{(n-k)!}$	$-(s-1)$	$(-1)^n\frac{n!}{(n-k)!}\frac{(-1)^{k-1}}{(k-1)!}\gamma_{k-1}Y(\log Y)^{n-k}$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
$\frac{(-1)^{n+1}n!}{(s-1)^{n+1}}$	$-\gamma_1(s-1)$	$\frac{(s-1)^{n-k}Y(\log Y)^{n-k}}{(n-k)!}$	$(-1)^{k-1}(s-1)^{k-1}$	$(-1)^{n+k}\frac{n!}{(n-k)!}(-\gamma_1)Y(\log Y)^{n-k}$
$\frac{(-1)^{n+1}n!}{(s-1)^{n+1}}$	γ_0	$\frac{(s-1)^{n-k}Y(\log Y)^{n-k}}{(n-k)!}$	$(-1)^k(s-1)^k$	$(-1)^{n+k+1}\frac{n!}{(n-k)!}\gamma_0 Y(\log Y)^{n-k}$
$\frac{(-1)^{n+1}n!}{(s-1)^{n+1}}$	$\frac{1}{s-1}$	$\frac{(s-1)^{n-k}Y(\log Y)^{n-k}}{(n-k)!}$	$(-1)^{k+1}(s-1)^{k+1}$	$(-1)^{n+k}\frac{n!}{(n-k)!}Y(\log Y)^{n-k}$

Table 3.1: Table to show which terms in the Laurent expansion of each piece of L combine to form a contribution to the $Y(\log Y)^{n-k}$ term in the residue ($k = 0, ..., n$).

3.1.8.1 The case $n = 1$ (Shanks' Conjecture)

We can use Theorem 3.1 to recover Fujii's asymptotic formula (2.3) (with an improved error term) and hence Shanks' Conjecture as first stated at the start of Chapter 2. To do this, set $n = 1$ in the theorem to obtain

$$\sum_{0<\gamma\leq T} \zeta'(\rho) = \frac{1}{2}\frac{T}{2\pi}\left(\log\frac{T}{2\pi}\right)^2 + \sum_{k=0}^{1}\binom{1}{k}(-1)^k k!\left(-1+\sum_{j=0}^{k}\frac{1}{j!}\gamma_j\right)\frac{T}{2\pi}\left(\log\frac{T}{2\pi}\right)^{1-k} + A_1\frac{T}{2\pi} + E_1(T).$$

Note that $A_1 = -2\gamma_1 - \gamma_0^2$. Substituting this into the expression above and simplifying gives

$$\sum_{0<\gamma\leq T} \zeta'(\rho) = \frac{T}{4\pi}\left(\log\frac{T}{2\pi}\right)^2 + (-1+\gamma_0)\frac{T}{2\pi}\log\frac{T}{2\pi} + (1-\gamma_0-\gamma_0^2-3\gamma_1)\frac{T}{2\pi} + E_1(T)$$

in perfect agreement with (3.1). In Figure 3.1 we show the accuracy of this asymptotic by considering the true value of the real part of the sum, and start subtracting the main terms, for T up to the height of the 100,000$^{\text{th}}$ zero.

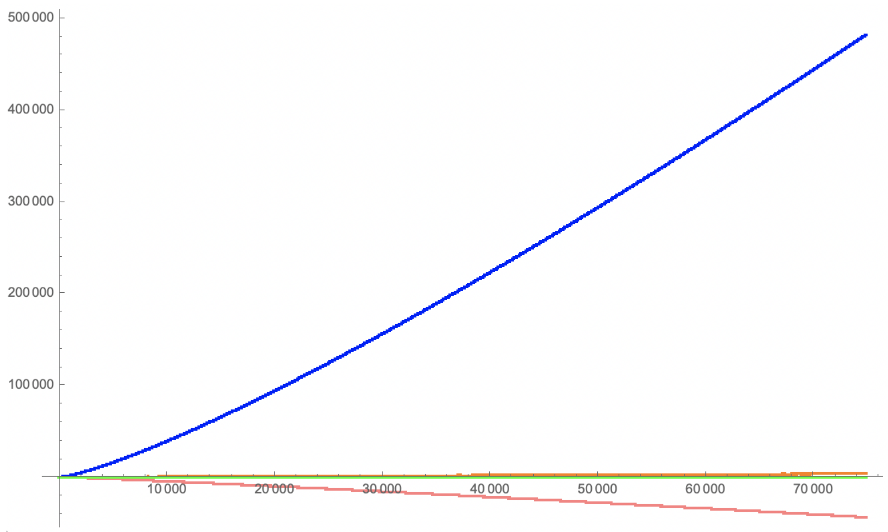

Figure 3.1: The real part of the sum $\sum_{0<\gamma\leq T}\zeta'(\rho)$ with true value (blue), the true - leading (pink), true - leading - subleading (orange) and true - leading - subleading - subsubleading (green) terms subtracted from the true value, for T up to the height of the 100,000$^{\text{th}}$ zero.

The error term $E_1(T)$ is $O\left(Te^{-C\sqrt{\log T}}\right)$ unconditionally. Note that under the Riemann Hypothesis, we have

$$E_1(T) = O\left(T^{1/2}(\log T)^{13/4}\right)$$

as previously claimed (and proved in [186]). This error term is then plotted in Figure 3.2, for T up to the height of the 100,000$^{\text{th}}$ zero.

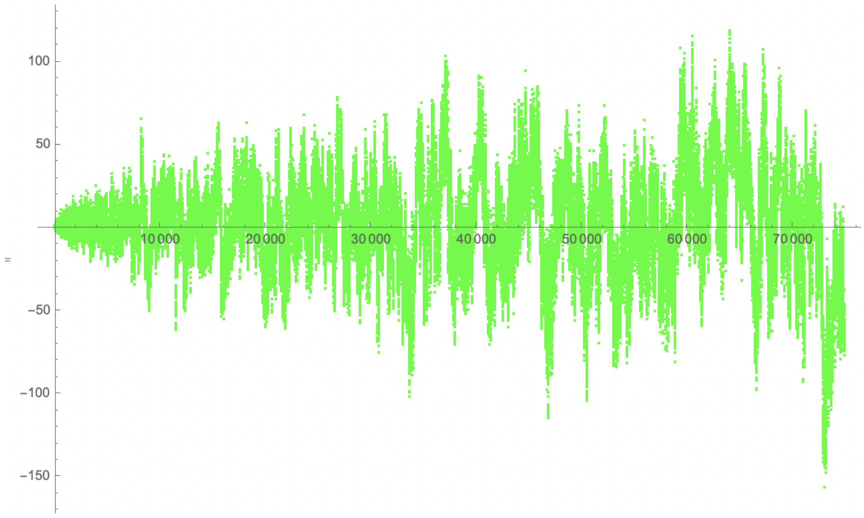

Figure 3.2: Difference in the real part of the actual value of $\sum_{0<\gamma\le T}\zeta'(\rho)$ and the whole asymptotic result, for T up to the height of the 100,000$^{\text{th}}$ zero, showing the real error at each point.

3.1.8.2 *The case $n = 2$*

We set $n = 2$ in Theorem 3.1 to obtain

$$\sum_{0<\gamma\le T}\zeta''(\rho) = -\frac{1}{3}\frac{T}{2\pi}\left(\log\frac{T}{2\pi}\right)^3 - \sum_{k=0}^{2}\binom{2}{k}(-1)^k k!\left(-1+\sum_{j=0}^{k}\frac{1}{j!}\gamma_j\right)\frac{T}{2\pi}\left(\log\frac{T}{2\pi}\right)^{2-k} + 2A_2\frac{T}{2\pi} + E_2(T).$$

Note that $A_2 = \frac{3}{2}\gamma_2 + 3\gamma_0\gamma_1 + \gamma_0^3$. Substituting this into the expression above and simplifying gives

$$\sum_{0<\gamma\le T}\zeta''(\rho) = -\frac{T}{6\pi}\left(\log\frac{T}{2\pi}\right)^3 - (-1+\gamma_0)\frac{T}{2\pi}\left(\log\frac{T}{2\pi}\right)^2 + (-2+2\gamma_0+2\gamma_1)\frac{T}{2\pi}\log\frac{T}{2\pi} + (2-2\gamma_0-2\gamma_1+2\gamma_2+6\gamma_0\gamma_1+2\gamma_0^3)\frac{T}{2\pi} + E_2(T).$$

In Figure 3.3 we show the accuracy of this asymptotic by considering the true value of the real part of the sum, and start subtracting the main terms, for T up to the height of the 100,000$^{\text{th}}$ zero.

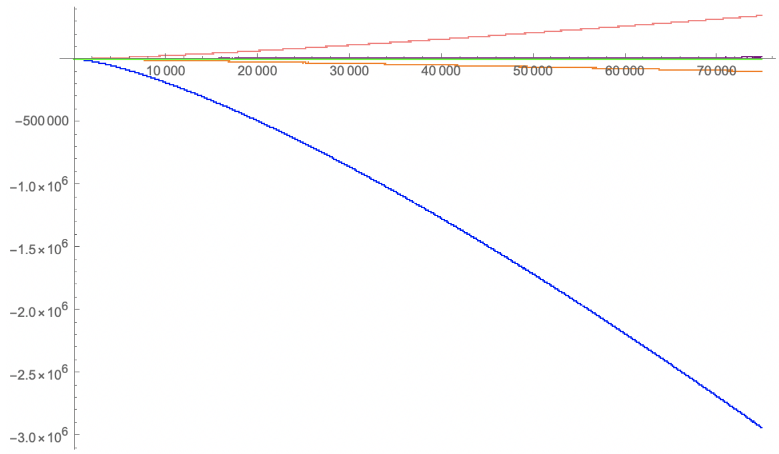

Figure 3.3: The real part of the sum $\sum_{0<\gamma\leq T}\zeta''(\rho)$ with true value (blue), the true - leading (pink), true - leading - subleading (orange), true - leading - subleading - subsubleading (green), true - leading - subleading - subsubleading - subsubsubleading (purple) terms subtracted from the true value, for T up to the height of the 100,000$^{\text{th}}$ zero.

The error term $E_2(T)$ is $O\left(Te^{-C\sqrt{\log T}}\right)$ unconditionally. Note that under the Riemann Hypothesis, we have

$$O\left(T^{1/2}(\log T)^{17/4}\right).$$

This error term is then plotted in Figure 3.4, for T up to the height of the 100,000$^{\text{th}}$ zero.

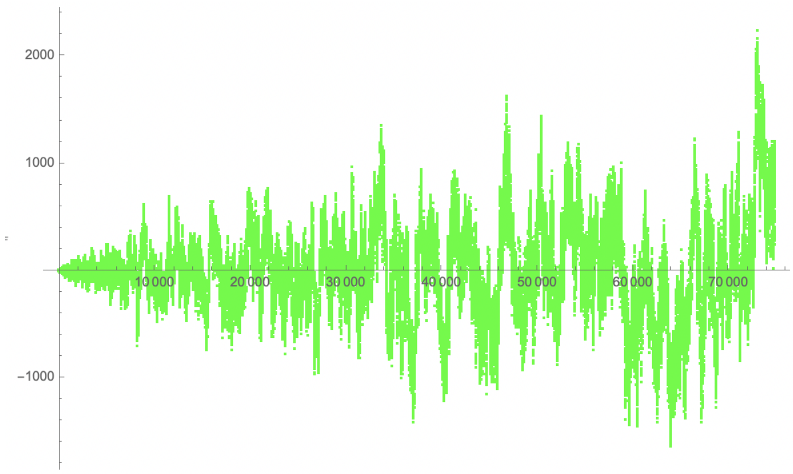

Figure 3.4: Difference in the real part of the actual value of $\sum_{0<\gamma\leq T}\zeta''(\rho)$ and the whole asymptotic result, for T up to the height of the 100,000$^{\text{th}}$ zero, showing the real error at each point.

3.2 THE GENERALISED SHANKS' CONJECTURE FROM A SHIFTED SUM

Fujii [126] also gave a shifted version of the Riemann zeta function at the non-trivial zeros of zeta, written in [22] in the case $\alpha = i\delta$, $0 \neq \delta \ll 1$ as

$$\sum_{0<\gamma\leq T} \zeta(\rho+\alpha) = \frac{T}{2\pi}\frac{\zeta'}{\zeta}(1+\alpha) - \left(\frac{T}{2\pi}\right)^{1-\alpha}\frac{\zeta(1-\alpha)}{1-\alpha} + \frac{T}{2\pi}\log\frac{T}{2\pi e} + O\left(Te^{-C\sqrt{\log T}}\right). \tag{3.12}$$

Fujii [126] shows the error term can be replaced by $O\left(T^{1/2}(\log T)^{5/2}\right)$ under the Riemann Hypothesis. By a similar argument to that given in Section 3.1.6, this can be improved to $O\left(T^{1/2}(\log T)^{9/4}\right)$.

In this section we use the above result (3.12) to recover the asymptotic in Theorem 3.1. As a theme that we see later in this thesis when using shifts, mainly in Chapters 5 and 6, we will Taylor expand the $\zeta(\rho+\alpha)$ term as

$$\zeta(\rho+\alpha) = \zeta'(\rho)\frac{\alpha}{1!} + \zeta''(\rho)\frac{\alpha^2}{2!} + \ldots + \zeta^{(n)}(\rho)\frac{\alpha^n}{n!} + \ldots, \tag{3.13}$$

recalling $\zeta(\rho) = 0$ by definition.

To do this, we begin by writing the appropriate functions in their Laurent expansions about $s = 1$. Specifically, with $L = \log\frac{T}{2\pi}$, we write

$$\frac{\zeta'}{\zeta}(1+\alpha) = -\frac{1}{\alpha} + \sum_{n=0}^{\infty} A_n\alpha^n \qquad \left(\frac{T}{2\pi}\right)^{1-\alpha} = \frac{T}{2\pi}\sum_{n=0}^{\infty}\frac{(-1)^n L^n\alpha^n}{n!}$$

$$\zeta(1-\alpha) = -\frac{1}{\alpha} + \sum_{m=0}^{\infty}\frac{\gamma_m\alpha^m}{m!} \qquad \frac{1}{1-\alpha} = \sum_{\ell=0}^{\infty}\alpha^\ell$$

where A_n is given explicitly in (3.3).

Next, substitute these into (3.12) to give

$$\begin{aligned}\sum_{0<\gamma\leq T}\zeta(\rho+\alpha) = \frac{T}{2\pi}&\left(-\frac{1}{\alpha} + \sum_{n=0}^{\infty}A_n\alpha^n\right)\\ &- \frac{T}{2\pi}\left(\sum_{n=0}^{\infty}\frac{(-1)^nL^n\alpha^n}{n!}\right)\left(-\frac{1}{\alpha} + \sum_{m=0}^{\infty}\frac{\gamma_m\alpha^m}{m!}\right)\left(\sum_{\ell=0}^{\infty}\alpha^\ell\right)\\ &+ \frac{T}{2\pi}\log\frac{T}{2\pi e} + O\left(Te^{-C\sqrt{\log T}}\right).\end{aligned}$$

After some simplifying, we have

$$\sum_{0<\gamma\leq T}\zeta(\rho+\alpha) = -\frac{T}{2\pi}\frac{1}{\alpha} + \frac{T}{2\pi}\left(\sum_{n=0}^{\infty}A_n\alpha^n\right) + \frac{T}{2\pi}\frac{1}{\alpha}\sum_{n=0}^{\infty}\left(\sum_{\ell=0}^{n}\frac{(-1)^{n-\ell}L^{n-\ell}}{(n-\ell)!}\right)\alpha^n + \frac{T}{2\pi}\sum_{n=0}^{\infty}\left(\sum_{m=0}^{n}\sum_{\ell=0}^{n-m}\frac{(-1)^{n-m-\ell+1}\gamma_m L^{n-m-\ell}}{(n-m-\ell)!m!}\right)\alpha^n + \frac{T}{2\pi}\log\frac{T}{2\pi e} + O\left(Te^{-C\sqrt{\log T}}\right).$$

Now extract the pole from the second line and re-index to obtain

$$\sum_{0<\gamma\leq T}\zeta(\rho+\alpha) = \frac{T}{2\pi}\left(\sum_{n=0}^{\infty}A_n\alpha^n\right) + \frac{T}{2\pi}\sum_{n=0}^{\infty}\left(\sum_{\ell=0}^{n+1}\frac{(-1)^{n-\ell+1}L^{n-\ell+1}}{(n-\ell+1)!}\right)\alpha^n + \frac{T}{2\pi}\sum_{n=0}^{\infty}\left(\sum_{m=0}^{n}\sum_{\ell=0}^{n-m}\frac{(-1)^{n-m-\ell+1}\gamma_m L^{n-m-\ell}}{(n-m-\ell)!m!}\right)\alpha^n + \frac{T}{2\pi}\log\frac{T}{2\pi e} + O\left(Te^{-C\sqrt{\log T}}\right).$$

For the general n^{th} derivative of $\zeta(s)$, where $n\in\mathbb{N}$, compare the coefficient of α^n on both sides of the previous equation. Recall that we have a Taylor expansion for $\zeta(\rho+\alpha)$ about $\alpha=0$, so

$$\sum_{0<\gamma\leq T}\frac{1}{n!}\zeta^{(n)}(\rho) = \frac{T}{2\pi}A_n + \frac{T}{2\pi}\sum_{\ell=0}^{n+1}\frac{(-1)^{n-\ell+1}L^{n-\ell+1}}{(n-\ell+1)!} + \frac{T}{2\pi}\sum_{m=0}^{n}\sum_{\ell=0}^{n-m}\frac{(-1)^{n-m-\ell+1}\gamma_m L^{n-m-\ell}}{(n-m-\ell)!m!} + O\left(Te^{-C\sqrt{\log T}}\right).$$

Multiplying through by $n!$ gives us an equivalent way of writing Theorem 3.1.

Theorem 3.17. *For $\rho=\beta+i\gamma$ a non-trivial zero of $\zeta(s)$, and where $\zeta^{(n)}(s)$ is the n^{th} derivative of $\zeta(s)$, we have for T sufficiently large,*

$$\sum_{0<\gamma\leq T}\zeta^{(n)}(\rho) = n!\sum_{\ell=0}^{n+1}\frac{(-1)^{n-\ell+1}}{(n-\ell+1)!}\frac{T}{2\pi}\left(\log\frac{T}{2\pi}\right)^{n-\ell+1} + n!\sum_{m=0}^{n}\sum_{\ell=0}^{n-m}\frac{(-1)^{n-m-\ell+1}\gamma_m}{(n-m-\ell)!m!}\frac{T}{2\pi}\left(\log\frac{T}{2\pi}\right)^{n-m-\ell} + n!A_n\frac{T}{2\pi} + O\left(Te^{-C\sqrt{\log T}}\right),$$

where the coefficients γ_j *are from the Laurent expansions of* $\zeta(s)$ *about* $s = 1$ *and the coefficients* A_n *are from the Laurent expansions of* $\zeta'(s)/\zeta(s)$ *about* $s = 1$*, given in* (3.3)*.*

It is clear then that the leading-order behaviour comes from the first sum with $\ell = 0$, and returns the expected leading-order coefficient.

We remark that care should be taken with regards to the error term; however it is fair that we should expect the error term from Theorem 3.1 to carry through, both unconditionally and under the Riemann Hypothesis.

3.3 THE GENERALISED SHANKS' CONJECTURE IN SHORT INTERVALS

We end this chapter by briefly considering sums of the derivative of the Riemann zeta function over the non-trivial zeros of the Riemann zeta function but instead over short intervals of length $T^{1/2+\varepsilon} \ll H \ll T$, rather than one of full length T. In an analogous method to that given in Section 3.1, we can show to leading order the following result.

Theorem. *Let* $T^{1/2+\varepsilon} \ll H \ll T$*. Then for* $\rho = \beta + i\gamma$ *a non-trivial zero of* $\zeta(s)$*, and where* $\zeta^{(n)}(s)$ *is the* n^{th} *derivative of* $\zeta(s)$*, we have*

$$\sum_{T<\gamma\leq T+H} \zeta^{(n)}(\rho) = (-1)^{n+1}\frac{1}{n+1}\frac{H}{2\pi}(\log T)^{n+1} + O\left(H(\log T)^n\right) + O\left(T^{1/2+\varepsilon}\right).$$

— 4 —

A Further Generalisation of Shanks' Conjecture

In this chapter we obtain a full asymptotic formula for the sum

$$\sum_{0<\gamma\leq T} \zeta^{(n)}(\rho)X^{\rho}$$

where $\zeta^{(n)}(s)$ denotes the n^{th} derivative of the Riemann zeta function, X is a positive real number, and $\rho = \beta + i\gamma$ denotes a non-trivial zero of the Riemann zeta function.

We also specify what the asymptotic formula becomes when X is a positive integer, highlighting the differences in the asymptotic expansions as X changes its arithmetic nature. This is interesting as the Landau–Gonek formula, as stated in (2.9) has numerous error terms but when X becomes a positive integer, as shown in (2.10), the behaviour changes. We see this phenomenon happening in the results in this chapter.

We have already seen the strength of the Landau–Gonek theorem in developing the heuristic presented in Chapter 2. The application of the Landau–Gonek theorem given here when combining with the Generalised Shanks' Conjecture takes a different form.

The work presented in this chapter has already appeared in print in [262]. Notation and cross-references have been updated for this thesis, as well as incorporating the improved error term given in Section 3.1.6.

4.1 HISTORICAL BACKGROUND OF COMBINATIONS OF THE LANDAU–GONEK THEOREM AND MOMENTS OF L-FUNCTIONS

Recall that the Landau–Gonek Theorem (2.9) is an explicit formula, a formula that relates the zeros of the Riemann zeta function to the prime numbers (and the further generalisations relating primes to zeros of other L-functions). By combining an explicit formula with an asymptotic for an L-function gives another type of explicit formula. Note that these combined formulae still link the zeros of an L-function with the prime numbers as will be highlighted in this historical section and in the new results we present.

Fujii started the idea of combining the asymptotic (2.9) from the Landau–Gonek Theorem and the derivatives of the Riemann zeta function in [128]. More specifically, he considers X to be a fixed positive real number, so he actually combines Landau's Theorem [219] with the derivatives of the Riemann zeta function (that is, the non-uniform version of the Landau–Gonek Theorem). For T sufficiently large, he gives the following explicit formula for a fixed positive real number X,

$$\begin{aligned}\sum_{0<\gamma\leq T}\zeta'(\rho)X^{\rho} = -\Delta(X)\frac{T}{2\pi}\left(\log X\left(\frac{1}{2}\log\frac{T}{2\pi}-\frac{1}{2}+\frac{\pi i}{4}\right)-\sum_{mr=X}\Lambda(r)\log m\right)\\ +X\sum_{m\leq\frac{T}{2\pi X}}e^{2\pi imX}(\log m)^2+\frac{1}{2}X\log X\sum_{m\leq\frac{T}{2\pi X}}e^{2\pi imX}\log m\\ -\left(\frac{1}{2}X(\log X)^2-\frac{\pi i}{4}X\log X\right)\sum_{m\leq\frac{T}{2\pi X}}e^{2\pi imX}\\ -X\sum_{mr\leq\frac{T}{2\pi X}}e^{2\pi imrX}\Lambda(r)\log m+O\left(T^{1/2}(\log T)^3\right)\end{aligned} \tag{4.1}$$

where $\Delta(X)$ is defined by

$$\Delta(X)=\begin{cases}1 & \text{if } X\in\mathbb{Z}\\ 0 & \text{otherwise.}\end{cases} \tag{4.2}$$

throughout this chapter.

Fujii then narrowed down X to be a positive integer and gave an asymptotic formula for this, again exhibiting the behaviour that Gonek noted in [128], about how the arithmetic nature of X can affect the asymptotic expansion. Specifically, he finds for X a positive integer,

$$\begin{aligned}\sum_{0<\gamma\leq T}\zeta'(\rho)X^{\rho} = \frac{T}{4\pi}\left(\log\frac{T}{2\pi}\right)^2+(-1+\gamma_0-\log X)\frac{T}{2\pi}\log\frac{T}{2\pi}\\ +\frac{T}{2\pi}\left(1-\gamma_0-\gamma_0^2-3\gamma_1+\sum_{X=mn}\Lambda(n)\log m-\left(\gamma_0-1+\frac{1}{2}\log X\right)\log X\right)\\ +O\left(Te^{-C\sqrt{\log T}}\right)\end{aligned} \tag{4.3}$$

where C is a positive constant. By assuming the Riemann Hypothesis, Fujii gives an improved error term of $O\left(T^{1/2}(\log T)^{7/2}\right)$. Clearly setting $X=1$ then recovers (2.3).

A generalisation of Fujii's result has been given in Jakhlouti and Mazhouda [202] to give an analogue of (4.1) for Dirichlet L-functions. This states for T sufficiently large and

X a positive real number,

$$\sum_{0<\gamma_\chi\le T} L'(\rho_\chi,\chi)X^{\rho_\chi} =$$
$$-\Delta(X)\chi[\Delta(X)X]\frac{T}{2\pi}\left(\log X\left(\frac{1}{2}\log\frac{qT}{2\pi}-\frac{1}{2}+\frac{\pi i}{4}\right)-\sum_{mr=X}\Lambda(r)\log m\right)$$
$$+\frac{X}{\sqrt{q}}\sum_{m\le\frac{qt}{2\pi X}} e^{2\pi im\frac{X}{q}}\overline{\chi}(m)(\log m)^2+\frac{1}{2\sqrt{q}}X\log X\sum_{m\le\frac{qt}{2\pi X}} e^{2\pi im\frac{X}{q}}\overline{\chi}(m)\log m$$
$$-\left(\frac{1}{2\sqrt{q}}X(\log X)^2-\frac{\pi i}{4\sqrt{q}}X\log X\right)\sum_{m\le\frac{qt}{2\pi X}} e^{2\pi im\frac{X}{q}}\overline{\chi}(m)$$
$$-\frac{X}{\sqrt{q}}\sum_{mr\le\frac{qt}{2\pi X}} e^{2\pi imr\frac{X}{q}}\Lambda(r)\overline{\chi}(r)\overline{\chi}(m)\log m+O\left(T^{1/2}(\log T)^3\right)$$

as $T\to\infty$ for a fixed positive number X and where χ is a primitive character mod q. Fixing $q=1$ gives (4.1) and setting $q=1$ and $X=1$ gives (2.3).

Other ideas have grown from (2.9). For example, Ford and Zaharescu [119] start (2.9) and investigate the distribution of the fractional parts of $\alpha\gamma$, where α is a fixed non-zero real number. This idea is then expanded upon by Ford, Soundararajan and Zaharescu in [118]. A further example of a result that begins with the Landau–Gonek Theorem can be found in [205], where Kaczorowski, Languasco, and Perelli consider a different weighted version of the Landau–Gonek Theorem.

4.2 COMBINING THE GENERALISED SHANKS' CONJECTURE WITH LANDAU'S THEOREM

We generalise Fujii's result to higher derivatives.

Theorem 4.1. *For X a fixed positive real number and T sufficiently large, we have*

$$\sum_{0<\gamma\le T}\zeta^{(n)}(\rho)X^\rho =$$
$$(-1)^n\left\{\Delta(X)\frac{T}{2\pi}\left((\log X)^n\left(\frac{1}{2}\log\frac{T}{2\pi}-\frac{1}{2}+\frac{\pi i}{4}\right)-\sum_{mr=X}\Lambda(r)(\log m)^n\right)\right.$$
$$+X(\log X)^n\left(\frac{1}{2}\log X-\frac{\pi i}{4}\right)\sum_{m\le\frac{T}{2\pi X}} e^{2\pi imX}+\frac{X}{2}(\log X)^n\sum_{m\le\frac{T}{2\pi X}} e^{2\pi imX}\log m$$
$$\left.-X\sum_{mr\le\frac{T}{2\pi X}} e^{2\pi imrX}\Lambda(r)(\log rX)^n\right\}+O\left(T^{1/2}(\log T)^{n+2}\right),$$

where $\Delta(X)$ is given in (4.2).

Remark. Setting $n = 1$ in the theorem recovers Fujii's result in (4.1).

When we restrict X to being a positive integer we obtain a special case of the above results. It is evident from the statement of the following corollary that we see the changing behaviour of our asymptotic expansions depending on whether $X > 0$ is any real number or when $X \geq 1$ is an integer.

Corollary 4.2. *If X is a positive integer and T is sufficiently large, we have*

$$\sum_{0<\gamma\leq T} \zeta^{(n)}(\rho)X^{\rho} =$$

$$(-1)^{n+1}\frac{T}{2\pi}(\log X)^n \Bigg\{ \sum_{k=0}^{n}\sum_{u=0}^{k+1}\binom{n}{k}\binom{k+1}{u}(-1)^u \frac{1}{k+1}\left(\log\frac{T}{2\pi}\right)^{k+1-u}(\log X)^{u-k}$$

$$+\sum_{k=0}^{n}\sum_{l=0}^{k}\sum_{u=0}^{k-l}\binom{n}{k}\binom{k}{l}\binom{k-l}{u}(-1)^l l!\left(-1+\sum_{j=0}^{l}\frac{1}{j!}\gamma_j\right)\left(\log\frac{T}{2\pi}\right)^{k-l-u}(\log X)^{u-k}$$

$$+\sum_{k=0}^{n}\binom{n}{k}(-1)^{k+1}k!A_k(\log X)^{-k} - \left(\log\frac{T}{2\pi} - 1 - \sum_{mr=X}\Lambda(r)(\log m)^n\right)\Bigg\} + E_n(T).$$

where $E_n(T)$ is given in Theorem 3.1. The γ_j are the coefficients in the Laurent expansion for $\zeta(s)$ about $s = 1$, and the A_j are the coefficients in the Laurent expansion for the logarithmic derivative of $\zeta(s)$ about $s = 1$, given in (3.3).

Remark. Setting $n = 1$ in the corollary recovers Fujii's result in (4.3). Setting $n = 1$ and $X = 1$ recovers Fujii's result in (2.3). Setting $X = 1$ recovers our result from [186], stated in Theorem 3.1.

4.2.1 Overview of the Proof

So far we have described the motivation for studying asymptotic expansions of the sums given in Section 4.1. We have stated the main results in Section 4.2 that we will prove in the following sections.

In Section 4.2.2 we will recall some basic facts about the Riemann zeta function $\zeta(s)$ and the Riemann xi function $\xi(s)$, which is a 'completed' version of the Riemann zeta function.

In Section 4.2.3 we will use the tools from Section 4.2.2 to prove Theorem 4.1. The integral we use to prove this theorem is given by

$$I = \frac{1}{2\pi i}\int_R \frac{\xi'}{\xi}(s)\zeta^{(n)}(s)X^s\, ds$$

where $\xi(s)$ is the Riemann xi function, $\zeta^{(n)}(s)$ denotes the n^{th} derivative of $\zeta(s)$ and R denotes the rectangular positively oriented contour with the vertices are $c + i, c + iT, 1 -$

$c+it, 1-c+i$ connected in this order and $c = 1 + \frac{1}{\log T}$. The non-trivial zeros of $\zeta(s)$ up to a height T are contained within R and so by Cauchy's Theorem the integral represents the summation

$$I = \sum_{0<\gamma\leq T} \zeta^{(n)}(\rho) X^{\rho}.$$

We split this section up into several subsections, each corresponding to different parts of the contour that we will be integrating over, to show that most of the contribution comes from the left-hand side of the contour, while the other sides mostly only contribute to the error term (apart from one term from the right-hand side).

Finally in Section 4.2.4 we will prove Corollary 4.2 which will highlight the differences between the general case proved in Section 4.2.3 for any positive number X and the case when X is a positive integer. As described above we will use a result from [186] to do most of the work here. This will again highlight the observation of Gonek's in [144] that the asymptotic formulae tend to change quite dramatically depending on the arithmetic nature of X.

4.2.2 Preliminary Lemmas

In this section we recall some basic information about $\zeta(s)$ and $\xi(s)$, as well as recalling some results from other papers that will be useful in our proof. Any facts that are not explicitly referenced in this section can be found in any good text about the Riemann zeta function, for example Titchmarsh [298].

We state a more general functional equation for $\zeta^{(n)}(s)$ that is proved using the functional equation (1.1) for $\zeta(s)$ and the Leibniz product rule.

Lemma 4.3. *The general functional equation for $\zeta^{(n)}(s)$ is given by the following formula*

$$\zeta^{(n)}(s) = \frac{1}{\chi(1-s)} \sum_{k=0}^{n} \binom{n}{k} (-1)^k \frac{\chi^{(n-k)}(s)}{\chi(s)} \zeta^{(k)}(1-s).$$

We will also need the following result that we proved in Lemma 3.7 in Section 3.1.3 for the integral along the top and the bottom of our contour.

Lemma 4.4. *For $c = 1 + \frac{1}{\log T}$, we have*

$$\int_{1-c}^{c} |\zeta^{(n)}(\sigma + iT)| \, d\sigma \ll T^{1/2} (\log T)^n.$$

For the Riemann xi function we write

$$\xi(s) = \frac{1}{2} s(s-1) \pi^{-s/2} \Gamma\left(\frac{s}{2}\right) \zeta(s)$$

so the functional equation for $\xi(s)$ is given by

$$\xi(s) = \xi(1-s).$$

We now observe that

$$\frac{\xi'}{\xi}(s) = \frac{2s-1}{s(s-1)} - \frac{1}{2}\log\pi + \frac{1}{2}\psi\left(\frac{s}{2}\right) + \frac{\zeta'}{\zeta}(s) \tag{4.4}$$

where we have written

$$\psi(s) = \frac{\Gamma'}{\Gamma}(s)$$

and for $|\arg s| < \pi - \delta$ with arbitrarily fixed positive δ and for $|s| \geq \frac{1}{2}$ we have

$$\psi(s) = \log s + O\left(\frac{1}{|s|}\right) = \log t + \frac{\pi i}{2} + O\left(\frac{1}{t}\right)$$

as $t \to \infty$.

Combining these two observations, we have the following lemma.

Lemma 4.5. *With the conditions written above, we have*

$$\frac{\xi'}{\xi}(s) = \frac{1}{2}\log\frac{t}{2\pi} + \frac{\pi i}{4} + \frac{\zeta'}{\zeta}(s) + O\left(\frac{1}{t}\right).$$

A key component to upcoming the proof is the method of stationary phase. Applications of this method to these types of problems can be found in Gonek [143, Sect.4, p.131], in Levinson [222] and in Jakhlouti and Mazhouda [202, Sect.2, p.13], amongst other places, including throughout this thesis. In an entirely analogous way to the proof that Gonek writes in [143], we are able to prove the following result.

Lemma 4.6. *Let X be a fixed positive real. Let $\{b_m\}_{m=1}^{\infty}$ be a sequence of complex numbers such that for any $\epsilon > 0, b_m \ll m^{\epsilon}$. Let $c > 1$ and let $k \geq 0$ be an integer. Then for T sufficiently large, we have*

$$\begin{aligned} &\frac{1}{2\pi}\int_1^T \chi(1-c-it)\left(\sum_{m=1}^{\infty} b_m m^{-c-it}\right)\left(\log\frac{t}{2\pi}\right)^k e^{-it\log X}\,dt \\ &\quad = X^c \sum_{1\leq m\leq \frac{T}{2\pi X}} b_m (\log mX)^k\, e^{-2\pi i m X} + O\left(T^{c-1/2}(\log T)^k\right). \end{aligned}$$

4.2.3 Proof of Theorem 4.1

Let X be a fixed positive real. We write $s = \sigma + it$ with $\sigma, t \in \mathbb{R}$ and $\rho = \beta + i\gamma$ for a non-trivial zero of the Riemann zeta function $\zeta(s)$. Suppose $T > T_0$ and T is not the imaginary part of the zeros of $\zeta(s)$ and further that $|T-\gamma| \gg \frac{1}{\log T}$ where γ is the imaginary part of any non-trivial zero ρ. This restriction on T is harmless within our remainder terms.

Set $c = 1 + \frac{1}{\log T}$ and consider the integral

$$I = \frac{1}{2\pi i}\int_R \frac{\xi'}{\xi}(s)\zeta^{(n)}(s)X^s \, ds \tag{4.5}$$

where $\xi(s)$ is the Riemann xi function, $\zeta^{(n)}(s)$ denotes the n^{th} derivative of $\zeta(s)$, and where R denotes the rectangular positively oriented contour with vertices given by $c+i, c+iT, 1-c+iT, 1-c+i$, connected in this order.

By Cauchy's Theorem,

$$I = \sum_{0<\gamma\leq T} \zeta^{(n)}(\rho)X^\rho. \tag{4.6}$$

We now need to evaluate I in another way to obtain our asymptotic expansion. We decompose the integral (4.5) along the sides of the contour as

$$\begin{aligned} I &= \frac{1}{2\pi i}\left(\int_{1-c+i}^{c+i} + \int_{c+i}^{c+iT} + \int_{c+iT}^{1-c+iT} + \int_{1-c+iT}^{1-c+i}\right)\frac{\xi'}{\xi}(s)\zeta^{(n)}(s)X^s \, ds \\ &= I_B + I_R + I_T + I_L. \end{aligned}$$

4.2.3.1 Bounding I_B and I_T

Notice that by our choice of T we may bound I_B and I_T trivially within our error. To do this, recall that for $-1 \leq \sigma \leq 2$ and since we are assuming $|T-\gamma| \gg \frac{1}{\log T}$, we have from [143, Sect.2, p.127] that

$$\frac{\xi'}{\xi}(s) \ll (\log T)^2.$$

Combining this with Lemma 4.4, since X is fixed we have

$$I_B + I_T \ll (\log T)^2 \int_{1-c}^{c} |\zeta^{(n)}(\sigma+it)X^{\sigma+it}| \, d\sigma \ll T^{1/2}(\log T)^{n+2}. \tag{4.7}$$

4.2.3.2 Evaluating I_R

Writing $s = c+it$ and using (4.4), we may write

$$\begin{aligned} I_R &= \frac{1}{2\pi}\int_1^T \frac{\xi'}{\xi}(c+it)\zeta^{(n)}(c+it)X^{c+it} \, dt \\ &= \frac{1}{2\pi}\int_1^T \left(\frac{2(c+it)-1}{(c+it)(c+it-1)} - \frac{1}{2}\log\pi + \psi\left(\frac{c+it}{2}\right) + \frac{\zeta'}{\zeta}(c+it)\right)\zeta^{(n)}(c+it)X^{c+it} \, dt. \end{aligned}$$

Using the Dirichlet series given in (3.7), and Lemma 4.5, we may rewrite this as

$$\begin{aligned}
I_R &= \frac{(-1)^n}{2\pi}\int_1^T \left(\frac{1}{2}\log\frac{t}{2\pi}+\frac{\pi i}{4}-\sum_{r=1}^{\infty}\frac{\Lambda(r)}{r^{c+it}}+O\left(\frac{1}{t}\right)\right)\sum_{m=1}^{\infty}\frac{(\log m)^n}{m^{c+it}}X^{c+it}\,dt\\
&= \frac{(-1)^n}{2\pi}X^c\sum_{m=1}^{\infty}\frac{(\log m)^n}{m^c}\int_1^T\left(\frac{1}{2}\log\frac{t}{2\pi}+\frac{\pi i}{4}+O\left(\frac{1}{t}\right)\right)\left(\frac{X}{m}\right)^{it}\,dt\\
&\quad+\frac{(-1)^{n+1}}{2\pi}X^c\sum_{m=1}^{\infty}\frac{(\log m)^n}{m^c}\sum_{r=1}^{\infty}\frac{\Lambda(r)}{r^c}\int_1^T\left(\frac{X}{mr}\right)^{it}\,dt\\
&= I_{R,1}+I_{R,2}.
\end{aligned}$$

Consider $I_{R,1}$ first. We have (with $\Delta(X)$ defined as in (4.2)),

$$\begin{aligned}
I_{R,1} &= \frac{(-1)^n}{2\pi}X^c\sum_{m=1}^{\infty}\frac{(\log m)^n}{m^c}\int_1^T\left(\frac{1}{2}\log\frac{t}{2\pi}+\frac{\pi i}{4}+O\left(\frac{1}{t}\right)\right)\left(\frac{X}{m}\right)^{it}\,dt\\
&= \frac{(-1)^n}{2\pi}\Delta(X)(\log X)^n\int_1^T\left(\frac{1}{2}\log\frac{t}{2\pi}+\frac{\pi i}{4}\right)\,dt\\
&\quad+\frac{(-1)^n}{2\pi}X^c\sum_{\substack{m=1\\ m\neq X}}^{\infty}\frac{(\log m)^n}{m^c}\int_1^T\left(\frac{1}{2}\log\frac{t}{2\pi}+\frac{\pi i}{4}\right)\left(\frac{X}{m}\right)^{it}\,dt\\
&\quad+O\left((\log T)^{n+2}\right)\\
&= I_{R,1,1}+I_{R,1,2}+O\left((\log T)^{n+2}\right).
\end{aligned}$$

Firstly,

$$I_{R,1,1}=(-1)^n\Delta(X)(\log X)^n\frac{T}{2\pi}\left(\frac{1}{2}\log\frac{T}{2\pi}-\frac{1}{2}+\frac{\pi i}{4}\right)+O(1).$$

Next, integrating by parts and summing we obtain

$$I_{R,1,2}\ll X^c\sum_{\substack{m=1\\ m\neq X}}^{\infty}\frac{(\log m)^n}{m^c}\frac{\log T}{\left|\log\frac{X}{m}\right|}\ll(\log T)^{n+2}.$$

If $0<X<1$ we can do slightly better than this error term. Recombining, we have

$$I_{R,1}=(-1)^n\Delta(X)(\log X)^n\frac{T}{2\pi}\left(\frac{1}{2}\log\frac{T}{2\pi}-\frac{1}{2}+\frac{\pi i}{4}\right)+O\left((\log T)^{n+2}\right). \tag{4.8}$$

Now consider $I_{R,2}$. We have

$$\begin{aligned}
I_{R,2} &= \frac{(-1)^{n+1}}{2\pi} X^c \sum_{m=1}^{\infty} \frac{(\log m)^n}{m^c} \sum_{r=1}^{\infty} \frac{\Lambda(r)}{r^c} \int_1^T \left(\frac{X}{mr}\right)^{it} dt \\
&= \frac{(-1)^{n+1}}{2\pi} X^c \sum_{k=1}^{\infty} \frac{1}{k^c} \sum_{k=mr} (\log m)^n \Lambda(r) \int_1^T \left(\frac{X}{k}\right)^{it} dt \\
&= \frac{(-1)^{n+1}}{2\pi} \Delta(X) \sum_{X=mr} (\log m)^n \Lambda(r) \int_1^T 1 \, dt \\
&\quad + \frac{(-1)^{n+1}}{2\pi} X^c \sum_{\substack{k=1 \\ k \neq X}}^{\infty} \frac{1}{k^c} \sum_{k=mr} (\log m)^n \Lambda(r) \int_1^T \left(\frac{X}{k}\right)^{it} dt \\
&= I_{R,2,1} + I_{R,2,2}.
\end{aligned}$$

Then

$$I_{R,2,1} = (-1)^{n+1} \Delta(X) \frac{T}{2\pi} \sum_{X=mr} (\log m)^n \Lambda(r) + O(1)$$

and as with the case for $I_{R,1,2}$ above, we have

$$I_{R,2,2} \ll X^c \sum_{\substack{k=1 \\ k \neq X}}^{\infty} \frac{1}{k^c} \sum_{k=mr} (\log m)^n \Lambda(r) \frac{1}{\log |X/k|} \ll (\log T)^{n+2}$$

where again the error can be improved slightly for $0 < X < 1$. Combining, we have

$$I_{R,2} = (-1)^{n+1} \Delta(X) \frac{T}{2\pi} \sum_{X=mr} (\log m)^n \Lambda(r) + O\left((\log T)^{n+2}\right). \tag{4.9}$$

Finally, we may combine (4.8) and (4.9) to obtain I_R, given by

$$\begin{aligned}
I_R = (-1)^n \Delta(X) \frac{T}{2\pi} &\left((\log X)^n \left\{ \frac{1}{2} \log \frac{T}{2\pi} - \frac{1}{2} + \frac{\pi i}{4} \right\} - \sum_{X=mr} (\log m)^n \, \Lambda(r) \right) \\
&+ O\left((\log T)^{n+2}\right).
\end{aligned} \tag{4.10}$$

4.2.3.3 Evaluating I_L

Finally we evaluate I_L, which is where most of the contribution to the asymptotic expansion comes from. Using Lemma 4.3 we have

$$\begin{aligned}
I_L &= -\frac{1}{2\pi i} \int_{1-c+i}^{1-c+iT} \frac{\xi'}{\xi}(s) \zeta^{(n)}(s) X^s \, ds \\
&= -\frac{1}{2\pi i} \int_{1-c+i}^{1-c+iT} \left(-\frac{\xi'}{\xi}(1-s)\right) \left(\frac{1}{\chi(1-s)} \sum_{k=0}^{n} \binom{n}{k} (-1)^k \frac{\chi^{(n-k)}(s)}{\chi(s)} \zeta^{(k)}(1-s) \right) X^s \, ds \\
&= -\frac{1}{2\pi} \int_1^T \left(-\frac{\xi'}{\xi}(c-it)\right) \\
&\qquad \times \left(\frac{1}{\chi(c-it)} \sum_{k=0}^{n} \binom{n}{k} (-1)^k \frac{\chi^{(n-k)}(1-c+it)}{\chi(1-c+it)} \zeta^{(k)}(c-it) \right) X^{1-c+it} \, dt.
\end{aligned}$$

By complex conjugation we obtain

$$\begin{aligned}
\overline{I_L} &= \frac{X^{1-c}}{2\pi}\int_1^T \frac{\xi'}{\xi}(c+it)\left(\frac{1}{\chi(c+it)}\sum_{k=0}^{n}\binom{n}{k}(-1)^k\frac{\chi^{(n-k)}(1-c-it)}{\chi(1-c-it)}\zeta^{(k)}(c+it)\right)X^{-it}\,dt\\
&= \frac{X^{1-c}}{2\pi}\int_1^T\left(\frac{1}{2}\log\frac{t}{2\pi}+\frac{\pi i}{4}-\sum_{r=1}^{\infty}\frac{\Lambda(r)}{r^{c+it}}+O\left(\frac{1}{t}\right)\right)\chi(1-c-it)\\
&\quad\times\left(\sum_{k=0}^{n}\binom{n}{k}(-1)^k\left((-1)^{n-k}\left(\log\frac{t}{2\pi}\right)^{n-k}+O\left(\frac{1}{t}\right)\right)(-1)^k\sum_{m=1}^{\infty}\frac{(\log m)^k}{m^{c+it}}\right)X^{-it}\,dt\\
&= \frac{X^{1-c}}{2\pi}\int_1^T\left(\frac{1}{2}\log\frac{t}{2\pi}+\frac{\pi i}{4}-\sum_{r=1}^{\infty}\frac{\Lambda(r)}{r^{c+it}}\right)\chi(1-c-it)\\
&\quad\times\left(\sum_{k=0}^{n}\binom{n}{k}(-1)^{n+k}\left(\log\frac{t}{2\pi}\right)^{n-k}\sum_{m=1}^{\infty}\frac{(\log m)^k}{m^{c+it}}\right)e^{-it\log X}\,dt+O\left(T^{1/2}(\log T)^{n+2}\right)
\end{aligned}$$

where the second line follows from Lemma 4.5.

We now split this integral and evaluate each part separately.

$$\begin{aligned}
\overline{I_L} &= \frac{X^{1-c}}{2\pi}\frac{1}{2}\int_1^T\chi(1-c-it)\sum_{k=0}^{n}\binom{n}{k}(-1)^{n+k}\left(\log\frac{t}{2\pi}\right)^{n-k+1}\sum_{m=1}^{\infty}\frac{(\log m)^k}{m^{c+it}}e^{-it\log X}\,dt\\
&+\frac{X^{1-c}}{2\pi}\frac{\pi i}{4}\int_1^T\chi(1-c-it)\sum_{k=0}^{n}\binom{n}{k}(-1)^{n+k}\left(\log\frac{t}{2\pi}\right)^{n-k}\sum_{m=1}^{\infty}\frac{(\log m)^k}{m^{c+it}}e^{-it\log X}\,dt\\
&+\frac{X^{1-c}}{2\pi}\int_1^T\chi(1-c-it)\sum_{r=1}^{\infty}\frac{\Lambda(r)}{r^{c+it}}\sum_{k=0}^{n}\binom{n}{k}(-1)^{n+k+1}\\
&\qquad\times\left(\log\frac{t}{2\pi}\right)^{n-k}\sum_{m=1}^{\infty}\frac{(\log m)^k}{m^{c+it}}e^{-it\log X}\,dt+O\left(T^{1/2}(\log T)^{n+2}\right)\\
&= J_1+J_2+J_3+O\left(T^{1/2}(\log T)^{n+2}\right).
\end{aligned}$$

Now apply Lemma 4.6 to each of the summations J_k, $k = 1, 2, 3$. For J_1, we have

$$\begin{aligned}
J_1 &= \frac{X^{1-c}}{2\pi}\frac{1}{2}\sum_{k=0}^{n}\binom{n}{k}(-1)^{n+k}\sum_{m=1}^{\infty}\frac{(\log m)^k}{m^c} \\
&\qquad\times\int_1^T \chi(1-c-it)\left(\log\frac{t}{2\pi}\right)^{n-k+1} e^{-it\log(mX)}\,dt \\
&= \frac{X}{2}\sum_{k=0}^{n}\binom{n}{k}(-1)^{n+k}\sum_{m\le\frac{T}{2\pi X}}(\log m)^k(\log mX)^{n-k+1}\,e^{-2\pi imX} + O\left(T^{1/2}(\log T)^{n+1}\right) \\
&= \frac{X}{2}\sum_{m\le\frac{T}{2\pi X}} e^{-2\pi imX}\left[\sum_{k=0}^{n}\binom{n}{k}(-1)^{n-k}(\log m)^k(\log mX)^{n-k}\right](\log(mX)) \\
&\quad + O\left(T^{1/2}(\log T)^{n+1}\right) \\
&= \frac{X}{2}\sum_{m\le\frac{T}{2\pi X}} e^{-2\pi imX}(\log mX)\left[-(\log mX)+\log m\right]^n + O\left(T^{1/2}(\log T)^{n+1}\right) \\
&= (-1)^n\frac{X}{2}\sum_{m\le\frac{T}{2\pi X}} e^{-2\pi imX}(\log mX)(\log X)^n + O\left(T^{1/2}(\log T)^{n+1}\right) \\
&= (-1)^n\frac{X}{2}(\log X)^{n+1}\sum_{m\le\frac{T}{2\pi X}} e^{-2\pi imX} \\
&\quad + (-1)^n\frac{X}{2}(\log X)^n\sum_{m\le\frac{T}{2\pi X}} e^{-2\pi imX}\log m + O\left(T^{1/2}(\log T)^{n+1}\right).
\end{aligned}$$

Similarly,

$$\begin{aligned}
J_2 &= \frac{X^{1-c}}{2\pi}\frac{\pi i}{4}\sum_{k=0}^{n}\binom{n}{k}(-1)^{n+k}\sum_{m=1}^{\infty}\frac{(\log m)^k}{m^c}\int_1^T \chi(1-c-it)\left(\log\frac{t}{2\pi}\right)^{n-k} e^{-it\log(mX)}\,dt \\
&= \frac{\pi i}{4}X\sum_{k=0}^{n}\binom{n}{k}(-1)^{n+k}\sum_{m\le\frac{T}{2\pi X}}(\log m)^k(\log mX)^{n-k}\,e^{-2\pi imX} + O\left(T^{1/2}(\log T)^n\right) \\
&= \frac{\pi i}{4}X\sum_{m\le\frac{T}{2\pi X}} e^{-2\pi imX}\left[\sum_{k=0}^{n}\binom{n}{k}(-1)^{n+k}(\log m)^k(\log mX)^{n-k}\right] + O\left(T^{1/2}(\log T)^n\right) \\
&= \frac{\pi i}{4}X\sum_{m\le\frac{T}{2\pi X}} e^{-2\pi imX}\left[\log m-(\log mX)\right]^n + O\left(T^{1/2}(\log T)^n\right) \\
&= (-1)^n\frac{\pi i}{4}X(\log X)^n\sum_{m\le\frac{T}{2\pi X}} e^{-2\pi imX} + O\left(T^{1/2}(\log T)^n\right).
\end{aligned}$$

Finally,

$$
\begin{aligned}
J_3 &= \frac{X^{1-c}}{2\pi} \sum_{k=0}^{n} \binom{n}{k} (-1)^{n+k+1} \sum_{r=1}^{\infty} \frac{\Lambda(r)}{r^c} \sum_{m=1}^{\infty} \frac{(\log m)^k}{m^c} \\
&\qquad \times \int_1^T \chi(1-c-it) \left(\log \frac{t}{2\pi} \right)^{n-k} e^{-it\log(mrX)} \, dt \\
&= X \sum_{k=0}^{n} \binom{n}{k} (-1)^{n+k+1} \sum_{mr \le \frac{T}{2\pi X}} \Lambda(r) (\log m)^k (\log mrX)^{n-k} \; e^{-2\pi i mrX} \\
&\quad + O\left(T^{1/2} (\log T)^n \right) \\
&= -X \sum_{mr \le \frac{T}{2\pi X}} e^{-2\pi i mrX} \Lambda(r) \left(\right) \sum_{k=0}^{n} \binom{n}{k} (-1)^{n+k} (\log m)^k (\log mrX)^{n-k} \Bigg] \\
&\quad + O\left(T^{1/2} (\log T)^n \right) \\
&= -X \sum_{mr \le \frac{T}{2\pi X}} e^{-2\pi i mrX} \Lambda(r) \left[-(\log mrX) + \log m \right]^n + O\left(T^{1/2} (\log T)^n \right) \\
&= (-1)^{n+1} X \sum_{mr \le \frac{T}{2\pi X}} e^{-2\pi i mrX} \Lambda(r) (\log rX)^n + O\left(T^{1/2} (\log T)^n \right).
\end{aligned}
$$

Recombining these, we have

$$
\begin{aligned}
\overline{I_L} = (-1)^n \Bigg\{ & X (\log X)^n \left(\frac{1}{2} \log X + \frac{\pi i}{4} \right) \sum_{m \le \frac{T}{2\pi X}} e^{-2\pi i mX} \\
& + \frac{1}{2} X (\log X)^n \sum_{m \le \frac{T}{2\pi X}} e^{-2\pi i mX} \log m - X \sum_{mr \le \frac{T}{2\pi X}} e^{-2\pi i mrX} \Lambda(r) (\log rX)^n \Bigg\} \\
& \qquad + O\left(T^{1/2} (\log T)^{n+2} \right).
\end{aligned}
$$

Taking complex conjugates,

$$
\begin{aligned}
I_L = (-1)^n \Bigg\{ & X (\log X)^n \left(\frac{1}{2} \log X - \frac{\pi i}{4} \right) \sum_{m \le \frac{T}{2\pi X}} e^{2\pi i mX} + \frac{X}{2} (\log X)^n \sum_{m \le \frac{T}{2\pi X}} e^{2\pi i mX} \log m \\
& - X \sum_{mr \le \frac{T}{2\pi X}} e^{2\pi i mrX} \Lambda(r) (\log rX)^n \Bigg\} + O\left(T^{1/2} (\log T)^{n+2} \right). \qquad (4.11)
\end{aligned}
$$

4.2.3.4 Finalising the Proof of Theorem 4.1

Combining (4.7), (4.10), and (4.11) gives I in the second way that we are looking for. Specifically, we have

$$\begin{aligned} I = (-1)^n \Bigg\{ &\Delta(X)\frac{T}{2\pi}\left((\log X)^n\left(\frac{1}{2}\log\frac{T}{2\pi} - \frac{1}{2} + \frac{\pi i}{4}\right) - \sum_{mr=X}\Lambda(r)(\log m)^n\right) \\ &+ X(\log X)^n\left(\frac{1}{2}\log X - \frac{\pi i}{4}\right)\sum_{m\le\frac{T}{2\pi X}} e^{2\pi imX} \\ &+ \frac{X}{2}(\log X)^n \sum_{m\le\frac{T}{2\pi X}} e^{2\pi imX}\log m - X\sum_{mr\le\frac{T}{2\pi X}} e^{2\pi imrX}\Lambda(r)(\log rX)^n\Bigg\} \\ &+ O\left(T^{1/2}(\log T)^{n+2}\right), \end{aligned}$$

Combining this asymptotic expansion with our observation that $I = \sum_{0<\gamma\le T}\zeta^{(n)}(\rho)X^\rho$ in (4.6) completes the proof of Theorem 4.1.

4.2.4 Proof of Corollary 4.2

We rewrite Theorem 4.1 in a slightly different way as follows.

Corollary 4.7. *For X a fixed positive real number, we have*

$$\begin{aligned} &\sum_{0<\gamma\le T}\zeta^{(n)}(\rho)X^\rho = \\ &\quad(-1)^n\Bigg\{\Delta(X)\frac{T}{2\pi}\left((\log X)^n\left(\frac{1}{2}\log\frac{T}{2\pi} - \frac{1}{2} + \frac{\pi i}{4}\right) - \sum_{mr=X}\Lambda(r)(\log m)^n\right) \\ &\quad+ X(\log X)^n\left(\frac{1}{2}\log X - \frac{\pi i}{4}\right)\sum_{m\le\frac{T}{2\pi X}} e^{2\pi imX} + \frac{X}{2}(\log X)^n\sum_{m\le\frac{T}{2\pi X}} e^{2\pi imX}\log m \\ &\quad- X\sum_{k=0}^{n}\binom{n}{k}(\log X)^{n-k}\sum_{mr\le\frac{T}{2\pi X}} e^{2\pi imrX}\Lambda(r)(\log r)^k\Bigg\} + O\left(T^{1/2}(\log T)^{n+2}\right), \end{aligned}$$

where $\Delta(X)$ is given in Theorem 4.1.

Proof. This follows from Theorem 4.1 by using the binomial expansion on $(\log rX)^n$ in the last summation in the braces in Theorem 4.1. □

Remark. The advantage to rewriting Theorem 4.1 in the form of Corollary 4.7 is that none of the summations involving exponentials have any reliance on powers of $\log X$.

When $X \ge 1$ and $X \in \mathbb{Z}$, notice that

$$\sum_{m\le\frac{T}{2\pi X}} e^{2\pi imX} = \frac{T}{2\pi X} + O(1),$$

$$\sum_{m\le\frac{T}{2\pi X}} e^{2\pi imX}\log m = \frac{T}{2\pi X}\log\frac{T}{2\pi X} - \frac{T}{2\pi X} + O(\log T),$$

$$\sum_{mr\le\frac{T}{2\pi X}} e^{2\pi imrX}\Lambda(r)(\log r)^k = \sum_{mr\le\frac{T}{2\pi X}} \Lambda(r)(\log r)^k.$$

Define

$$S = (-1)^{k+1}\sum_{mr\le\frac{T}{2\pi X}} \Lambda(r)(\log r)^k \tag{4.12}$$

Then in an entirely analogous way to that done in Chapter 3 and in Hughes and Pearce-Crump [186], we have

$$\begin{aligned} S = {} & (-1)^{k+1}\frac{1}{k+1}\frac{T}{2\pi X}\left(\log\frac{T}{2\pi X}\right)^{k+1} \\ & + (-1)^{k+1}\sum_{l=0}^{k}\binom{k}{l}(-1)^l l!\left(-1+\sum_{j=0}^{l}\frac{1}{j!}\gamma_j\right)\frac{T}{2\pi X}\left(\log\frac{T}{2\pi X}\right)^{k-l} \\ & + k!A_k\frac{T}{2\pi X} + E_k(T) \end{aligned}$$

where

$$E_k(T) = \begin{cases} O\left(Te^{-C\sqrt{\log T}}\right) & \text{unconditionally} \\ O\left(T(\log T)^{k+9/4}\right) & \text{under the Riemann Hypothesis} \end{cases}$$

and $C > 0$ is a constant. Multiplying S by $(-1)^{k+1}$ gives the summation that we were originally looking for.

Substituting these expressions into the asymptotic expansion from Corollary 4.7 gives

$$\begin{aligned} \sum_{0<\gamma\le T}\zeta^{(n)}(\rho)X^\rho = (-1)^n\Bigg\{ & \frac{T}{2\pi}\left((\log X)^n\left(\frac{1}{2}\log\frac{T}{2\pi} - \frac{1}{2} + \frac{\pi i}{4}\right) - \sum_{mr=X}\Lambda(r)(\log m)^n\right) \\ & + (\log X)^n\left(\frac{1}{2}\log X - \frac{\pi i}{4}\right)\frac{T}{2\pi} + \frac{1}{2}(\log X)^n\left(\frac{T}{2\pi}\log\frac{T}{2\pi X} - \frac{T}{2\pi}\right) \\ & - \sum_{k=0}^{n}\binom{n}{k}(\log X)^{n-k}\Bigg(\frac{1}{k+1}\frac{T}{2\pi}\left(\log\frac{T}{2\pi X}\right)^{k+1} \\ & + \sum_{l=0}^{k}\binom{k}{l}(-1)^l l!\left(-1+\sum_{j=0}^{l}\frac{1}{j!}\gamma_j\right)\frac{T}{2\pi}\left(\log\frac{T}{2\pi X}\right)^{k-l} \\ & + (-1)^{k+1}k!A_k\frac{T}{2\pi}\Bigg)\Bigg\} + E_n(T), \end{aligned}$$

where the γ_j and A_k are defined in the statement of Corollary 4.2 and $E_n(T)$ is defined in Theorem 3.1.

We want to simplify this so that the $\log \frac{T}{2\pi X}$ terms can be written separately in terms of $\log \frac{T}{2\pi}$ and $\log X$. To do this, we begin by writing this previous expansion in a slightly different form and do some simplifying.

$$\begin{aligned}\sum_{0<\gamma\le T} \zeta^{(n)}(\rho)X^{\rho} = (-1)^n \frac{T}{2\pi}(\log X)^n \left(\log \frac{T}{2\pi} - 1 - \sum_{mr=X} \Lambda(r)(\log m)^n\right) \\ + (-1)^{n+1} \sum_{k=0}^{n} \binom{n}{k} (\log X)^{n-k} \Bigg\{ \frac{1}{k+1}\frac{T}{2\pi}\left(\log \frac{T}{2\pi} - \log X\right)^{k+1} \\ + \sum_{l=0}^{k} \binom{k}{l} (-1)^l l! \left(-1 + \sum_{j=0}^{l} \frac{1}{j!}\gamma_j\right) \frac{T}{2\pi}\left(\log\frac{T}{2\pi} - \log X\right)^{k-l} \\ + (-1)^{k+1} k! A_k \frac{T}{2\pi}\Bigg\} + E_n(T).\end{aligned}$$

Applying the binomial theorem, we have

$$\begin{aligned}\sum_{0<\gamma\le T} \zeta^{(n)}(\rho)X^{\rho} = (-1)^n \frac{T}{2\pi}(\log X)^n \left(\log \frac{T}{2\pi} - 1 - \sum_{mr=X} \Lambda(r)(\log m)^n\right) \\ + (-1)^{n+1}\frac{T}{2\pi}\Bigg\{ \sum_{k=0}^{n}\sum_{u=0}^{k+1} \binom{n}{k}\binom{k+1}{u}(-1)^u \frac{1}{k+1}\left(\log\frac{T}{2\pi}\right)^{k+1-u} (\log X)^{n-k+u} \\ + \sum_{k=0}^{n}\sum_{l=0}^{k}\sum_{u=0}^{k-l} \binom{n}{k}\binom{k}{l}\binom{k-l}{u}(-1)^l l! \\ \times \left(-1 + \sum_{j=0}^{l}\frac{1}{j!}\gamma_j\right)\left(\log\frac{T}{2\pi}\right)^{k-l-u} (\log X)^{n-k+u} \\ + \sum_{k=0}^{n}\binom{n}{k}(-1)^{k+1}k! A_k (\log X)^{n-k}\Bigg\} + E_n(T).\end{aligned}$$

Finally, we may rearrange slightly to complete the proof of Corollary 4.2 to give

$$\begin{aligned}\sum_{0<\gamma\le T} \zeta^{(n)}(\rho)X^{\rho} = (-1)^{n+1}\frac{T}{2\pi}(\log X)^n \\ \Bigg\{ \sum_{k=0}^{n}\sum_{u=0}^{k+1} \binom{n}{k}\binom{k+1}{u}(-1)^u \frac{1}{k+1}\left(\log\frac{T}{2\pi}\right)^{k+1-u} (\log X)^{u-k} \\ + \sum_{k=0}^{n}\sum_{l=0}^{k}\sum_{u=0}^{k-l} \binom{n}{k}\binom{k}{l}\binom{k-l}{u}(-1)^l l! \left(-1 + \sum_{j=0}^{l}\frac{1}{j!}\gamma_j\right)\left(\log\frac{T}{2\pi}\right)^{k-l-u} (\log X)^{u-k} \\ + \sum_{k=0}^{n}\binom{n}{k}(-1)^{k+1}k! A_k \log^{-k} X - \left(\log\frac{T}{2\pi} - 1 - \sum_{mr=X}\Lambda(r)(\log m)^n\right)\Bigg\} + E_n(T).\end{aligned}$$

— 5 —

Higher Moments of the Derivatives of the Riemann Zeta Function via RMT and the Hybrid Model

In this chapter we assume the Riemann Hypothesis, unless otherwise stated. Note that in this chapter we have divided through by $N(T)$, while in most of the rest of the thesis we do not make this normalisation. This is because in this chapter we develop the heuristic RMT connection to model higher moments of zeta, and that model works at the level of averages.

We will develop the philosophy of Keating and Snaith [211] and Hughes, Keating and O'Connell [182] from RMT to study the discrete moments of the n^{th} derivative of $\zeta(s)$, denoted $\zeta^{(n)}(s)$. That is, we study

$$\frac{1}{N(T)} \sum_{0<\gamma\leq T} \zeta^{(n)}\left(\frac{1}{2}+i\gamma\right)^k, \tag{5.1}$$

where $N(T)$ is given in (1.4). In fact, we will study the more general problem of moments of mixed derivatives,

$$\frac{1}{N(T)} \sum_{0<\gamma\leq T} \zeta^{(n_1)}\left(\frac{1}{2}+i\gamma\right) \dots \zeta^{(n_k)}\left(\frac{1}{2}+i\gamma\right).$$

Clearly if $n_1 = \cdots = n_k = n$, then we recover (5.1).

Recall that the model proposed by Keating and Snaith [211] is that the characteristic polynomial of a large random unitary matrix can be used to model the value distribution of the Riemann zeta function near a large height T. They used the characteristic polynomial

$$Z_N(\theta) = \det(I - Ue^{-i\theta}) = \prod_{m=1}^{N} (1 - e^{i(\theta_m - \theta)}), \tag{5.2}$$

where the θ_m are the eigenangles of an $N \times N$ random unitary matrix U, to model $\zeta(s)$. The motivation for studying this is that it has been conjectured that the limiting distribution of the non-trivial zeros of $\zeta(s)$, on the scale of their mean spacing, is asymptotically the same as that of the eigenangles θ_m of matrices chosen according to Haar measure, in the limit as $N \to \infty$, as previously discussed in Section 1.3.3. Recall that equating the mean densities yields the connection between matrix size and height up the critical line

$$N = \log \frac{T}{2\pi}.$$

Averaging over all Haar-distributed $N \times N$ unitary matrices, Keating and Snaith [211] calculated the moments of $|Z(\theta)|$, leading them to form Conjecture 1.9. Hughes, Keating and O'Connell [182] followed a similar approach and calculated the discrete moments of $|Z'(\theta)|$ and formed Conjecture 1.19.

In both of these conjectures, the arithmetic factor was inserted artificially after studying the analogous problem in RMT. The hybrid model was formed to fix this problem, treating the zeros and primes part of the Riemann zeta function equally, recreating Conjectures 1.9 and 1.19, as previously discussed in Section 1.3.4.

Both of the problems discussed considered moments of a real function, where an absolute value of the characteristic polynomial (and so zeta) was taken. For our problem (5.1) and its generalisation, we consider the moments of the complex function. In this chapter we attack our problem in two ways. First, by direct calculation of the characteristic polynomial, and then by modelling zeta using the hybrid approach. We also consider some problems relating to negative moments, and to a 'hidden' recurrence relation in our characteristic polynomial approach. The problem of considering lower order terms is taken up in Chapter 6.

Other than the work presented in Section 5.4 and in Section 5.5, the work presented in this chapter has already appeared in print in [187]. Notation and cross-references have been updated for this thesis.

5.1 STATEMENT OF RESULTS

In Section 5.2 we will calculate

$$\mathbb{E}_N \left[\frac{1}{N} \sum_{m=1}^{N} Z_N(\theta_m + \alpha_1) \dots Z_N(\theta_m + \alpha_k) \right]$$

where recall from Section 1.2.1 that $\mathbb{E}_N$ denotes expectation with respect to Haar measure. By Taylor expanding each characteristic polynomial about their respective shift, we will be able to prove the following theorem.

Theorem 5.1. *For fixed positive integers $n_1, \ldots, n_k$, we have*

$$\mathbb{E}_N\left[\frac{1}{N}\sum_{m=1}^{N} Z_N^{(n_1)}(\theta_m)\ldots Z_N^{(n_k)}(\theta_m)\right] \sim (-1)^{n_1+\ldots+n_k+k}\ i^{n_1+\ldots+n_k}\frac{n_1!\ldots n_k!}{(n_1+\ldots+n_k+1)!}N^{n_1+\ldots+n_k},$$

as $N\to\infty$.

Setting $n_1=\cdots=n_k=n$ gives the following Corollary.

Corollary 5.2. *For fixed positive integers n, k, we have*

$$\mathbb{E}_N\left[\frac{1}{N}\sum_{m=1}^{N} Z_N^{(n)}(\theta_m)^k\right] \sim (-1)^{k(n+1)}\ i^{kn}\frac{(n!)^k}{(kn+1)!}N^{kn}$$

as $N\to\infty$.

In order to use this to create a conjecture for zeta, we need to know what the arithmetic term equals. To do that, we take the hybrid approach, discussed in Section 5.3. In Section 5.3.1 (Theorems 5.8 and 5.9) we calculate the discrete moments of $P_X^{(n_1)}\ldots P_X^{(n_k)}$ and show that they asymptotically vanish unless all the n_j are 0 (that is, no derivatives are taken), in which case the mean is 1. Furthermore, we predict that the discrete moments of Z_X are accurately modelled by the characteristic polynomial, and we will verify this in the case of the first derivative in Theorem 5.12 in Section 5.3.2. That is, we conjecture that there is no arithmetic term at the leading order for these moments of the complex Riemann zeta function.

Note that the derivative of $Z_N(\theta)$ is with respect to θ, and this acts like the derivative of $\zeta(1/2+it)$ with respect to t. This is obviously equal to $i\zeta'(1/2+it)$, and so we expect there to be no factors of i for the Riemann zeta function. To be precise, we make the following prediction.

Conjecture 5.3. *For fixed positive integers $n_1, \ldots, n_k$, the moments of mixed derivatives of $\zeta(s)$, evaluated at the non-trivial zeros of $\zeta(s)$, are given by*

$$\frac{1}{N(T)}\sum_{0<\gamma\le T}\zeta^{(n_1)}\left(\frac{1}{2}+i\gamma\right)\ldots\zeta^{(n_k)}\left(\frac{1}{2}+i\gamma\right) \sim (-1)^{n_1+\ldots+n_k+k}\frac{n_1!\ldots n_k!}{(n_1+\ldots+n_k+1)!}\left(\log\frac{T}{2\pi}\right)^{n_1+\ldots+n_k}$$

as $T\to\infty$.

Setting $n_1=\cdots=n_k=n$ gives the following conjecture.

Conjecture 5.4. *For fixed positive integers n, k, the k^{th} moment of the n^{th} derivative of $\zeta(s)$ is given by*

$$\frac{1}{N(T)}\sum_{0<\gamma\leq T}\zeta^{(n)}\left(\frac{1}{2}+i\gamma\right)^k \sim (-1)^{k(n+1)}\frac{(n!)^k}{(kn+1)!}\left(\log\frac{T}{2\pi}\right)^{kn}$$

as $T\to\infty$.

Very little is rigorously known about these types of results. For $k=0$ the result is trivial, as the sum is just $N(T)$, defined in equation (1.5). For $k=1$, they have been previously studied in relation to Shanks' Conjecture, a full history of which can be found in Chapter 2, and in [184], and the theoretical results as given in Chapter 3 agree with Conjecture 5.4 in this case.

These results are for leading order only. In Chapter 6 and in a forthcoming paper [185], we use a different method to conjecture the full asymptotic for zeta.

These results and conjectures are stated for k a positive integer. However, in the case of the first derivative, when $n=1$, Section 5.3.2 applies for $k\in\mathbb{C}$ with $\Re(k)>-3$, and some of our results in Section 5.3.1 (namely Theorem 5.9) also apply for non-integer k. Therefore it is plausible that in the case of the first derivative, Conjecture 5.4 also holds for complex k.

Conjecture 5.5. *For $\Re(k)>-3$ as $T\to\infty$*

$$\frac{1}{N(T)}\sum_{0<\gamma\leq T}\zeta'\left(\frac{1}{2}+i\gamma\right)^k \sim \frac{1}{\Gamma(k+2)}\left(\log\frac{T}{2\pi}\right)^{k}.$$

In the case $k=-1$, this result is already known under the additional assumption of simple zeros (but without the Riemann Hypothesis), and can be found as equation (3.9) in a paper of Garaev and Sankaranarayanan, [134], and in (2.14).

When $k=-2$, the right hand side of Conjecture 5.5 vanishes. A separate calculation that will be shown explicitly in Section 5.4 shows that

$$\mathbb{E}_N\left[\frac{1}{N}\sum_{m=1}^{N}Z_N'(\theta_m)^{-2}\right]=0$$

exactly. For the case of zeta, what we mean is the left hand side is bounded by some error terms with no leading-order asymptotic. An educated guess suggests the error terms will be $O(T^{-1/2+\varepsilon})$. We discuss this further in Section 5.4.

5.2 THE CHARACTERISTIC POLYNOMIAL APPROACH

In this section we prove Theorem 5.1 concerning moments of characteristic polynomials. We start with the product representation of the characteristic polynomial of an $N\times N$

random unitary matrix $Z_N(\theta)$ in (5.2), given by

$$Z_N(\theta) = \prod_{m=1}^{N} (1 - e^{i(\theta_m - \theta)}).$$

The Haar probability density of $U(N)$ equals [311]

$$d\,\text{Haar} = \frac{1}{N!(2\pi)^N} \prod_{1 \le j < \ell \le N} |e^{i\theta_j} - e^{i\theta_\ell}|^2 \; d\theta_1 \ldots d\theta_N. \tag{5.3}$$

To extract the moments that we wish to calculate, we use shifts and calculate

$$\mathbb{E}_N \left[\frac{1}{N} \sum_{m=1}^{N} Z_N(\theta_m + \alpha_1) \ldots Z_N(\theta_m + \alpha_k) \right].$$

By invariance of Haar measure there are no distinguished eigenvalues, so this expectation equals

$$\mathbb{E}_N \left[Z_N(\theta_N + \alpha_1) \ldots Z_N(\theta_N + \alpha_k) \right].$$

Since we can Taylor expand assuming the α_j are very small, we obtain

$$\mathbb{E}_N \Bigg[\left(Z_N'(\theta_N) \frac{\alpha_1}{1!} + Z_N''(\theta_N) \frac{\alpha_1^2}{2!} + \ldots + Z_N^{(n_1)}(\theta_N) \frac{\alpha_1^{n_1}}{n_1!} + \ldots \right) \\ \times \ldots \times \left(Z_N'(\theta_N) \frac{\alpha_k}{1!} + Z_N''(\theta_N) \frac{\alpha_k^2}{2!} + \ldots + Z_N^{(n_k)}(\theta_N) \frac{\alpha_k^{n_k}}{n_k!} + \ldots \right) \Bigg],$$

where obviously $Z_N(\theta_N) = 0$. By calculating the $\alpha_1^{n_1} \ldots \alpha_k^{n_k}$-th coefficient, we can find moments of the mixed derivatives of the characteristic polynomial.

Writing out the expectation in terms of the Weyl density (5.3), we have

$$\mathbb{E}_N \left[\prod_{r=1}^{k} Z_N(\theta_N + \alpha_r) \right] = \\ \frac{1}{N!(2\pi)^N} \int \cdots \int_0^{2\pi} \prod_{1 \le j < \ell \le N} |e^{i\theta_j} - e^{i\theta_\ell}|^2 \prod_{m=1}^{N} \prod_{r=1}^{k} (1 - e^{i\theta_m} e^{-i\theta_N} e^{-i\alpha_r}) \; d\theta_m.$$

We split off the terms in the first product with $\ell = N$, and all the terms in the second product with $m = N$ (which can then be pulled out of the integral) to give

$$\frac{1}{N!(2\pi)^N} \prod_{r=1}^{k} (1 - e^{-i\alpha_r}) \int \cdots \int_0^{2\pi} \prod_{1 \le j < \ell \le N-1} |e^{i\theta_j} - e^{i\theta_\ell}|^2 \\ \times \prod_{m=1}^{N-1} \left| e^{i\theta_m} - e^{i\theta_N} \right|^2 \prod_{r=1}^{k} (1 - e^{i\theta_m} e^{-i\theta_N} e^{-i\alpha_r}) \; d\theta_m.$$

We may make a change of variables $\phi_m = \theta_m - \theta_N$ for $m = 1, \ldots, N-1$ and trivially perform the θ_N integral to obtain

$$\frac{1}{N!(2\pi)^{N-1}} \prod_{r=1}^{k} (1 - e^{-i\alpha_r}) \int \cdots \int_0^{2\pi} \prod_{1 \le j < \ell \le N-1} \left| e^{i\phi_j} - e^{i\phi_\ell} \right|^2 \\ \times \prod_{m=1}^{N-1} (1 - e^{i\phi_m})(1 - e^{-i\phi_m}) \prod_{r=1}^{k} (1 - e^{i\phi_m} e^{-i\alpha_r}) \, d\phi_m .$$

Notice then that we can rewrite the integrals back in terms of Haar measure for $(N-1) \times (N-1)$ unitary matrices, obtaining

$$\begin{aligned} &\frac{1}{N} \prod_{r=1}^{k} (1 - e^{-i\alpha_r}) \times \mathbb{E}_{N-1} \left[\prod_{m=1}^{N-1} (1 - e^{i\phi_m})(1 - e^{-i\phi_m}) \prod_{r=1}^{k} (1 - e^{i\phi_m} e^{-i\alpha_r}) \right] \\ &\quad = \frac{(-1)^{(k+1)(N-1)}}{N} \prod_{r=1}^{k} A_r^{-N} (A_r - 1) \times \mathbb{E}_{N-1} \left[\prod_{m=1}^{N-1} e^{-i\phi_m} (e^{i\phi_m} - 1)^2 \prod_{r=1}^{k} (e^{i\phi_m} - A_r) \right] \end{aligned} \tag{5.4}$$

where we have done some simple algebraic manipulations to put it into a suitable form for later, and written $A_r = e^{i\alpha_r}$. We may then use Heine's Lemma [295] to write the expectation as a Toeplitz determinant, and thus we have

$$\mathbb{E}_{N-1} \left[\prod_{m=1}^{N-1} e^{-i\phi_m} (e^{i\phi_m} - 1)^2 \prod_{r=1}^{k} (e^{i\phi_m} - A_r) \right] = D_{N-1}[f]$$

where

$$D_{N-1}[f] := \det \left| \hat{f}_{j-\ell} \right|_{1 \le j, \ell \le N-1}$$

with

$$\hat{f}_{j-\ell} = \frac{1}{2\pi} \int_0^{2\pi} f(\vartheta) e^{-i(j-\ell)\vartheta} \, d\vartheta$$

for the symbol

$$f(z) = z^{-1} (z-1)^2 \prod_{r=1}^{k} (z - A_r) . \tag{5.5}$$

As a historical aside, though the identity was first written down in 1939 by Szegő [295], he gave the credit to Heine (who lived from 1821 to 1881).

Putting this together, we have

$$\mathbb{E}_N \left[\prod_{r=1}^{k} Z_N(\theta_N + \alpha_r) \right] = \frac{(-1)^{(k+1)(N-1)}}{N} \prod_{r=1}^{k} A_r^{-N} (A_r - 1) \times D_{N-1}[f]. \tag{5.6}$$

Basor and Forrester [21] evaluate $D_{N-1}[f]$ with symbols of the form (5.5) as a $(k+2)\times(k+2)$ determinant,

$$D_{N-1}[f] = \frac{(-1)^{(k+1)(N-1)}\prod_{r=1}^{k+2}(-A_r)}{\prod_{1\le j<\ell\le k+2}(A_\ell - A_j)} \times \det \begin{bmatrix} A_1^{N-1} & A_1^{N} & A_1^{N+1} & \dots & A_1^{N-1+k} & (-A_1)^{-1} \\ A_2^{N-1} & A_2^{N} & A_2^{N+1} & \dots & A_2^{N-1+k} & (-A_2)^{-1} \\ A_3^{N-1} & A_3^{N} & A_3^{N+1} & \dots & A_3^{N-1+k} & (-A_3)^{-1} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ A_k^{N-1} & A_k^{N} & A_k^{N+1} & \dots & A_k^{N-1+k} & (-A_k)^{-1} \\ A_{k+1}^{N-1} & A_{k+1}^{N} & A_{k+1}^{N+1} & \dots & A_{k+1}^{N-1+k} & (-A_{k+1})^{-1} \\ A_{k+2}^{N-1} & A_{k+2}^{N} & A_{k+2}^{N+1} & \dots & A_{k+2}^{N-1+k} & (-A_{k+2})^{-1} \end{bmatrix},$$

where we write A_{k+1} and A_{k+2} for now, but will let them both tend to 1 later.

We can manipulate this determinant through elementary row operations. We begin by factoring A_r^{N-1} from each row, and factor the -1 from the last column. This determinant becomes

$$D_{N-1}[f] = \frac{(-1)^{N(k+1)}\prod_{r=1}^{k+2}A_r^{N}}{\prod_{1\le j<\ell\le k+2}(A_\ell - A_j)} \det \begin{bmatrix} 1 & A_1 & A_1^2 & \dots & A_1^k & A_1^{-N} \\ 1 & A_2 & A_2^2 & \dots & A_2^k & A_2^{-N} \\ 1 & A_3 & A_3^2 & \dots & A_3^k & A_3^{-N} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & A_k & A_k^2 & \dots & A_k^{N-1+k} & A_k^{-N} \\ 1 & A_{k+1} & A_{k+1}^2 & \dots & A_{k+1}^k & A_{k+1}^{-N} \\ 1 & A_{k+2} & A_{k+2}^2 & \dots & A_{k+2}^k & A_{k+2}^{-N} \end{bmatrix}.$$

Subtract the first row from each other row, and bring the factor of $1/(A_r - A_1)$ inside the determinant for each row $r = 2, \dots k+2$ to show that $D_{N-1}[f]$ equals

$$\frac{(-1)^{N(k+1)}\prod_{r=1}^{k+2}A_r^N}{\prod_{2\le j<\ell\le k+2}(A_\ell - A_j)}\det\begin{bmatrix} 1 & A_1 & A_1^2 & \dots & A_1^k & A_1^{-N} \\ 0 & 1 & A_1+A_2 & \dots & \sum_{j_1=0}^{k-1} A_1^{j_1}A_2^{k-1-j_1} & C_{2,2} \\ 0 & 1 & A_1+A_3 & \dots & \sum_{j_1=0}^{k-1} A_1^{j_1}A_3^{k-1-j_1} & C_{3,2} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 1 & A_1+A_k & \dots & \sum_{j_1=0}^{k-1} A_1^{j_1}A_k^{k-1-j_1} & C_{k,2} \\ 0 & 1 & A_1+A_{k+1} & \dots & \sum_{j_1=0}^{k-1} A_1^{j_1}A_{k+1}^{k-1-j_1} & C_{k+1,2} \\ 0 & 1 & A_1+A_{k+2} & \dots & \sum_{j_1=0}^{k-1} A_1^{j_1}A_{k+2}^{k-1-j_1} & C_{k+2,2} \end{bmatrix}$$

where in the r^{th} row and m^{th} column we make use of the following identity

$$\frac{A_r^{m-1} - A_1^{m-1}}{A_r - A_1} = \sum_{j_1=0}^{m-2} A_1^{j_1}A_r^{m-2-j_1} \tag{5.7}$$

for m from 2 to $k+1$, and for the $(k+2)^{\text{nd}}$ column we use the identity

$$C_{r,2} := \frac{A_r^{-N} - A_1^{-N}}{A_r - A_1} = -\sum_{j_1=1}^{N} A_1^{-j_1}A_r^{-(N+1-j_1)}. \tag{5.8}$$

Now subtract the second row from each other row below it and bring the factor of $1/(A_r - A_2)$ inside the determinant for each row $r = 3, \dots k+2$ to give $D_{N-1}[f]$ as

$$\frac{(-1)^{N(k+1)}\prod_{r=1}^{k+2}A_r^N}{\prod_{3\le j<\ell\le k+2}(A_\ell - A_j)}\det\begin{bmatrix} 1 & A_1 & \dots & A_1^k & A_1^{-N} \\ 0 & 1 & \dots & \sum_{j_1=0}^{k-1} A_1^{j_1}A_2^{k-1-j_1} & C_{2,2} \\ 0 & 1 & \dots & \sum_{j_1=0}^{k-2}\sum_{j_2=0}^{k-2-j_1} A_1^{j_1}A_2^{j_2}A_3^{k-2-j_1-j_2} & C_{3,3} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 1 & \dots & \sum_{j_1=0}^{k-2}\sum_{j_2=0}^{k-2-j_1} A_1^{j_1}A_2^{j_2}A_k^{k-2-j_1-j_2} & C_{k,3} \\ 0 & 1 & \dots & \sum_{j_1=0}^{k-2}\sum_{j_2=0}^{k-2-j_1} A_1^{j_1}A_2^{j_2}A_{k+1}^{k-2-j_1-j_2} & C_{k+1,3} \\ 0 & 1 & \dots & \sum_{j_1=0}^{k-2}\sum_{j_2=0}^{k-2-j_1} A_1^{j_1}A_2^{j_2}A_{k+2}^{k-2-j_1-j_2} & C_{k+2,3} \end{bmatrix}$$

where we have used (5.7) for the r^{th} row and m^{th} column for $m = 3, ..., k+1$ and where the last column uses the identity (5.8) with A_2 instead of A_1 with

$$\begin{aligned} C_{r,3} &= -\sum_{j_1=1}^{N} A_1^{-j_1} \left(\frac{A_r^{-(N+1-j_1)} - A_2^{-(N+1-j_1)}}{A_r - A_2} \right) \\ &= (-1)^2 \sum_{j_1=1}^{N} \sum_{j_2=1}^{N+1-j_1} A_1^{-j_1} A_2^{-j_2} A_r^{-(N+2-j_1-j_2)}. \end{aligned}$$

Continuing in this manner, it is clear that $D_{N-1}[f]$ becomes

$$D_{N-1}[f] = (-1)^{N(k+1)} \prod_{r=1}^{k+2} A_r^N$$
$$\times \det \begin{bmatrix} 1 & A_1 & A_1^2 & \dots & A_1^k & A_1^{-N} \\ 0 & 1 & A_1 + A_2 & \dots & \sum_{j_1=0}^{k-1} A_1^{j_1} A_2^{k-1-j_1} & C_{2,2} \\ 0 & 0 & 1 & \dots & \sum_{j_1=0}^{k-2} \sum_{j_2=0}^{k-2-j_1} A_1^{j_1} A_2^{j_2} A_3^{k-2-j_1-j_2} & C_{3,3} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & A_1 + A_2 + \dots + A_k & C_{k,k} \\ 0 & 0 & 0 & \dots & 1 & C_{k+1,k+1} \\ 0 & 0 & 0 & \dots & 0 & C_{k+2,k+2} \end{bmatrix},$$

that is, we have an upper-triangular matrix with 1's on the diagonal and zeros underneath. This means that the determinant equals the bottom right-most element, which is

$$\begin{aligned} C_{k+2,k+2} = (-1)^{(k+1)} \sum_{j_1=1}^{N} \sum_{j_2=1}^{N+1-j_1} \cdots \sum_{j_k=1}^{N+k-1-j_1-\dots-j_{k-1}} A_1^{-j_1} \dots A_k^{-j_k} \\ \times \sum_{j_{k+1}=1}^{N+k-j_1-\dots-j_k} A_{k+1}^{j_{k+1}} A_{k+2}^{-(N+k+2-j_1-\dots-j_{k+1})}. \end{aligned}$$

We now combine $D_{N-1}[f]$ with the other terms in (5.6), and let $A_{k+1}, A_{k+2} \to 1$. This gives

$$\begin{aligned} &\mathbb{E}_N \left[\prod_{r=1}^{k} Z(\theta_N + \alpha_r) \right] \\ &\quad = \frac{1}{N} \prod_{r=1}^{k} (A_r - 1) \sum_{j_1=1}^{N} \sum_{j_2=1}^{N+1-j_1} \cdots \sum_{j_k=1}^{N+k-1-j_1-\dots-j_{k-1}} A_1^{-j_1} \dots A_k^{-j_k} \sum_{j_{k+1}=1}^{N+k-j_1-\dots-j_k} 1. \end{aligned}$$

Re-indexing the summations to start from 0 instead of 1 and evaluating the last sum, we have

$$\mathbb{E}_N\left[\prod_{r=1}^{k} Z(\theta_N+\alpha_r)\right]$$
$$=\frac{1}{N}\prod_{r=1}^{k} A_r^{-1}\left(A_r-1\right)\sum_{j_1=0}^{N-1}\sum_{j_2=0}^{N-1-j_1}\cdots\sum_{j_k=0}^{N-1-j_1-\cdots-j_{k-1}} A_1^{-j_1}\ldots A_k^{-j_k}(N-j_1-\cdots-j_k). \tag{5.9}$$

Recall that the coefficient of $\alpha_1^{n_1}\ldots\alpha_k^{n_k}$, which we denote by $[\alpha_1^{n_1}\ldots\alpha_k^{n_k}]$, from (5.9) will yield the desired mixed derivative, and we wish to find this to leading order as $N\to\infty$. It is clear that to do this, we want to obtain the highest possible power of N from the summations as they depend upon N, and the smallest possible contribution from the product $\prod_{r=1}^{k} A_r^{-1}\left(A_r-1\right)$ as there is no N dependence in that product.

Recalling that $A_r=e^{i\alpha_r}$ and Taylor expanding gives

$$\prod_{r=1}^{k} A_r^{-1}\left(A_r-1\right)=i^k\alpha_1\ldots\alpha_k+\text{ higher order terms.} \tag{5.10}$$

Therefore we need to find the large N behaviour of $[\alpha_1^{n_1-1}\ldots\alpha_k^{n_k-1}]$ from the summations in (5.9), that is from

$$\sum_{j_1=0}^{N-1}\sum_{j_2=0}^{N-1-j_1}\cdots\sum_{j_k=0}^{N-1-j_1-\cdots-j_{k-1}} e^{-ij_1\alpha_1}\ldots e^{-ij_k\alpha_k}(N-j_1-\cdots-j_k).$$

The coefficient of $\alpha_1^{n_1-1}$ in the Taylor expansion of $e^{-ij_1\alpha_1}$ equals $(-ij_1)^{n_1-1}/(n_1-1)!$, so the coefficient $[\alpha_1^{n_1-1}...\alpha_k^{n_k-1}]$ equals

$$\sum_{j_1=0}^{N-1}\cdots\sum_{j_k=0}^{N-1-j_1-\cdots-j_{k-1}}\frac{(-ij_1)^{n_1-1}}{(n_1-1)!}\cdots\frac{(-ij_k)^{n_k-1}}{(n_k-1)!}(N-j_1-\cdots-j_k)$$
$$=\frac{(-i)^{n_1+\cdots+n_k-k}}{(n_1-1)!\ldots(n_k-1)!}\sum_{j_1=0}^{N-1}\cdots\sum_{j_k=0}^{N-1-j_1-\cdots-j_{k-1}} j_1^{n_1-1}\ldots j_k^{n_k-1}(N-j_1-\cdots-j_k).$$

To evaluate the leading order coefficient of these sums, we will turn them into Riemann sums and hence into an integral. The sums equal

$$N^{n_1+\cdots+n_k+1}\sum_{j_1=0}^{N-1}\sum_{j_2=0}^{N-1-j_1}\cdots$$
$$\sum_{j_k=0}^{N-1-j_1-\cdots-j_{k-1}}\frac{1}{N^k}\left(\frac{j_1}{N}\right)^{n_1-1}\cdots\left(\frac{j_k}{N}\right)^{n_k-1}\left(1-\frac{j_1}{N}-\cdots-\frac{j_k}{N}\right)$$

and now each summation can be considered as a Riemann sum and so we can rewrite the summation in the above line as the k-fold integral

$$\int_0^1 \int_0^{1-x_1} \cdots \int_0^{1-x_1-\cdots-x_{k-1}} x_1^{n_1-1} \dots x_k^{n_k-1}(1-x_1-\cdots-x_k)\ dx_1 dx_2 \dots dx_k.$$

By Theorem 1.8.6 in [3], this integral equals

$$\frac{(n_1-1)!\dots(n_k-1)!}{(n_1+\dots+n_k+1)!}$$

and so we have

$$[\alpha_1^{n_1-1}...\alpha_k^{n_k-1}] \sim \frac{(-i)^{n_1+\cdots+n_k-k}}{(n_1-1)!\dots(n_k-1)!}\frac{(n_1-1)!\dots(n_k-1)!}{(n_1+\dots+n_k+1)!}N^{n_1+\dots+n_k+1}. \tag{5.11}$$

Combining (5.10) with (5.11) and the term $1/N$ in (5.9), we obtain the coefficient $[\alpha_1^{n_1}...\alpha_k^{n_k}]$ of $\mathbb{E}_N\left[Z(\theta_N+\alpha_1)\dots Z(\theta_N+\alpha_k)\right]$ is asymptotic to

$$\frac{(-1)^{n_1+\cdots+n_k+k}\ i^{n_1+\cdots+n_k}}{(n_1+\dots+n_k+1)!}N^{n_1+\dots+n_k}.$$

Recalling that the coefficient of $\alpha_r^{n_r}$ in the Taylor expansion of $Z(\theta_N+\alpha_r)$ equals $Z^{(n_r)}(\theta_N)/n_r!$, we see that

$$\mathbb{E}_N\left[Z^{(n_1)}(\theta_N)\dots Z^{(n_k)}(\theta_N)\right] \sim (-1)^{n_1+\cdots+n_k+k}\ i^{n_1+\cdots+n_k}\frac{n_1!\dots n_k!}{(n_1+\dots+n_k+1)!}N^{n_1+\dots+n_k},$$

and this completes the proof of Theorem 5.1.

5.3 THE HYBRID MODEL APPROACH

As discussed in Section 1.3.4, in 2007, Gonek, Hughes and Keating [149] proved a hybrid formula for the zeta function, expressing it as a partial product over primes times a rapidly decaying product over non-trivial zeros. We state a result with slightly more control over the smoothing (in [149] and other later papers, $X=Y$ is taken).

Theorem 5.6 (Gonek–Hughes–Keating). *Let $s=\sigma+it$ with $\sigma\geq 0$ and $|t|\geq 2$, let $X,Y\geq 2$ be real parameters, and let K be any fixed positive integer. Let $f(x)$ be a non-negative C^∞ function of mass 1 supported on $[0,1]$ and set $u(x)=Yf(Y\log\frac{x}{e}+1)/x$. Thus, $u(x)$ is a function of mass 1 supported on $[e^{1-1/Y},e]$. Set*

$$U(z)=\int_1^e u(y)E_1(z\log y)\ \ dy\,, \tag{5.12}$$

where $\mathbb{E}_1(z)$ is the exponential integral $\int_z^\infty e^{-w}/w\ \ dw$. Then

$$\zeta(s)=P_X(s)Z_X(s)\left(1+O\left(\frac{Y^{K+1}X^{\max(1-\sigma,0)}}{(|s|\log X)^K}\right)+O\left(\frac{X^{1-\sigma}\log X}{Y}\right)\right)\ ,$$

where

$$P_X(s) = \exp\left(\sum_{n\le X}\frac{\Lambda(n)}{\log n}\frac{1}{n^s}\right), \tag{5.13}$$

$\Lambda(n)$ *is von Mangoldt's function, and*

$$Z_X(s) = \exp\left(-\sum_{\rho_n} U((s-\rho_n)\log X)\right). \tag{5.14}$$

The constants implied by the O terms depend only on f and K.

Remark. The proof of this result follows precisely the method in [149], with obvious changes for the different smoothing.

Note that $U(z)$ is not an analytic function; it has a logarithmic singularity at $z=0$. However, recall the formula

$$E_1(z) = -\log z - \gamma_0 - \sum_{m=1}^{\infty}\frac{(-1)^m z^m}{m!\,m}, \tag{5.15}$$

where $|\arg z| < \pi$, $\log z$ denotes the principal branch of the logarithm, and γ_0 is Euler's constant. (It is clear that the sum is an entire function of z since it is absolutely convergence for all $z\in\mathbb{C}$.) From this and (5.12) we observe that we may interpret $\exp(-U(z))$ to be an analytic function, asymptotic to Cz as $z\to 0$, for some constant C which depends upon the smoothing function u.

Just as in work of Bui, Gonek and Milinovich [47], we can differentiate whilst still obtaining the asymptotic, obtaining under the Riemann Hypothesis

$$\zeta'(\rho) = P_X(\rho)Z_X'(\rho)\left(1 + O\left(\frac{Y^{K+1}X^{1/2}}{(|\rho|\log X)^K}\right) + O\left(\frac{X^{1/2}\log X}{Y}\right)\right).$$

It is believed that P_X and Z_X operate pseudo-independently. Hence the moments of zeta are products of moments of P_X and Z_X. This is known as the Splitting Conjecture, given in Conjecture 1.10 for the analogous continuous moment case. We conjecture it here in our case, where it will become clear later in the section where the technical assumptions come from.

Conjecture 5.7. *Let $X,T\to\infty$ with $X = O(\log T)$. Then for $k > -3$, we have*

$$\frac{1}{N(T)}\sum_{0<\gamma\le T}\zeta'(\rho)^k \sim \left(\frac{1}{N(T)}\sum_{0<\gamma\le T}P_X(\rho)^k\right)\left(\frac{1}{N(T)}\sum_{0<\gamma\le T}Z_X'(\rho)^k\right).$$

In the next section we will evaluate the moments of mixed derivatives of P_X, when averaged over zeros of zeta. We will show that the moments only really contribute when no derivatives are taken. In the last section we will model the moments of the first derivative of Z_X when averaged over zeros of zeta, using a method that allows non-integer moments to be taken. Taken collectively, these results give weight to Conjectures 5.4 and 5.5.

5.3.1 The moments of P_X

In this section we will show that the mixed moments of P_X vanish if any derivatives are taken, whilst the mean of P_X^k is asymptotically 1, when averaged over zeros of the zeta function.

Theorem 5.8. *Under the Riemann Hypothesis, for $X > 2$ with $X = O(\log T)$, for any non-negative integers $n_1, \ldots, n_k$ we have,*

$$\sum_{0<\gamma\leq T} P_X^{(n_1)}(\rho)\ldots P_X^{(n_k)}(\rho) = \begin{cases} N(T) + O(T\log\log T) & \text{if } n_1 = \cdots = n_k = 0 \\ O\left(T(\log\log T)^{1+n_1}\right) & \text{if } n_1 > 0 \text{ and } n_2 = \cdots = n_k = 0 \\ O\left(T\right) & \text{if more than one } n_i > 0 \end{cases}$$

as $T \to \infty$, where $\rho = \frac{1}{2} + i\gamma$ is a non-trivial zero of the Riemann zeta function, $P_X(s)$ is given in (5.13) *and $N(T)$ is the number of such zeros up to height T, given by* (1.5)*.*

In the case that no derivatives are taken, one can permit k to be real and positive.

Theorem 5.9. *Under the Riemann Hypothesis, for $X > 2$ with $X = O(\log T)$, for k a fixed positive real number,*

$$\sum_{0<\gamma\leq T} P_X(\rho)^k = N(T) + O(T\log\log T)$$

as $T \to \infty$.

This should be compared to a result of Bui, Gonek and Milinovich (Theorem 2.2 of [47]) which stated that, under the Riemann Hypothesis, for $\varepsilon > 0$ and $X, T \to \infty$ with $X = O\left((\log T)^{2-\varepsilon}\right)$ then for any $k \in \mathbb{R}$ one has

$$\frac{1}{N(T)} \sum_{0<\gamma\leq T} |P_X(\rho)|^{2k} = a_k \left(e^{\gamma_0}\log X\right)^{k^2} \left(1 + O_k\left((\log X)^{-1}\right)\right)$$

where a_k is an explicit product over primes given by (1.19).

Before we prove Theorem 5.8, we need to state and prove some preliminary lemmas.

Lemma 5.10. *For k a fixed positive real number, the function $P_X(s)^k$ can be written as a non-vanishing absolutely convergent Dirichlet series*

$$P_X(s)^k = \sum_{m=1}^{\infty} \frac{a_k(m)}{m^s}$$

with $0 \leq a_k(m) \leq d_k(m)$, where $d_k(m)$ is the k^{th} divisor function.

Proof. Since $P_X(s)$ given in (5.13) is the exponential of a finite Dirichlet polynomial, so its k^{th} power is an entire non-vanishing function, so can be written as a Dirichlet series

$$P_X(s)^k = \exp\left(k \sum_{n \le X} \frac{\Lambda(n)}{\log n} \frac{1}{n^s}\right)$$
$$= \sum_{m=1}^{\infty} \frac{a_k(m)}{m^s}$$

where the sum converges absolutely for any s, and $a_k(m) = 0$ if m has any prime divisor greater than X. If $p \le X$ is a prime, then $a_k(p) = k$. Since these coefficients come from the exponential of positive terms, the $a_k(m)$ are positive. In the case when $m \le X$, these coefficients will equal $d_k(m)$ and in the case when $m > X$ they will be less than $d_k(m)$ due to missing contributions from terms with $n > X$ in the exponent. □

In the proofs of the two theorems, it will be important to truncate the infinite sum.

Lemma 5.11 (Gonek-Hughes-Keating)**.** *For $2 \le X \ll (\log T)^{2-\varepsilon}$ with $\varepsilon > 0$, and k a fixed positive real number, and θ a small positive number, we have*

$$P_X\left(\frac{1}{2} + it\right)^k = \sum_{m \le T^\theta} \frac{a_k(m)}{m^{1/2+it}} + O_k\left(T^{-\varepsilon\theta/2}\right).$$

Proof. This follows immediately from the proof of Lemma 2 in [149]. □

As previously discussed, Gonek [146] proved unconditionally a uniform version of Landau's formula concerning sums over the non-trivial zeros of the Riemann zeta function, including the corollary given in Lemma 2.2 under the assumption of the Riemann Hypothesis. We restate it below for ease of reference.

Lemma (Gonek)**.** *Under the Riemann Hypothesis, for $T > 1, m \in \mathbb{N}$ with $m \ge 2$ and ρ a non-trivial zero of the Riemann zeta function $\zeta(s)$,*

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

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

Remark. Recall that this result does not apply in the case when $m = 1$, when the sum over zeros trivially equals $N(T)$.

Proof of Theorem 5.8. To differentiate $P_X(\sigma)$ j-times, we return to the exponential form (5.13). The Faà di Bruno formula on multiple derivatives of e^f states

$$\frac{d^j}{d\sigma^j} e^{f(\sigma)} = \left(f^{(j)} + \cdots + (f')^j\right) e^f$$

where the sum ranges over all possible combinations of derivatives of f so that total derivative is j, with certain multinomial coefficients that don't matter for us.

In our case, one can check that the longest sum comes from the first derivative raised to the j^{th} power, essentially giving a sum of length X^j. That is

$$P_X^{(j)}(s) = \sum_{n \le X^j} \frac{\tilde{\beta}_j(n)}{n^s} \exp\left(\sum_{n \le X} \frac{\Lambda(n)}{\log n} \frac{1}{n^s}\right)$$

for coefficients $\tilde{\beta}_j(n)$ that come from appropriate combinations of derivatives of the sum in the exponential, whose precise nature does not concern us, other than noting that

$$\tilde{\beta}_j(1) = \begin{cases} 0 & \text{if } j \neq 0 \\ 1 & \text{if } j = 0 \end{cases}$$

and for prime $p \le X$,

$$\tilde{\beta}_j(p) = \begin{cases} (-\log p)^j & \text{if } j \neq 0 \\ 0 & \text{if } j = 0 \end{cases}$$

(this comes from differentiating the sum in the exponential j times; other terms in the Faà di Bruno formula contribute to coefficients of higher powers of p). If n is divisible by any prime greater than X, $\tilde{\beta}_j(n) = 0$.

Combining k of these expressions together (replacing j with derivatives $n_1, n_2, \ldots, n_k$, we have

$$P_X^{(n_1)}(s) \ldots P_X^{(n_k)}(s) = \sum_{n \le X^{n_1+n_2+\cdots+n_k}} \frac{\beta(n)}{n^s} P_X(s)^k \tag{5.16}$$

where

$$\beta(n) = (\tilde{\beta}_{n_1} * \tilde{\beta}_{n_2} * \cdots * \tilde{\beta}_{n_k})(n)$$

is the convolution of the appropriate $\tilde{\beta}_j$.

In the case when $\Re(s) = 1/2$ and $X = (\log T)^{2-\varepsilon}$, using Lemma 5.11 we have

$$\begin{aligned} P_X^{(n_1)}(s) \ldots P_X^{(n_k)}(s) &= \sum_{n \le X^{n_1+n_2+\cdots+n_k}} \frac{\beta(n)}{n^s} \left(\sum_{m \le T^\theta} \frac{a_k(m)}{m^s} + O_k\left(T^{-\varepsilon\theta/2}\right)\right) \\ &= \sum_{m \le T^{\theta'}} \frac{b(m)}{m^s} + O\left(T^{-\varepsilon'}\right) \end{aligned} \tag{5.17}$$

for some $\varepsilon' > 0$ and $\theta' > \theta$, which both depend upon ε, k, θ, and $n_1, \ldots, n_k$. Essentially, since the first sums length is only a power of $\log T$, the two sums together are truncated at $T^{\theta'}$ for some $\theta' > \theta$, as T gets large.

Shortly we will use some facts about the $b(m)$, which we record here:

- Only if $n_1 = n_2 = \cdots = n_k = 0$ does $b(1) = 1$, otherwise $b(1) = 0$ (essentially because $\tilde{\beta}_j(1) = 0$ for any $j \neq 0$ since differentiation kills constants).
- If $n_1 = n_2 = \cdots = n_k = 0$, then $b(p) = a_k(p)$ and for prime $p \leq X$, $a_k(p) = k$.
- If exactly all bar one of the n_i vanish (say $n_1 \neq 0$, and $n_2 = n_3 = \cdots = n_k = 0$) then $b(p) = \beta(p) = \tilde{\beta}_{n_1}(p) = (-\log p)^{n_1}$. To see this, note that $\tilde{\beta}_{n_1}(1) = 0$, which kills all other contributions in the convolution other than $\tilde{\beta}_{n_1}(p)$.
- If more than one $n_i \neq 0$, then $b(p) = 0$ since there will be at least two pieces in the convolution that have $\tilde{\beta}_{n_1}(1) = 0$ and $\tilde{\beta}_{n_2}(1) = 0$, so every term vanishes.

Assuming the Riemann Hypothesis, we can sum (5.16) over the zeros of zeta, obtaining

$$\sum_{0<\gamma\leq T} P_X^{(n_1)}(\rho)\ldots P_X^{(n_k)}(\rho) = b(1)N(T) + \sum_{0<\gamma\leq T}\ \sum_{2\leq m\leq T^{\theta'}} \frac{b(m)}{m^\rho} + O\left(N(T)T^{-\varepsilon'}\right) \quad (5.18)$$

and applying Corollary 2.2 to the middle sum yields

$$\sum_{0<\gamma\leq T}\ \sum_{2\leq m\leq T^{\theta}} \frac{b(m)}{m^\rho} = -\frac{T}{2\pi} \sum_{2\leq m\leq T^{\theta'}} \frac{b(m)\Lambda(m)}{m} + \sum_{2\leq m\leq T^{\theta}} b(m)O(\log(2mT)\log\log(3m)). \quad (5.19)$$

To bound the first term on the right-hand side of (5.19), note that the $\Lambda(m)$ forces the sum to be over primes and prime powers only, and the $b(m)$ ensures we only need primes $p \leq X$. Since $b(m) \ll m^\varepsilon$, the square and higher powers of primes form a convergent sum, so

$$-\frac{T}{2\pi} \sum_{2\leq m\leq T^{\theta'}} \frac{b(m)\Lambda(m)}{m} = O\left(T \sum_{\substack{p\leq X \\ p \text{ prime}}} \frac{b(p)\log p}{p}\right) + O(T).$$

The value of $b(p)$ depends on how many $n_i = 0$

$$b(p) = \begin{cases} k & \text{if } n_1 = \cdots = n_k = 0 \\ (-\log p)^{n_1} & \text{if } n_1 > 0 \text{ and } n_i = 0 \text{ otherwise} \\ 0 & \text{if more than one } n_i > 0. \end{cases}$$

Hence, summing over all primes up to X and using the Prime Number Theorem,

$$\sum_{p\leq x} \frac{b(p)\log p}{p} \ll \begin{cases} \log X & \text{if } n_1 = \cdots = n_k = 0 \\ (\log X)^{1+n_1} & \text{if } n_1 > 0 \text{ and } n_i = 0 \text{ otherwise} \\ 0 & \text{if more than one } n_i > 0. \end{cases}$$

For the second error term in (5.19), since the $b(m)$ all have the same sign (for any given fixed $n_1, \ldots, n_k$), we have that this equals

$$O\left(\log T \log\log T \sum_{m=1}^{\infty} b(m)\right).$$

By (5.17) and (5.16) the sum is simply

$$\sum_{m=1}^{\infty} b(m) = \sum_{n \leq X^{n_1+n_2+\cdots+n_k}} \beta(n) P_X(0)^k.$$

To bound the first sum on the right-hand side, recall that $\beta(n) \ll n^{\varepsilon}$, and to bound the $P_X(0)^k$ note that since

$$\begin{aligned} \log P_X(0) &= \sum_{n \leq X} \frac{\Lambda(n)}{\log n} \\ &= \frac{X}{\log X} + O\left(\frac{X}{(\log X)^2}\right) \end{aligned}$$

by the Prime Number Theorem, we have

$$\sum_{m=1}^{\infty} b(m) = O\left(\exp\left(c' \frac{X}{\log X}\right)\right)$$

for any fixed $c' > k$.

Plugging these two error terms back into (5.19), we have shown

$$\sum_{0<\gamma\leq T} \sum_{2\leq m\leq T^{\theta}} \frac{b(m)}{m^{\rho}} = O\left(T(\log X)^{1+n_1}\right) + O(T) + O\left(\log T \log\log T \exp\left(c' \frac{X}{\log X}\right)\right)$$

where the first error term is only present if $n_2 = \cdots = n_k = 0$.

To complete the proof we now choose X to balance the various error terms that appear when we substitute this into (5.18). If we insist $X = O(\log T)$ then we have

$$\sum_{0<\gamma<T} P_X^{(n_1)}(\rho) \dots P_X^{(n_k)}(\rho) = \frac{T}{2\pi} \log T + O\left(T(\log\log T)\right)$$

in the case when $n_1 = \cdots = n_k = 0$,

$$\sum_{0<\gamma<T} P_X^{(n_1)}(\rho) \dots P_X^{(n_k)}(\rho) = O\left(T(\log\log T)^{1+n_1}\right)$$

if $n_1 > 0$ and $n_2 = \cdots = n_k = 0$, and

$$\sum_{0<\gamma<T} P_X^{(n_1)}(\rho) \dots P_X^{(n_k)}(\rho) = O\left(T\right)$$

if more than one $n_i > 0$.

This completes the proof of Theorem 5.8. □

Proof of Theorem 5.9. In the case when no derivatives are taken, we can exploit the multiplicative nature of P_X to allow k to be a fixed positive real number, not just an integer. Much of the proof goes through unchanged.

By Lemma 5.11 and Lemma 2.2 we have

$$\begin{aligned}\sum_{0<\gamma\le T} P_X(\rho)^k &= N(T) + \sum_{0<\gamma\le T}\sum_{2\le m\le T^\theta} \frac{a_k(m)}{m^\rho} + O\left(N(T)T^{-\varepsilon'}\right)\\ &= N(T) - \frac{T}{2\pi}\sum_{2\le m\le T^\theta}\frac{a_k(m)\Lambda(m)}{m} + O\left(\log T\log\log T \sum_{2\le m\le T^\theta} a_k(m)\right)\end{aligned}$$

since $a_k(1) = 1$.

As in the case of Theorem 5.8, assuming $X < T^\theta$ we can bound

$$\begin{aligned}\sum_{2\le m\le T^\theta}\frac{a_k(m)\Lambda(m)}{m} &= \sum_{p<X}\frac{k\log p}{p} + O(1)\\ &\ll \log X\end{aligned}$$

and, exactly as before,

$$\sum_{m=1}^{\infty} a_k(m) = P_X(0)^k \ll \exp\left(c'\frac{X}{\log X}\right)$$

for any fixed $c' > k$.

Therefore

$$\sum_{0<\gamma\le T} P_X(\rho)^k = N(T) + O\left(T\log X\right) + O\left(\log T\log\log T\exp\left(c'\frac{X}{\log X}\right)\right).$$

As before, the error terms can be made to approximately match when $X = O(\log T)$. □

Remark. In the previous proofs we can take X to be anything up to $o(\log T\log\log T)$ before the second error term dominates the main term of $\frac{T}{2\pi}\log T$. Since the error term as we have written it comes from a subsidiary main term, we cannot reduce the error down to $O(T)$.

5.3.2 The moments of Z'_X

In this section we will concentrate on the random matrix equivalent for Z_X, given in (5.14), and for simplicity just look at its first derivative. Again in this section, we will not require k to be an integer. Taking an $N \times N$ unitary matrix with eigenvalues $e^{i\theta_1}, \ldots, e^{i\theta_N}$, we wish to calculate

$$\mathbb{E}_N\left[Z'_{N,X}(\theta_N)^k\right]$$

where

$$Z_{N,X}(\theta) = \prod_{m=1}^{N}\exp\left(-\sum_{j=-\infty}^{\infty} U(i(\theta-\theta_m+2\pi j)\log X)\right)$$

plays the role of $Z_X(s)$ in Theorem 5.6, and where U is given in (5.12).

Remark. The sum over j makes the arguments 2π-periodic, thus permitting the move from $e^{i\theta}$ to θ without any branch-cut ambiguities. The decay of U for large inputs means that the infinite sum over j is absolutely summable.

Theorem 5.12. *If $k \in \mathbb{C}$ is such that $k \notin \{-3, -4, -5, \dots\}$, then*

$$\mathbb{E}_N\left[\frac{1}{N}\sum_{m=1}^{N} Z'_{N,X}(\theta_m)^k\right] \sim \frac{e^{ik\pi/2}}{\Gamma(k+2)}N^k$$

as $N \to \infty$.

Remark. The proof deals with the analytic continuation of the objects under consideration. However, for our purposes as a model for zeta, we must stop before the first singularity; that is, in Conjecture 5.5 we take $\Re(k) > -3$.

Remark. Restricting to $k \in \mathbb{N}$, we see this Theorem has the same right hand side as Corollary 5.2 in the case $n = 1$. That is, $Z'_{N,X}$ and the first derivative of the characteristic polynomial asymptotically have the same moments.

Proof. It is convenient to factor out the behaviour around the eigenvalues (where $Z_{N,X}$ vanishes) as follows

$$Z_{N,X}(\theta) = \prod_{m=1}^{N}\left(1 - e^{-i(\theta-\theta_m)}\right)e^{F_X(\theta-\theta_m)}$$

where

$$F_X(\vartheta) = -\log\left(1 - e^{-i\vartheta}\right) - \sum_{j=-\infty}^{\infty} U\big(i(\vartheta + 2\pi j)\log X\big) \tag{5.20}$$

is a 2π-periodic function which is continuously differentiable for all real ϑ - the logarithmic singularities cancel out. The first statement is obvious. The second statement can be seen from the definition of $U(z)$ given in (5.12) and the series expansion of $E_1(z)$ around $z = 0$ given in (5.15) (and indeed, this fact will be made clear when we look at the decay of its Fourier coefficients in Lemma 5.13).

Differentiating,

$$\begin{aligned}Z'_{N,X}(\theta) = &\sum_{n=1}^{N} ie^{-i(\theta-\theta_n)}e^{F_X(\theta-\theta_n)}\prod_{\substack{m=1\\m\neq n}}^{N}\left(1 - e^{-i(\theta-\theta_m)}\right)e^{F_X(\theta-\theta_m)}\\&+\sum_{n=1}^{N}\left(1 - e^{-i(\theta-\theta_n)}\right)F'_X(\theta-\theta_n)e^{F_X(\theta-\theta_n)}\prod_{\substack{m=1\\m\neq n}}^{N}\left(1 - e^{-i(\theta-\theta_m)}\right)e^{F_X(\theta-\theta_m)}\end{aligned}$$

and substituting $\theta = \theta_N$, we see that for every $n \neq N$ there is a term in the product that vanishes (so only the $n = N$ terms survives), and every term in the second term vanishes, including the $n = N$ term. That is,

$$Z'_{N,X}(\theta_N) = ie^{F_X(0)} \prod_{m=1}^{N-1} \left(1 - e^{-i(\theta_N - \theta_m)}\right) e^{F_X(\theta_N - \theta_m)}.$$

Remark. There is nothing special about picking θ_N over any of the other eigenvalues. This is made for notational convenience. The true calculation would be to evaluate

$$\frac{1}{N} \sum_{m=1}^{N} Z'_{N,X}(\theta_m)$$

similar to what we do in Section 5.2, but by rotation invariance the result will be the same.

We now calculate the expected value of $Z'_{N,X}(\theta_N)^k$ for $k \in \mathbb{C}$ when averaged over all $N \times N$ unitary matrices distributed according to Haar measure, employing a trick found in [182] and written in this thesis as Lemma 1.18.

$$\begin{aligned} \mathbb{E}_N \left[Z'_{N,X}(\theta_N)^k \right] &= e^{ik\pi/2} e^{kF_X(0)} \mathbb{E}_N \left[\prod_{m=1}^{N-1} \left(1 - e^{-i(\theta_N - \theta_m)}\right)^k e^{kF_X(\theta_N - \theta_m)} \right] \\ &= e^{ik\pi/2} e^{kF_X(0)} \frac{1}{N} \mathbb{E}_{N-1} \left[\prod_{m=1}^{N-1} \left|1 - e^{i\vartheta_m}\right|^2 \left(1 - e^{i\vartheta_m}\right)^k e^{kF_X(-\vartheta_m)} \right] \end{aligned} \tag{5.21}$$

where we interpret $e^{i\vartheta_m}$ as the eigenvalues of an $(N-1) \times (N-1)$ unitary matrix. (Briefly, what we have done is write the first expectation out as a N-dimensional Weyl integral, then change variables to $\vartheta_m = \theta_m - \theta_N$ for $m = 1, \dots, N-1$. Making use of the fact the integrand is 2π-periodic, we turn it back into a $(N-1)$-dimension Weyl integral, plus an extra trivial integral over θ_N.)

Because k is complex, we need to be precise about the choice of branch taken. We define $\left(1 - e^{i\vartheta}\right)^k$ to be the value obtained from continuous variation of $\left(1 - e^{i\vartheta} e^{-\varepsilon}\right)^k$ for $\varepsilon > 0$, converging to the value 1 as $\varepsilon \to \infty$.

As in Section 5.2, the inner expectation can be calculated by Heine's identity to be equal to the Toeplitz determinant

$$D_{N-1}[f] := \det \left| \hat{f}_{j-\ell} \right|_{1 \le j, \ell \le N-1}$$

with symbol

$$f(\vartheta) = \left|1 - e^{i\vartheta}\right|^2 \left(1 - e^{i\vartheta}\right)^k e^{kF_X(-\vartheta)}.$$

Note that $f(\vartheta)$ has only one singularity at $\vartheta = 0$. Toeplitz determinants with such symbols have been calculated asymptotically by Ehrhardt and Silbermann in [110] (building on extensive previous work by several other authors).

They show (in their Theorem 2.5) that if $b(\vartheta)$ is a suitably smooth (defined in their paper) 2π-periodic function with winding number zero and whose logarithm has the Fourier series expansion

$$\log b(\vartheta) = \sum_{m=-\infty}^{\infty} s_m e^{im\vartheta},$$

then for symbols of the form

$$f(\vartheta) = b(\vartheta)\left(1 - e^{i\vartheta}\right)^{\gamma}\left(1 - e^{-i\vartheta}\right)^{\delta}$$

subject to $\gamma + \delta \notin \{-1, -2, -3, \dots\}$, then for any $\varepsilon > 0$

$$D_{N-1}[f] = C_1 N^{\gamma\delta} C_2^{N-1}\left(1 + O\left(\frac{1}{N^{1-\varepsilon}}\right)\right)$$

where

$$C_1 = \frac{G(1+\gamma)G(1+\delta)}{G(1+\gamma+\delta)} \exp\left(\sum_{m=1}^{\infty} m s_m s_{-m}\right) \exp\left(-\delta \sum_{m=1}^{\infty} s_m\right) \exp\left(-\gamma \sum_{m=1}^{\infty} s_{-m}\right)$$

where G is the Barnes G-function, and where

$$C_2 = \exp(s_0).$$

In our case, $\gamma = k + 1$ and $\delta = 1$ and $b(\vartheta) = \exp(kF_X(-\vartheta))$. To complete the proof, we simply need to calculate the Fourier coefficients of $kF_X(-\vartheta)$ (those coefficients being the desired s_m).

We will, in fact, delay the exact calculation of s_m to Lemma 5.13 to quickly complete the proof of the theorem. All we need from the lemma is that $s_m = 0$ if $m \leq 0$. From (5.21) and using Ehrhardt and Silbermann's formula above, with the values $\gamma = k + 1$ and $\delta = 1$, we have

$$\mathbb{E}_N\left[Z'_{N,X}(\theta_N)^k\right] \sim e^{ik\pi/2} e^{kF_X(0)} \frac{1}{N} \frac{G(k+2)G(2)}{G(k+3)} \exp\left(-\sum_{m=1}^{\infty} s_m\right) N^{k+1}.$$

Finally, note that $G(2) = 1$, $G(k+3) = \Gamma(k+2)G(k+2)$ and

$$e^{kF_X(0)} = \exp\left(\sum_{m=-\infty}^{\infty} s_m\right) = \exp\left(\sum_{m=1}^{\infty} s_m\right)$$

(the first equality following from setting $\vartheta = 0$ in the Fourier series expansion; the second equality comes from knowing $s_m = 0$ for $m \leq 0$). Therefore,

$$\mathbb{E}_N\left[Z'_{N,X}(\theta_N)^k\right] \sim \frac{e^{ik\pi/2}}{\Gamma(k+2)} N^k$$

as $N \to \infty$, as required. □

Lemma 5.13. *Let $F_X(\vartheta)$ be defined in* (5.20)*, then*

$$kF_X(-\vartheta) = \sum_{m=-\infty}^{\infty} s_m e^{im\vartheta}$$

where

$$s_m = \begin{cases} 0 & \text{if } m \leq 0 \\ \frac{k}{m}\left(1 - \int_1^{\exp(m/\log X)} u(y)\ dy\right) & \text{if } 1 \leq m < \log X \\ 0 & \text{if } m \geq \log X. \end{cases}$$

Remark. Since u has total mass 1, for $m > 0$ we can write

$$1 - \int_1^{\exp(m/\log X)} u(y)\ dy = \int_{\exp(m/\log X)}^{\infty} u(y)\ dy$$

although due to the support condition on u, if $m \geq \log X$ then $\exp(m/\log X) > e$ and so the integral vanishes.

Proof of Lemma 5.13. Note that

$$s_m = \frac{1}{2\pi}\int_{-\pi}^{\pi} kF_X(-\vartheta)e^{-im\vartheta}\ d\vartheta.$$

From (5.20) we have

$$kF_X(-\vartheta) = -k\log\left(1 - e^{i\vartheta}\right) - k\sum_{j=-\infty}^{\infty} U(i(-\vartheta + 2\pi j)\log X).$$

For m an integer, we have

$$\frac{1}{2\pi}\int_{-\pi}^{\pi} -k\log\left(1 - e^{i\vartheta}\right)e^{-im\vartheta}\ d\vartheta = \begin{cases} 0 & \text{if } m \leq 0 \\ \frac{k}{m} & \text{if } m \geq 1. \end{cases} \tag{5.22}$$

(To non-rigorously see why, note that $\log\left(1 - e^{i\vartheta}\right) = -\sum_{\ell=1}^{\infty} e^{i\ell\vartheta}/\ell$ and the only term in the sum that survives the integration is when $\ell = m$ for positive integers m.)

Furthermore, we have

$$\begin{aligned}\frac{1}{2\pi}\int_{-\pi}^{\pi} -k\sum_{j=-\infty}^{\infty} U\left(i(-\vartheta + 2\pi j)\log X\right)e^{-im\vartheta}\ d\vartheta &= \frac{-k}{2\pi}\int_{-\infty}^{\infty} U(-i\vartheta\log X)e^{-im\vartheta}\ d\vartheta \\ &= \frac{-k}{2\pi}\int_{-\infty}^{\infty}\int_1^e u(y)E_1(-i\vartheta\log X\log y)e^{-im\vartheta}\ \ dy\ d\vartheta\end{aligned}$$

where the final equality comes from inserting the definition of U from (5.12) and the support of u. Swapping the order of integration, this is

$$\frac{-k}{2\pi}\int_1^e u(y)\int_{-\infty}^{\infty} E_1(-i\vartheta\log X\log y)e^{-im\vartheta}\ \ d\vartheta\ dy.$$

The Fourier transform of the exponential integral is

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} E_1(-i\vartheta\log X\log y)e^{-im\vartheta}\ \ d\vartheta = \begin{cases} 0 & \text{if } m < \log X\log y \\ \frac{1}{2m} & \text{if } m = \log X\log y \\ \frac{1}{m} & \text{if } m > \log X\log y. \end{cases}$$

Therefore, making use of the fact that u is supported on $[1, e]$ and has total mass 1, we have

$$\frac{-k}{2\pi}\int_1^e u(y)\int_{-\infty}^{\infty} E_1(-i\vartheta\log X\log y)e^{-im\vartheta}\ \ d\vartheta\ dy = \frac{-k}{m}\int_1^{\max(1,\exp(m/\log X))} u(y)\ dy$$
$$= \begin{cases} 0 & \text{if } m \le 0 \\ -\frac{k}{m}\int_1^{\exp(m/\log X)} u(y)\ dy & \text{if } 1 \le m < \log X \\ -\frac{k}{m} & \text{if } m \ge \log X. \end{cases}$$

The Fourier coefficient, s_m is the sum of this and (5.22). Note that both terms are zero for $m \le 0$ and the two terms perfectly cancel each other if $m \ge \log X$. □

5.4 NEGATIVE MOMENTS OF THE DERIVATIVES OF THE CHARACTERISTIC POLYNOMIAL

As we have seen in Section 1.3.6, Section 1.4.1 and Section 2.4, negative moments are of interest. Recall that Conjecture 5.5 states that we can take any $\Re(k) > -3$. We consider some small negative moments, specifically the cases when $k = -1, -2, -3$ (pushing our model to the point of breaking). We consider

$$\mathbb{E}_N\left[\frac{1}{N}\sum_{m=1}^{N} Z_N'(\theta_m)^k\right],$$

where we remind the reader that $Z_N(\theta)$ is the characteristic polynomial of a random unitary matrix, given by

$$Z_N(\theta) = \det(I - Ue^{-i\theta}) = \prod_{m=1}^{N}(1 - e^{i(\theta_m-\theta)}).$$

For the analogous symbol to (5.5) for the negative moments problem, we need to consider for $k = -1, -2, -3$,

$$f(z) = |1 - e^{iz}|^2(1 - e^{iz})^k.$$

For $k = -1$, we have

$$f(z) = |1 - e^{iz}|^2(1 - e^{iz})^{-1} = (1 - e^{-it})$$

so the Fourier coefficients are $c_{-1} = -1, c_0 = 1$, and $c_j = 0$ for $j \geq 1$. Then the Toeplitz determinant is given by

$$\mathbb{E}_N\left[\frac{1}{N}\sum_{m=1}^{N} Z_N'(\theta_m)^{-1}\right] = \frac{1}{N}\det\begin{bmatrix} 1 & 0 & 0 & \dots \\ -1 & 1 & 0 & \dots \\ 0 & -1 & 1 & \dots \\ \vdots & \vdots & \vdots & \vdots \end{bmatrix} = \frac{1}{N}.$$

This suggests as $T \to \infty$,

$$\frac{1}{N(T)}\sum_{0<\gamma\leq T} \zeta'\left(\frac{1}{2}+i\gamma\right)^{-1} \sim \frac{1}{\log T}.$$

Multiplying through by $N(T)$ gives the result from Theorem 2.3.

For $k = -2$, our symbol is of the form

$$f(z) = |1-e^{iz}|^2(1-e^{iz})^{-2} = (1-e^{-it})(1-e^{it})^{-1} = (1-e^{-it})\left(\sum_{k=0}^{\infty} e^{ikt}\right).$$

This sum telescopes to give

$$f(z) = -e^{-it}$$

so the Fourier coefficients are $c_{-1} = -1$, and $c_j = 0$ for $j \geq 0$. Then the Toeplitz determinant is given by

$$\mathbb{E}_N\left[\frac{1}{N}\sum_{m=1}^{N} Z_N'(\theta_m)^{-2}\right] = \frac{1}{N}\det\begin{bmatrix} 0 & 0 & 0 & \dots \\ -1 & 0 & 0 & \dots \\ 0 & -1 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots \end{bmatrix} = 0.$$

This suggests as $T \to \infty$,

$$\frac{1}{N(T)}\sum_{0<\gamma\leq T} \zeta'\left(\frac{1}{2}+i\gamma\right)^{-2} = O\left(T^{-1/2+\varepsilon}\right),$$

with some numerical evidence given in Figure 5.1, where we suggest an error term of ‘typical’ size for the zeta function.

Finally for $k = -3$, our symbol is of the form

$$f(z) = |1-e^{iz}|^2(1-e^{iz})^{-3} = (1-e^{-it})(1-e^{it})^{-2} = (1-e^{-it})(1-e^{it})^{-1}(1-e^{it})^{-1}.$$

Then by the $k = -2$ case, the first two terms in the last equality cancel to give $-e^{-it}$ so we have

$$f(z) = -e^{-it}\left(\sum_{k=0}^{\infty} e^{ikt}\right) = -e^{-it} - 1 - e^{it} - e^{2it} - \dots$$

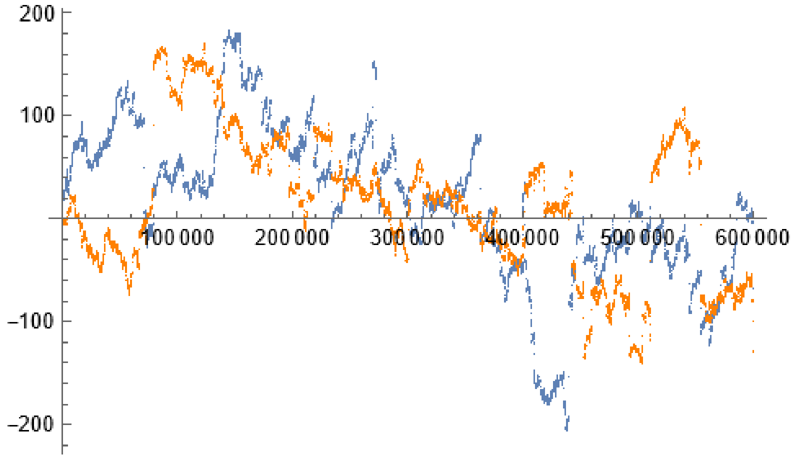

Figure 5.1: The real (blue) and imaginary (orange) part of $\sum_{0<\gamma\le T}\zeta'\left(\frac{1}{2}+i\gamma\right)^{-2}$ plotted over the first million zeros.

so the Fourier coefficients are $c_j = -1$ for $j \ge -1$. Hence,

$$\mathbb{E}_N\left[\frac{1}{N}\sum_{m=1}^{N} Z_N'(\theta_m)^{-3}\right] = \frac{1}{N}\det\begin{bmatrix} -1 & -1 & -1 & \dots \\ -1 & -1 & -1 & \dots \\ 0 & -1 & -1 & \dots \\ \vdots & \vdots & \vdots & \vdots \end{bmatrix}.$$

Then expanding along the first column gives two copies of the same matrix, with a minus sign from expanding a determinant, meaning that this expectation is also zero.

Therefore, we could conjecture the follow result for the Riemann zeta function. As $T \to \infty$,

$$\frac{1}{N(T)}\sum_{0<\gamma\le T}\zeta'\left(\frac{1}{2}+i\gamma\right)^{-3} = O\left(T^{-1/2+\varepsilon}\right),$$

where again we suggest an error term of 'typical' size for the zeta function.

However, we do emphasise that our model breaks down exactly at $k = -3$ so we can't give this conjecture with a huge degree of confidence, unlike the above which we have given good supporting evidence for. It would be of great interest to explore how to model the Riemann zeta function at this breaking point, and for higher negative moments.

5.5 A RECURRENCE RELATION HIDDEN IN THE RMT CALCULATION

Consider the left-hand side of (5.4), given by

$$\frac{1}{N}\prod_{r=1}^{k}(1-e^{-i\alpha_r}) \times \mathbb{E}_{N-1}\left[\prod_{m=1}^{N-1}(1-e^{i\phi_m})(1-e^{-i\phi_m})\prod_{r=1}^{k}(1-e^{i\phi_m}e^{-i\alpha_r})\right].$$

By following the method in Section 5.2, that is, following the method from Basor and Forrester [21], we have shown in (5.9) that this equals (after a trivial simplification)

$$\frac{1}{N}\prod_{r=1}^{k}\left(1-A_r^{-1}\right)\sum_{j_1=0}^{N-1}\sum_{j_2=0}^{N-1-j_1}\cdots\sum_{j_k=0}^{N-1-j_1-\cdots-j_{k-1}} A_1^{-j_1}\dots A_k^{-j_k}(N-j_1-\cdots-j_k),$$

where $A_r=e^{i\alpha_r}$.

Hidden behind this method is a recurrence relation, which we now derive and give a solution for. Our previous method in Section 5.2 proves that the solution we give here is the correct one.

Rather than using Heine's Lemma [295] to write the expectation of the right-hand side of (5.4) as a Toeplitz determinant, and then applying the method of Basor and Forrester [21], we instead consider the left-hand side of (5.4) and rearrange it in a naïve way. That is, we first use Heine's Lemma to write

$$\mathbb{E}_{N-1}\left[\prod_{m=1}^{N-1}(1-e^{i\phi_m})(1-e^{-i\phi_m})\prod_{r=1}^{k}(1-e^{i\phi_m}e^{-i\alpha_r})\right]=D_{N-1}[f] \tag{5.23}$$

for the symbol

$$f(z)=(1-z)(1-1/z)\prod_{r=1}^{k}(1-zA_r^{-1}).$$

For ease of notation, we relabel $A_r^{-1}=\mathcal{A}_r$. Expanding $f(z)$ gives

$$\begin{aligned}
f(z)&=(1-z)(1-1/z)(1-\mathcal{A}_1 z)\dots(1-\mathcal{A}_k z)\\
&=(-1/z+2-z)(1-\mathcal{A}_1 z)\dots(1-\mathcal{A}_k z)\\
&=(-1/z+2-z)(B_0-B_1z+B_2z^2+\ldots+(-1)^kB_kz^k)\\
&=-\frac{1}{z}+(2B_0+B_1)-z(B_0+2B_1+B_2)+z^2(B_1+2B_2+B_3)+\ldots+\\
&\quad+(-1)^{k-1}z^{k-1}(B_{k-2}+2B_{k-1}+B_k)+(-1)^kz^k(B_{k-1}+2B_k)+(-1)^{k+1}z^{k+1}B_k
\end{aligned}$$

where

$$\begin{aligned}
B_0&=1\\
B_1&=\sum_{1\le r\le k}\mathcal{A}_r\\
B_2&=\sum_{1\le r_1<r_2\le k}\mathcal{A}_{r_1}\mathcal{A}_{r_2}\\
B_3&=\sum_{1\le r_1<r_2<r_3\le k}\mathcal{A}_{r_1}\mathcal{A}_{r_2}\mathcal{A}_{r_3}\\
&\vdots\\
B_k&=\mathcal{A}_1\dots\mathcal{A}_k
\end{aligned}$$

are the elementary symmetric polynomials in k variables.

The Fourier coefficients we need to write this expectation as the Toeplitz determinant $D_{N-1}[f]$ are then given by

$$f_j = \begin{cases} 0 & \text{for } j \leq -2 \\ -1 & \text{for } j = -1 \\ 2B_0 + B_1 & \text{for } j = 0 \\ (-1)^j(B_{j-1} + 2B_j + B_{j+1}) & \text{for } 1 \leq j \leq k-1 \\ (-1)^k(B_{k-1} + 2B_k) & \text{for } j = k \\ (-1)^{k+1}B_k & \text{for } j = k+1 \\ 0 & \text{for } j \geq k+2. \end{cases}$$

The expectation in (5.23) (with $N \geq k+4$) may be written as the $(N-1) \times (N-1)$ Toeplitz determinant

$$D_{N-1}[f] = \det \begin{bmatrix} f_0 & f_1 & f_2 & f_3 & \dots & f_{k+1} & 0 & 0 & \dots \\ -1 & f_0 & f_1 & f_2 & \dots & f_k & f_{k+1} & 0 & \dots \\ 0 & -1 & f_0 & f_1 & \dots & f_{k-1} & f_k & f_{k+1} & \dots \\ 0 & 0 & -1 & f_0 & \dots & f_{k-2} & f_{k-1} & f_k & \dots \\ \vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \dots \end{bmatrix}$$

with the f_j for $j \geq 0$ as given above. Expanding this determinant along the leading column repeatedly, we are lead to the following recurrence relation (where we have not substituted the f_j given above for ease of notation)

$$D_{N-1}[f] = f_0 D_{N-2}[f] + f_1 D_{N-3}[f] + \ldots + f_{k+1} D_{N-k-3}[f]. \tag{5.24}$$

We then know by (5.9) that the solution to this recurrence relation is

$$\sum_{j_1=0}^{N-1} \sum_{j_2=0}^{N-1-j_1} \cdots \sum_{j_k=0}^{N-1-j_1-\cdots-j_{k-1}} A_1^{-j_1} \ldots A_k^{-j_k} (N - j_1 - \cdots - j_k),$$

which can be written as

$$D_{N-1}[f] = N + (N-1)C_1 + (N-2)C_2 + \ldots + C_{N-1}$$

where

$$C_j = \sum_{1 \leq r_1 \leq r_2 \leq r_3 \cdots \leq r_j \leq k} \mathcal{A}_{r_1} \mathcal{A}_{r_2} \mathcal{A}_{r_3} \ldots \mathcal{A}_{r_j}$$

are defined similarly to the B_j other than none of the inequalities are strict. Note that this gives a solution to the hidden recurrence relation (5.24) as claimed.

— 6 —

Higher Moments of the Riemann Zeta Function via the Ratios Conjecture

In this chapter we assume the Riemann Hypothesis, unless otherwise stated.

In Section 6.1 we begin this chapter with a summary of some results that one can obtain from the Ratios Conjecture, many of which are rigorously known. Its strength is in deriving these results in a generally easier way, and often giving more information, such as the lower order terms for asymptotics. The Ratios Conjecture is a heuristic argument based on certain RMT results. For an integral containing quotients of products of zeta functions (or more generally L-functions), we perform the follow steps (ignoring all error terms at all steps):

1. Replace all zeta functions in the denominator by its Dirichlet series (which we know conditionally converges up to the critical line under the Riemann Hypothesis).
2. Replace all zeta functions in the numerator by the approximate functional equation.
3. Expand the new terms in the integral, keeping only those terms with an equal number of $\chi(s)$ and $\chi(1-s)$ terms. These are the terms that are not rapidly oscillating.
4. In these remaining terms, keep only the diagonal terms.
5. Complete the resulting sums, factoring out various zeta factors to make the resulting terms converge.
6. A power-saving error term is then conjectured for the final result.

A full example will be seen when we use the Ratios Conjecture to calculate our conjectures in Section 6.2.

In Section 6.2 we will use the Ratios Conjecture in several different ways. First we give a general closed integral form to find a full asymptotic expansion for any moment for any number of derivatives. Then we re-derive Conjectures 5.3 and 5.4 following the Ratios Conjecture methodology.

We have discussed that the Ratios Conjecture can be used to find lower order terms for discrete moments of the Riemann zeta function. Applying similar ideas, we can use the Ratios Conjecture to find lower order terms for the conjectures formulated in Chapter 5.

Finally we give two examples of our result, the first of which is to find an integral form of the full asymptotic for the Generalised Shanks' Conjecture, first given in Theorem 3.1. This integral form is simpler than our previous result, and as has been seen in recent times, the 'correct' way of writing moments are as integrals.

Theorem 6.1. *For n a positive integer and $\rho = 1/2 + i\gamma$ a non-trivial zero of the Riemann zeta function,*

$$\sum_{0<\gamma\leq T} \zeta^{(n)}\left(\frac{1}{2}+i\gamma\right) = \frac{n!}{2\pi}\int_1^T \left(A_n + \frac{(-1)^{n+1}L^{n+1}}{(n+1)!} + \sum_{m=0}^{n} \frac{(-1)^{m+1}L^m\gamma_{n-m}}{m!(n-m)!}\right) dt + O\left(T^{1/2+\varepsilon}\right),$$

where $L = \log\frac{t}{2\pi}$, and the γ_m are the coefficients in the Laurent expansion of $\zeta(s)$ about $s = 1$, and the A_n are the coefficients in the Laurent expansion of $\zeta'(s)/\zeta(s)$ about $s = 1$.

Note that while we assume the Riemann Hypothesis in this chapter, but as previously seen, this result is actually unconditional with the only change in the error term.

The second example is a conjecture for the second moment of the first derivative of the Riemann zeta function, a previously unknown result. Specifically, we conjecture the following result.

Conjecture 6.2. *For $L = \log\frac{t}{2\pi}$ and $\rho = 1/2 + i\gamma$ a non-trivial zero of the Riemann zeta function,*

$$\begin{aligned}\sum_{0<\gamma\leq T} \zeta'\left(\frac{1}{2}+i\gamma\right)^2 = \\ \frac{1}{2\pi}\int_1^T &\left(\frac{1}{6}L^3 + \frac{1}{2}L^2\left(2\gamma_0 + A^{(0,0,1)}\right) + \frac{1}{2}L\left(-8\gamma_1 + 4\gamma_0 A^{(0,0,1)} + A^{(0,0,2)} + 2A^{(0,1,1)}\right)\right. \\ &+ \frac{1}{6}\left(-12\gamma_0^3 - 36\gamma_0\gamma_1 + 6\gamma_2 - 24\gamma_1 A^{(0,0,1)} + 6\gamma_0 A^{(0,0,2)} + A^{(0,0,3)}\right. \\ &\left.\left. + 12\gamma_0 A^{(0,1,1)} + 3A^{(0,1,2)} - 3A^{(0,2,1)} + 6A^{(1,1,1)}\right)\right) dt + O\left(T^{1/2+\varepsilon}\right)\end{aligned}$$

where the γ_m are the coefficients in the Laurent expansion of $\zeta(s)$ about $s = 1$ and the $A^{(i,j,k)}$ are arithmetic terms that are various products and sums over primes.

Much of this chapter is based on an upcoming paper, and will soon appear in [185]. Notation and cross-references have been updated for this thesis.

6.1 THE RATIOS CONJECTURE

The recipe of Conrey, Farmer, Keating, Rubinstein and Snaith [60] is used to calculate products of L-functions averaged over a family with full asymptotic formula with a power-saving error term. The Ratios Conjecture generalises the recipe to quotients of products of L-functions. The recipe was created through comparison with the analogous quantities for the characteristic polynomials of matrices averaged over classical compact groups [60], and various analogous RMT results for the Ratios Conjecture can be found in [63, 62, 36, 64, 180].

A conjecture of Farmer [112] states that for $s = \sigma + it$ and for complex shifts $\alpha, \beta, \gamma, \delta$ with small positive real parts,

$$\frac{1}{T}\int_0^T \frac{\zeta(s+\alpha)\zeta(1-s+\beta)}{\zeta(s+\gamma)\zeta(1-s+\delta)}\,dt \sim \frac{(\alpha+\delta)(\beta+\gamma)}{(\alpha+\beta)(\gamma+\delta)} - T^{-(\alpha+\beta)}\frac{(\alpha-\gamma)(\beta-\delta)}{(\alpha+\beta)(\gamma+\delta)}.$$

The Ratios Conjecture generalises Farmer's conjecture to quotients of an arbitrary number of L-functions averaged over a family, with a full asymptotic expansion and a power-saving error term in each case. It does so through a similar process to the recipe, with one extra step. In the first step of the Ratios Conjecture, for any L-function in the denominator, we replace it by its Dirichlet series, and carry on the recipe as usual. This is acceptable as under the (Generalised) Riemann Hypothesis, the Dirichlet series converges up to the critical line.

The reason we are so interested in the Ratios Conjecture is that it has numerous applications to a number of questions that arise from number theory. We give a brief overview of some of these applications below. Conrey and Snaith [87] go into a great deal of detail in their paper but we give a short summary of some of their results here. The versatility of the Ratios Conjecture allows us to recover many previously known or conjectured results, and often pushes these further.

Throughout the following subsections we assume the truth of both the Ratios Conjecture, and of the Riemann Hypothesis.

6.1.1 Pair Correlation and n-level Correlations

Farmer noted that his original conjecture implies the leading order terms of Montgomery's Pair Correlation Conjecture. The Ratios Conjecture can be used to calculate full asymptotics of all $n-$level correlations of zeros, as predicted heuristically by Bogomolny and Keating [30, 31], and stated by Rudnick and Sarnark [274] and later proved by them in [275], albeit in a restricted range.

As an example, Conrey and Snaith [87] explicitly calculate the full asymptotic for Pair Correlation, and show how one can recover the leading order behaviour, exactly as in Conjecture 1.3.

Additionally, Conrey and Snaith have found full asymptotics for other n-level correlations via the Ratios Conjecture, for example in [89, 88, 86].

6.1.2 Moments of Logarithmic Derivatives of the Riemann zeta function

Goldston, Gonek and Montgomery [141] considered a second continuous moment of the logartihmic derivative of the Riemann zeta function, and found an equivalence with it and Montgomery's Pair Correlation Conjecture. Using the Ratios Conjecture, lower order terms for such a problem were found. Higher moments are considered in [12, 139], and a weighted moment version is studied in [114]. Similarly, Farmer [112] considered discrete moments of the ratio $\zeta(\rho+\alpha)/\zeta(\rho+\beta)$ for small shifts α, β and obtained a leading order asymptotic. Using the Ratios Conjecture, Conrey, Farmer and Zirnbauer [63] found a full asymptotic for moments of this form.

6.1.3 Mollified Moments of L-functions

As we discussed in detail in Section 1.3.7.2, mollifying moments is used for computing information about zeros, for example for obtaining lower bounds for the proportion of zeros on the critical line as in 1.3.7.3, and as have seen in Section 1.4.3.1, for obtaining lower bounds for the proportion of simple zeros as in [75, 39].

Recall that when we want to perform a mollified moment calculation, we take our L-function and multiply it by a Dirichlet polynomial which acts as an approximation to the inverse of the L-function. As discussed in Section 1.3.7.3, mollifier calculations are generally very complicated. The Ratios Conjecture gives us a relatively simple way to obtain the relevant asymptotic formulae, and serves as a guide and goal to aim for. Recall that we described how Young [316] shortened Levinson's result that one-third of the zeros of $\zeta(s)$ lie on the critical line from 50 pages to 8 pages, using this idea.

These mollified calculations via the Ratios Conjecture also provide evidence that mean-value formulae, that can be proved for short mollifiers, remain true for long mollifiers. This gives more evidence for Farmer's $\theta = \infty$ conjecture. While we have assumed the Riemann Hypothesis in this section, these calculations retain their value.

6.1.4 Non-vanishing results for various families of L-functions

While we have not discussed other L-functions in much detail in this thesis, we note that the Ratios Conjecture can be used to show that the proportion of non-vanishing for

$L^{(k)}(1/2, \chi)$ approaches 100% as $k \to \infty$ for this family. The Ratios Conjecture can also be used to deduce results about the non-vanishing of automorphic L-functions, and with non-vanishing of Dirichlet L-functions for real quadratic characters, at the central point and on the real axis. For further reading see [201, 232, 289].

6.1.5 Discrete Moments of $\zeta(s)$ and Lower Order Terms

The Ratios Conjecture can be used to recover discrete moment results, with full asymptotic expansions. Conrey and Snaith [87] show how to obtain this asymptotic for the second moment, and in particular, preempted Milinovich's result [233], referred to in (1.33) (albeit in integral form), for the full asymptotic for the second discrete moment. In particular, they showed that assuming the Ratios Conjecture, we have

$$\sum_{0<\gamma\le T} |\zeta'(\rho)|^2 = \int_0^T \left(\frac{1}{24\pi}\left(\log\frac{t}{2\pi}\right)^4 + \frac{\gamma_0}{3\pi}\left(\log\frac{t}{2\pi}\right)^3 + \left(\frac{\gamma_0^2}{2\pi} - \frac{\gamma_1}{\pi}\right)\left(\log\frac{t}{2\pi}\right)^2 \right.$$
$$- \left(\frac{\gamma_0^3}{\pi} + \frac{5\gamma_0\gamma_1}{\pi} + \frac{\gamma_2}{2\pi}\right)\log\frac{t}{2\pi} + \left.\left(\frac{\gamma_0^4}{\pi} + \frac{6\gamma_0^2\gamma_1}{\pi} + \frac{7\gamma_1^2}{\pi} + \frac{4\gamma_0\gamma_2}{\pi} + \frac{5\gamma_3}{3\pi}\right)\right)$$
$$\times \left(1 + O\left(t^{-1/2+\varepsilon}\right)\right)\, dt.$$

Note that performing the integral recovers Gonek's [143] result to leading order. Milinovich's theorem [233] is proved in a different way but he obtains the same asymptotic which can be seen by computing the integral. Milinovich's asymptotic also follows from a result of Fujii's [127]. Note that none of these proofs require the Ratios Conjecture.

6.2 LOWER ORDER TERMS FOR MOMENTS OF THE DERIVATIVES OF THE RIEMANN ZETA FUNCTION

The aim of this chapter is to extend the Conjectures 5.3 and 5.4 to include the lower order terms with a power-saving error term. We do this by evaluating discrete moments of zeta with small shifts α_j. Throughout this chapter we assume that $|\Re(\alpha_j)| < \frac{1}{4}$ and $|\Im(\alpha_j)| \ll_\varepsilon T^{1-\varepsilon}$ for every $\varepsilon > 0$. We will also assume the Riemann Hypothesis.

Specifically, from the ratios methodology we will obtain the following conjecture.

Conjecture 6.3. *Assume the Riemann Hypothesis. For $|\delta| < 1/4$, let*

$$A_{\{\alpha_1,\ldots,\alpha_k\}}(\delta) := \prod_p \frac{1 + F_1(p,\delta) + F_2(p,\delta) + \cdots + F_k(p,\delta)}{(1-p^{-(1+\alpha_1)})\ldots(1-p^{-(1+\alpha_k)})} \tag{6.1}$$

where for $1 \le m \le k$

$$F_m(p,\delta) = (-1)^m \sum_{\substack{J\subset\{1,\ldots,k\}\\ |J|=m}} p^{-\left(m+(m-1)\delta+\sum_{j\in J}\alpha_j\right)}.$$

The discrete moments of shifts of $\zeta(s)$, evaluated at the non-trivial zeros $\rho = 1/2 + i\gamma$ of $\zeta(s)$, are given by

$$\sum_{0<\gamma\leq T} \zeta\left(\frac{1}{2}+i\gamma+\alpha_1\right)\dots\zeta\left(\frac{1}{2}+i\gamma+\alpha_k\right)$$
$$= \frac{1}{2\pi}\int_1^T \left(A'_{\{\alpha_1,\dots,\alpha_k\}}(0) + \sum_{j=1}^{k} W_{\{\alpha_1,\dots,\alpha_k\}\setminus\{\alpha_j\}}(\alpha_j,t)\right)\,dt + O\left(T^{1/2+\varepsilon}\right),$$

where

$$W_{\{\alpha_1,\dots,\alpha_k\}\setminus\{\alpha_j\}}(\alpha_j,t) = \frac{\zeta'(1+\alpha_j)}{\zeta(1+\alpha_j)}$$
$$- \left(\frac{t}{2\pi}\right)^{-\alpha_j}\zeta(1-\alpha_j)A_{\{\alpha_1,\dots\alpha_{j-1},0,\alpha_{j+1},\dots,\alpha_k\}}(-\alpha_j)\prod_{\substack{\ell=1\\ \ell\neq j}}^{k}\frac{\zeta(1+\alpha_\ell-\alpha_j)}{\zeta(1+\alpha_\ell)}.$$

Remark. Note that if $\delta = 0$ we write $F_m(p,0) = F_m(p)$, and in this case have

$$1 + F_1(p) + F_2(p) + \dots + F_k(p) = (1-p^{-(1+\alpha_1)})\dots(1-p^{-(1+\alpha_k)}),$$

so $A_{\{\alpha_1,\dots,\alpha_k\}}(0) = 1$.

Remark. To obtain the mixed derivative that we are interested in, Taylor expand each $\zeta(1/2 + i\gamma + a_j)$ about $a_j = 0$, take derivatives with respect to a_j and then set each α_j equal to zero.

Remark. As we previously discussed, the error term here can be contentious. While some authors prefer an error term of $O\left(T^{1-\delta}\right)$ for $0 < \delta < 1/2$, in this conjecture and our later examples, we suggest an error term of $O\left(T^{1/2+\varepsilon}\right)$, in keeping with the original statements of the recipe/Ratios Conjecture.

6.2.1 Preliminary Lemmas on Vandermonde Determinants

As part of our later calculations, a certain identity between Vandemonde determinants will prove useful.

Let

$$\Delta_k(\alpha_1,\dots,\alpha_k) = \det\begin{pmatrix} 1 & \alpha_1 & \alpha_1^2 & \dots & \alpha_1^{k-1} \\ 1 & \alpha_2 & \alpha_2^2 & \dots & \alpha_2^{k-1} \\ \vdots & \vdots & \vdots & \dots & \vdots \\ 1 & \alpha_k & \alpha_k^2 & \dots & \alpha_k^{k-1} \end{pmatrix}$$
$$= \prod_{1\leq i<j\leq k}(\alpha_j - \alpha_i)$$

denote the Vandermonde determinant with k parameters, and also let

$$\Delta_{k-1}(\alpha_1,\dots,\alpha_k;\alpha_\ell) = \prod_{\substack{1\le i<j\le k\\ i\neq\ell\\ j\neq\ell}} (\alpha_j-\alpha_i)$$

denote the Vandermonde determinant with the ℓ^{th} element removed.

Lemma 6.4. *For $k\in\mathbb{N}$ and $n\in\mathbb{Z}$, if $\alpha_1,\dots,\alpha_k\neq 0$ then*

$$\sum_{\ell=1}^{k}(-1)^{k+\ell}\Delta_{k-1}(\alpha_1,\dots,\alpha_k;\alpha_\ell)\,\alpha_\ell^{n-1}$$
$$= \begin{cases} \Delta_k(\alpha_1,\dots,\alpha_k) \displaystyle\sum_{\substack{n_1\ge0,\dots,n_k\ge0\\ n_1+\dots+n_k=n-k}} \alpha_1^{n_1}\alpha_2^{n_2}\dots\alpha_k^{n_k} & \text{if } n\ge k\\ 0 & \text{if } 1\le n\le k-1\\ (-1)^{k+1}\Delta_k(\alpha_1,\dots,\alpha_k) \displaystyle\sum_{\substack{n_1\ge0,\dots,n_k\ge0\\ n_1+\dots+n_k=|n|}} \alpha_1^{-n_1-1}\alpha_2^{-n_2-1}\dots\alpha_k^{-n_k-1} & \text{if } n\le 0. \end{cases}$$

Proof. Let

$$X = \sum_{\ell=1}^{k}(-1)^{k+\ell}\Delta_{k-1}(\alpha_1,\dots,\alpha_k;\alpha_\ell)\,\alpha_\ell^{n-1}.$$

Observe that X can be expressed as a determinant,

$$X = \det\begin{pmatrix} 1 & \alpha_1 & \alpha_1^2 & \dots & \alpha_1^{k-2} & \alpha_1^{n-1}\\ 1 & \alpha_2 & \alpha_2^2 & \dots & \alpha_2^{k-2} & \alpha_2^{n-1}\\ \vdots & \vdots & \vdots & \dots & \vdots & \vdots\\ 1 & \alpha_k & \alpha_k^2 & \dots & \alpha_k^{k-2} & \alpha_k^{n-1} \end{pmatrix}$$

where the terms in the last column are replaced by α_j^{n-1} (in the standard Vandermonde these terms would be α_j^{k-1}). Expanding the determinant down its last column, it is clear that it equals X.

Note that if $n\le k-1$ then the last column will be equal to one of the other columns in the matrix, and thus the determinant will be zero.

To complete the proof of the lemma, we now evaluate X in a different manner, via row manipulations.

Subtract the first row from all subsequent rows. Pull out a factor of $(\alpha_j-\alpha_1)$ from the j^{th} row (for $j\ge2$).

Then subtract the new second row from all subsequent rows, and pull out a factor of $(\alpha_j-\alpha_2)$ from the j^{th} row (for $j\ge3$ this time).

Repeat this process all the way down to subtracting what remains in the the $k-1^{\text{st}}$ row from what remains in the k^{th} row, and pulling out a factor of $(\alpha_k - \alpha_{k-1})$.

The terms that are factored out during this process are

$$\prod_{\ell=1}^{k-1} \prod_{j=\ell+1}^{k} (\alpha_j - \alpha_\ell) = \Delta_k(\alpha_1, \dots, \alpha_k)$$

and the remaining matrix determinant is

$$\det \begin{pmatrix} A_{1,1} & A_{1,2} & \dots & A_{1,k-1} & B_1 \\ A_{2,1} & A_{2,2} & \dots & A_{2,k-1} & B_2 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ A_{k,1} & A_{k,2} & \dots & A_{k,k-1} & B_k \end{pmatrix}$$

where

$$A_{\ell,m} = \sum_{\substack{n_1,\dots,n_\ell \geq 0 \\ n_1+\dots+n_\ell = m-\ell}} \alpha_1^{n_1} \dots \alpha_\ell^{n_\ell}$$

and where $B_\ell = A_{\ell,n}$ in the case $n \geq 1$, and in the case $n \leq 0$,

$$B_\ell = (-1)^{\ell+1} \sum_{\substack{n_1,\dots,n_\ell \geq 0 \\ n_1+\dots+n_\ell = |n|}} \alpha_1^{-n_1-1} \dots \alpha_\ell^{-n_\ell-1}.$$

Crucially note that $A_{\ell,m} = 0$ for $m < \ell$ and $A_{\ell,\ell} = 1$. This makes the determinant trivial to evaluate - the matrix is upper triangular, and so the determinant will equal B_k.

That is, we have shown that

$$X = \Delta_k(\alpha_1, \dots, \alpha_k) B_k$$

and this is the right-hand of the statement of the lemma. □

From this we can derive two useful combinatorial sums.

Lemma 6.5. *For $k \in \mathbb{N}$ and distinct nonzero $\alpha_1, \dots, \alpha_k \in \mathbb{C}$, we have*

$$\sum_{\ell=1}^{k} \frac{1}{\alpha_\ell} \prod_{\substack{j=1 \\ j \neq \ell}}^{k} \frac{\alpha_j}{(\alpha_j - \alpha_\ell)} = \sum_{\ell=1}^{k} \frac{1}{\alpha_\ell}.$$

Proof. From Lemma 6.4 with $n = -1$ we have

$$\sum_{\ell=1}^{k} (-1)^{k+\ell} \Delta_{k-1}(\alpha_1, \dots, \alpha_k; \alpha_\ell) \alpha_\ell^{-2} = (-1)^{k+1} \Delta_k(\alpha_1, \dots, \alpha_k) \frac{1}{\alpha_1 \dots \alpha_k} \sum_{\ell=1}^{k} \frac{1}{\alpha_\ell}.$$

Since the α_i are all distinct, Δ_k is nonzero, so dividing both sides by

$$(-1)^{k+1} \frac{\Delta_k(\alpha_1, \dots, \alpha_k)}{\alpha_1 \dots \alpha_k}$$

yields

$$\sum_{\ell=1}^{k} \frac{(-1)^{\ell-1}\Delta_{k-1}\left(\alpha_1,\dots,\alpha_k;\alpha_\ell\right)}{\Delta_k(\alpha_1,\dots,\alpha_k)} \frac{\alpha_1\dots\alpha_k}{\alpha_\ell^2} = \sum_{\ell=1}^{k} \frac{1}{\alpha_\ell}.$$

Note that

$$\frac{(-1)^{\ell-1}\Delta_{k-1}\left(\alpha_1,\dots,\alpha_k;\alpha_\ell\right)}{\Delta_k(\alpha_1,\dots,\alpha_k)} = \prod_{\substack{j=1\\ j\neq\ell}}^{k} \frac{1}{\alpha_j-\alpha_\ell}$$

where we observe that for $j = 1,\dots,\ell-1$ there are terms $\alpha_\ell - \alpha_j$ in the Vandermonde, whereas in the product on the RHS they are $\alpha_j - \alpha_\ell$, thus accounting for the $(-1)^{\ell-1}$ term). Therefore we have shown

$$\frac{(-1)^{\ell-1}\Delta_{k-1}\left(\alpha_1,\dots,\alpha_k;\alpha_\ell\right)}{\Delta_k(\alpha_1,\dots,\alpha_k)} \frac{\alpha_1\dots\alpha_k}{\alpha_\ell^2} = \frac{1}{\alpha_\ell}\prod_{\substack{j=1\\ j\neq\ell}}^{k} \frac{\alpha_j}{\alpha_j-\alpha_\ell}$$

as required. □

Lemma 6.6. *For distinct $\alpha_j \in \mathbb{C}$, for $n \in \mathbb{N}$ and $k \in \mathbb{N}$ we have*

$$\sum_{\ell=1}^{k} \alpha_\ell^n \prod_{\substack{j=1\\ j\neq\ell}}^{k} \frac{\alpha_j}{(\alpha_j-\alpha_\ell)} = \begin{cases} (-1)^{k+1} \displaystyle\sum_{\substack{n_1\geq1,\dots,n_k\geq1\\ n_1+\dots+n_k=n}} \alpha_1^{n_1}\alpha_2^{n_2}\dots\alpha_k^{n_k} & \text{if } n \geq k \\ 0 & \text{if } n < k. \end{cases}$$

Proof. As in the previous lemma, we multiply both sides of the statement of Lemma 6.4 for the case $n \geq 1$ by $\prod_{j=1}^k \alpha_j$, and divide by the Vandermonde determinant $\Delta_k(\alpha_1,\dots,\alpha_k)$. Again, note that the assumption that all the variables α_j are distinct means their Vandermonde determinant is non-zero, so this is a valid division.

On the left-hand side of Lemma 6.4 this yields terms such as

$$(-1)^{k+\ell}\frac{\Delta_{k-1}(\alpha_1,\dots,\alpha_k;\alpha_\ell)}{\Delta_k(\alpha_1,\dots,\alpha_k)}\alpha_\ell^{n-1}\prod_{j=1}^{k}\alpha_j = (-1)^{k-1}\alpha_\ell^n \prod_{\substack{j=1\\ j\neq\ell}}^{k} \frac{\alpha_j}{\alpha_j-\alpha_\ell}$$

and the effect on the right-hand side of Lemma 6.4 is that

$$\prod_{j=1}^{k}\alpha_j \sum_{\substack{n_1\geq0,\dots,n_k\geq0\\ n_1+\dots+n_k=n-k}} \alpha_1^{n_1}\alpha_2^{n_2}\dots\alpha_k^{n_k} = \sum_{\substack{n_1\geq1,\dots,n_k\geq1\\ n_1+\dots+n_k=n}} \alpha_1^{n_1}\alpha_2^{n_2}\dots\alpha_k^{n_k}$$

which yields the statement of this lemma, when we note that if $1 \leq n \leq k$ then the sum is empty, so equals 0. □

6.2.2 Deriving Conjecture 6.3

We are required to find

$$\sum_{0<\gamma\le T}\prod_{j=1}^{k}\zeta\left(\frac{1}{2}+i\gamma+\alpha_j\right)$$

where the α_j satisfy certain conditions as specified at the start of Section 6.2.

We may use Cauchy's theorem to write

$$\sum_{0<\gamma\le T}\prod_{j=1}^{k}\zeta\left(\frac{1}{2}+i\gamma+\alpha_j\right)=\frac{1}{2\pi i}\int_R\frac{\zeta'}{\zeta}(s)\zeta\left(s+\alpha_1\right)\ldots\zeta\left(s+\alpha_k\right)\,ds,$$

where R is a positively oriented rectangular contour with vertices $c+i$, $c+iT$, $1-c+iT$, and $1-c+i$, where $1/2<c<3/4$. For simplicity we assume that $|T-\gamma|\gg 1/\log T$ for any zero γ and T sufficiently large, although this constraint has no effect on the final answer.

One can prove that the bottom, right, and top sides of the contour do not contribute anything except to the error term, with the largest contribution coming from the top piece of the contour at $O\left(T^{1/2+\varepsilon}\right)$.

We use the functional equation of $\zeta(s)$ given in (1.1) to write

$$\frac{\zeta'}{\zeta}(s)=\frac{\chi'}{\chi}(s)-\frac{\zeta'}{\zeta}(1-s)$$

and rewrite the left-hand side of the contour. Again the part that comes from the $\chi'(s)/\chi(s)$ term is also small and only contributes to the error term.

Therefore we have shown that

$$\sum_{0<\gamma\le T}\prod_{j=1}^{k}\zeta\left(\frac{1}{2}+i\gamma+\alpha_j\right)=\frac{1}{2\pi i}\int_{c+i}^{c+iT}\frac{\zeta'}{\zeta}(s)\zeta(1-s+\alpha_1)\ldots\zeta(1-s+\alpha_k)\,ds+O\left(T^{1/2+\varepsilon}\right).$$

This integral can be rewritten as

$$\frac{d}{d\delta}\frac{1}{2\pi}\int_1^T\frac{\zeta(c+it+\delta)}{\zeta(c+it)}\zeta(1-c-it+\alpha_1)\ldots\zeta(1-c-it+\alpha_k)\,ds\Bigg|_{\delta=0}\tag{6.2}$$

for some small shift δ.

We now apply the recipe from the Ratios Conjecture. Step 1 tells us that for the $\zeta(s)$ term in the denominator, we replace it with its Dirichlet series

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

noting that, assuming the Riemann Hypothesis, this is conditionally convergent on the line of integration. Step 2 tells us that for any $\zeta(s)$ terms in the numerator, we replace them using the approximate functional equation

$$\zeta(s) = \sum_{n \le \sqrt{t/2\pi}} \frac{1}{n^s} + \chi(s) \sum_{n \le \sqrt{t/2\pi}} \frac{1}{n^{1-s}}$$

ignoring the error terms.

Step 3 of the Ratio's Conjecture tells us to now expand the numerator, yielding 2^{k+1} terms coming from picking either the sum without a χ factor or the sum with a χ factor in each zeta function.

For example, we can keep every term from each of the approximate functional equations without a $\chi(s)$ factor, which gives

$$\sum_m \frac{1}{n^{c+it+\delta}} \sum_{n_1} \frac{1}{n_1^{1-c-it+\alpha_1}} \cdots \sum_{n_k} \frac{1}{n_k^{1-c-it+\alpha_1}} \sum_h \frac{\mu(h)}{h^{c+it}}.$$

Step 4 tells us that when we integrate over t we want to keep only the "diagonal terms", which are the terms in the sum where there are no oscillations in t, namely where

$$mh = n_1 \dots n_k.$$

The ratios methodology assumes all the non-diagonal terms oscillate away, and so we are left with

$$\sum_{mh = n_1 \dots n_k} \frac{\mu(h)}{m^{1/2+\delta} h^{1/2} n_1^{1/2+\alpha_1} \dots n_k^{1/2+\alpha_k}}.$$

Since this sum is multiplicative, we may write this as an Euler product. Writing

$$n_j = p^{a_j}, m = p^c, h = p^d$$

we have

$$\prod_p \sum_{c+d = a_1 + \dots + a_k} \frac{\mu(p^d)}{p^{c(1/2+\delta)} p^{d(1/2)} p^{a_1(1/2+\alpha_1)} \dots p^{a_k(1/2+\alpha_k)}}.$$

We may only have $d = 0$ (in which case $\mu(1) = 1$), or $d = 1$ (in which case $\mu(p) = -1$).

Summing over both possibilities for d gives

$$\prod_p \sum_{a_1=0}^{\infty} \cdots \sum_{a_k=0}^{\infty} \frac{1}{p^{a_1(1+\alpha_1+\delta)}} \cdots \frac{1}{p^{a_k(1+\alpha_k+\delta)}} - \prod_p p^{\delta} \left(\sum_{a_1=0}^{\infty} \cdots \sum_{a_k=0}^{\infty} \frac{1}{p^{a_1(1+\alpha_1+\delta)}} \cdots \frac{1}{p^{a_k(1+\alpha_k+\delta)}} - 1 \right).$$

Factorising and using the sum of the geometric formula gives

$$\prod_p \frac{1}{1 - p^{-(1+\alpha_1+\delta)}} \cdots \frac{1}{1 - p^{-(1+\alpha_k+\delta)}} \left(1 - p^{\delta}(1 - (1 - p^{-(1+\alpha_1+\delta)}) \dots (1 - p^{-(1+\alpha_k+\delta)})\right).$$

The Euler product for $\zeta(s)$ allows us to rewrite this as

$$\zeta(1+\alpha_1+\delta)\dots\zeta(1+\alpha_k+\delta)$$
$$\prod_p \Big(1-p^{-(1+\alpha_1)}-\dots-p^{-(1+\alpha_k)}+p^{-(2+\alpha_1+\alpha_2+\delta)}+\dots+p^{-(2+\alpha_{k-1}+\alpha_k+\delta)}$$
$$+\dots+(-1)^k p^{-(k+\alpha_1+\dots+\alpha_k+(k-1)\delta)}\Big).$$

Finally, in Step 5, to make this product over primes converge we take out factors of $\zeta(1+\alpha_j)$ for each $j=1,\dots,k$. In doing so, we have

$$\frac{\zeta(1+\alpha_1+\delta)\dots\zeta(1+\alpha_k+\delta)}{\zeta(1+\alpha_1)\dots\zeta(1+\alpha_k)}\prod_p \frac{1-p^{-(1+\alpha_1)}+\dots+(-1)^k p^{-(k+\alpha_1+\dots+\alpha_k+(k-1)\delta)}}{(1-p^{-(1+\alpha_1)})\dots(1-p^{-(1+\alpha_k)})}$$
$$=: Z_{\alpha_1,\dots,\alpha_k,\delta}.$$

For later simplicity, noticing the symmetry in the parameters $\alpha_1,\dots,\alpha_k$, we will denote the product over primes in the previous line by

$$A_{\{\alpha_1,\dots,\alpha_k\}}(\delta) := \prod_p \frac{1-p^{-(1+\alpha_1)}+\dots+(-1)^k p^{-(k+\alpha_1+\dots+\alpha_k+(k-1)\delta)}}{(1-p^{-(1+\alpha_1)})\dots(1-p^{-(1+\alpha_k)})}.$$

We now return to the numerator in (6.2) when the zeta terms have been replaced by the appropriate approximate functional equation. The ratios methodology tells us to keep only the terms with an equal number of $\chi(s)$ and $\chi(1-s)$ terms, since all the other terms will be highly oscillatory, and hence are assumed to not contribute to the final answer.

Other than the case when there are no χ terms (dealt with above), it is clear from (6.2) that the only such terms will come from $\chi(c+it+\delta)$ and $\chi(1-c-it+\alpha_j)$ for each j.

Note that

$$\chi(c+it+\delta)\chi(1-c-it+\alpha_j) = \left(\frac{t}{2\pi}\right)^{-\delta-\alpha_j}\left(1+O\left(\frac{1}{|t|}\right)\right)$$

and the rest of the calculation (namely, the summing over the diagonal terms) proceeds as in the "no swap" case, given above. Thus the term arising from the swap of α_j with δ contributes

$$\left(\frac{t}{2\pi}\right)^{-\alpha_j-\delta} Z_{\alpha_1,\dots,\alpha_{j-1},-\delta,\alpha_{j+1},\dots,\alpha_k,-\alpha_j}.$$

Overall, we have

$$\sum_{0<\gamma\le T}\zeta\left(\frac{1}{2}+i\gamma+\alpha_1\right)\dots\zeta\left(\frac{1}{2}+i\gamma+\alpha_k\right)=$$
$$\frac{d}{d\delta}\frac{1}{2\pi}\int_1^T Z_{\alpha_1,\dots,\alpha_k,\delta}+\left(\frac{t}{2\pi}\right)^{-\alpha_1-\delta}Z_{-\delta,\alpha_2,\dots,\alpha_k,-\alpha_1}+\dots+\left(\frac{t}{2\pi}\right)^{-\alpha_k-\delta}Z_{\alpha_1,\dots,-\delta,-\alpha_k}\,dt\Bigg|_{\delta=0}$$
$$+O\left(T^{1/2+\varepsilon}\right), \quad (6.3)$$

where

$$Z_{\alpha_1,\ldots,\alpha_k,\delta}=\frac{\zeta(1+\alpha_1+\delta)\ldots\zeta(1+\alpha_k+\delta)}{\zeta(1+\alpha_1)\ldots\zeta(1+\alpha_k)}A_{\{\alpha_1,\ldots,\alpha_k\}}(\delta).$$

Remark. It is not obvious from inspection that the main term of (6.3) is holomorphic in terms of the shift parameters. However the symmetries of the expression imply that the poles cancel to form a holomorphic function. Lemma 6.7 of [63] exhibits an integral representation for the permutation sum that proves the holomorphy.

We proceed to pull the $\frac{d}{d\delta}$ inside the integral. Note that

$$\frac{d}{d\delta}Z_{\alpha_1,\ldots,\alpha_k,\delta}\Big|_{\delta=0}=A'_{\{\alpha_1,\ldots,\alpha_k\}}(0)+\sum_{j=1}^{k}\frac{\zeta'(1+\alpha_j)}{\zeta(1+\alpha_j)}$$

and due to the fact that $\frac{1}{\zeta(1-\delta)}\Big|_{\delta=0}=0$ and $\lim_{\delta\to 0}\frac{\zeta'}{\zeta^2}(1-\delta)=-1$ we have

$$\begin{aligned}&\frac{d}{d\delta}\left(\frac{t}{2\pi}\right)^{-\alpha_1-\delta}Z_{-\delta,\alpha_2,\ldots,\alpha_k,-\alpha_1}\Big|_{\delta=0}\\&=-\left(\frac{t}{2\pi}\right)^{-\alpha_1}Z_{0,\alpha_2,\ldots,\alpha_k,-\alpha_1}-\left(\frac{t}{2\pi}\right)^{-\alpha_1}\zeta(1-\alpha_1)A_{\{0,\alpha_2,\ldots,\alpha_k\}}(-\alpha_1)\prod_{j=2}^{k}\frac{\zeta(1+\alpha_j-\alpha_1)}{\zeta(1+\alpha_j)}\\&=-\left(\frac{t}{2\pi}\right)^{-\alpha_1}\zeta(1-\alpha_1)A_{\{0,\alpha_2,\ldots,\alpha_k\}}(-\alpha_1)\prod_{j=2}^{k}\frac{\zeta(1+\alpha_j-\alpha_1)}{\zeta(1+\alpha_j)}\end{aligned}$$

where the first term in the second line vanishes (again due to the fact that $\frac{1}{\zeta(1-\delta)}\Big|_{\delta=0}=0$). Therefore, if we let

$$\begin{aligned}W_{\{\alpha_1,\ldots,\alpha_k\}\backslash\{\alpha_j\}}(\alpha_j,t)&=\frac{\zeta'(1+\alpha_j)}{\zeta(1+\alpha_j)}\\&-\left(\frac{t}{2\pi}\right)^{-\alpha_j}\zeta(1-\alpha_j)A_{\{\alpha_1,\ldots\alpha_{j-1},0,\alpha_{j+1},\ldots,\alpha_k\}}(-\alpha_j)\prod_{\substack{\ell=1\\ \ell\neq j}}^{k}\frac{\zeta(1+\alpha_\ell-\alpha_j)}{\zeta(1+\alpha_\ell)}\end{aligned}$$

then we see that the Ratios Conjecture yields

$$\begin{aligned}&\sum_{0<\gamma\leq T}\zeta\left(\frac{1}{2}+i\gamma+\alpha_1\right)\ldots\zeta\left(\frac{1}{2}+i\gamma+\alpha_k\right)=\\&=\frac{1}{2\pi}\int_1^T\left(A'_{\{\alpha_1,\ldots,\alpha_k\}}(0)+\sum_{j=1}^{k}W_{\{\alpha_1,\ldots,\alpha_k\}\backslash\{\alpha_j\}}(\alpha_j,t)\right)dt+O\left(T^{1/2+\varepsilon}\right),\quad(6.4)\end{aligned}$$

which is Conjecture 6.3.

6.2.3 Recovering Conjectures 5.3 and 5.4

We aim to find the coefficient of $\alpha_1^{n_1} \dots \alpha_k^{n_k}$, or rather its leading order in term of the largest power of $L = \log \frac{t}{2\pi}$. We will follow the Ratios methodology, which is to replace each arithetmic piece by its leading order, which in our case means

$$A_{\{\alpha_1,\dots,\alpha_k\}}(0) \sim 1.$$

We also replace each zeta function by its expansion about its pole, that is,

$$\zeta(1+x) = \frac{1}{x} + O(1).$$

Then we can write

$$\frac{\zeta'}{\zeta}(1+x) = -\frac{1}{x} + O(1).$$

Writing $L = \log \frac{t}{2\pi}$ we have

$$\left(\frac{t}{2\pi}\right)^{-\alpha_1} = 1 - L\alpha_1 + \frac{1}{2!}L^2\alpha_1^2 + \dots.$$

Combing all this, we have shown that

$$W_{\{\alpha_1,\dots,\alpha_k\}\setminus\{\alpha_\ell\}}(\alpha_\ell, t) \sim -\frac{1}{\alpha_\ell} + \left(1 - L\alpha_1 + \frac{1}{2!}L^2\alpha_1^2 + \dots\right)\frac{1}{\alpha_\ell}\prod_{\substack{1\le j\le k\\ j\ne\ell}}\frac{\alpha_j}{\alpha_j - \alpha_\ell}.$$

Returning to (6.4), we see that

$$\begin{aligned}
&\sum_{0<\gamma\le T}\zeta\left(\frac{1}{2} + i\gamma + \alpha_1\right)\dots\zeta\left(\frac{1}{2} + i\gamma + \alpha_k\right)\\
&= \frac{1}{2\pi}\int_1^T \left(A'_{\{\alpha_1,\dots,\alpha_k\}}(0) + \sum_{\ell=1}^k W_{\{\alpha_1,\dots,\alpha_k\}\setminus\{\alpha_\ell\}}(\alpha_\ell, t)\right)\, dt + O\left(T^{1/2+\varepsilon}\right)\\
&\sim \frac{1}{2\pi}\int_1^T -\sum_{\ell=1}^k \frac{1}{\alpha_\ell} + \sum_{\ell=1}^k\left(1 - L\alpha_1 + \frac{1}{2!}L^2\alpha_1^2 + \dots\right)\frac{1}{\alpha_\ell}\prod_{\substack{1\le j\le k\\ j\ne\ell}}\frac{\alpha_j}{\alpha_j-\alpha_\ell}\, dt.
\end{aligned}$$

We can now see by Lemma 6.5 that the poles from the sums over ℓ, where we take the 1-term in the bracket containing the logarithms, cancels perfectly. This means that we have to evaluate

$$\begin{aligned}
&\sum_{0<\gamma\le T}\zeta\left(\frac{1}{2} + i\gamma + \alpha_1\right)\dots\zeta\left(\frac{1}{2} + i\gamma + \alpha_k\right)\\
&\qquad\sim \frac{1}{2\pi}\int_1^T \sum_{\ell=1}^k\left(-L\alpha_1 + \frac{1}{2!}L^2\alpha_1^2 + \dots\right)\frac{1}{\alpha_\ell}\prod_{\substack{1\le j\le k\\ j\ne\ell}}\frac{\alpha_j}{\alpha_j-\alpha_\ell}\, dt.
\end{aligned}$$

To find the coefficient of the α_ℓ^n term, say, we need to take the $(-1)^{n+1}\alpha_\ell^{n+1}/(n+1)!$ term for each α_ℓ from the bracket containing the logarithms, as one α_ℓ will cancel with the one in the denominator for each ℓ. Summing over all such ℓ, we have

$$\sum_{0<\gamma\leq T} \zeta\left(\frac{1}{2}+i\gamma+\alpha_1\right)\dots\zeta\left(\frac{1}{2}+i\gamma+\alpha_k\right) \sim \frac{1}{2\pi}\int_1^T \left(\frac{(-1)^{n+1}}{(n+1)!}L^{n+1}\right)\sum_{\ell=1}^k \alpha_\ell^n \prod_{\substack{j=1\\ j\neq\ell}}^k \frac{\alpha_j}{\alpha_j-\alpha_\ell}\,dt.$$

By Lemma 6.6, for $n \geq k$, this is

$$\sum_{0<\gamma\leq T} \zeta\left(\frac{1}{2}+i\gamma+\alpha_1\right)\dots\zeta\left(\frac{1}{2}+i\gamma+\alpha_k\right) \sim \frac{1}{2\pi}\int_1^T \left(\frac{(-1)^{n+1}}{(n+1)!}L^{n+1}\right)(-1)^{k+1}\sum_{\substack{n_1\geq 1,\dots,n_k\geq 1\\ n_1+\dots+n_k=n}} \alpha_1^{n_1}\alpha_2^{n_2}\dots\alpha_k^{n_k}\,dt.$$

Since $n = n_1 + \dots n_k$, we have

$$\sum_{0<\gamma\leq T} \zeta\left(\frac{1}{2}+i\gamma+\alpha_1\right)\dots\zeta\left(\frac{1}{2}+i\gamma+\alpha_k\right) \sim \frac{1}{2\pi}\int_1^T \left(\frac{(-1)^{n_1+\dots n_k+k}}{(n_1+\dots n_k+1)!}L^{n_1+\dots n_k+1}\right)\sum_{\substack{n_1\geq 1,\dots,n_k\geq 1\\ n_1+\dots+n_k=n}} \alpha_1^{n_1}\alpha_2^{n_2}\dots\alpha_k^{n_k}\,dt.$$

Finally, Taylor expand the left-hand side around each α_ℓ, differentiate with respect of each α_ℓ n_ℓ-times and set $\alpha_\ell = 0$. Multiplying through by n_ℓ for each ℓ gives

$$\sum_{0<\gamma\leq T} \zeta^{(n_1)}\left(\frac{1}{2}+i\gamma\right)\dots\zeta^{(n_k)}\left(\frac{1}{2}+i\gamma\right) \sim \frac{1}{2\pi}\int_1^T \left((-1)^{n_1+\dots n_k+k}\frac{n_1!\dots n_k!}{(n_1+\dots n_k+1)!}L^{n_1+\dots n_k+1}\right)\,dt.$$

Integrating gives Conjecture 5.3 and additionally, setting all n_ℓ equal to n gives Conjecture 5.4.

6.2.4 EXAMPLES

6.2.4.1 Recovering the Shanks' conjecture asymptotic ($k = 1$)

For the case $k = 1$ we will recover the full Generalised Shanks' Conjecture in an integral form, including the lower order terms, which is equivalent to the asymptotic found in Chapter 3 and in [186] for all derivatives.

By Conjecture 6.3 we can write

$$\sum_{0<\gamma\leq T} \zeta\left(\frac{1}{2}+i\gamma+\alpha\right) = \frac{1}{2\pi}\int_1^T \left(A'_{\{\alpha\}}(0)+W(\alpha,t)\right)\, dt + O\left(T^{1/2+\varepsilon}\right) \tag{6.5}$$

where

$$W(\alpha,t) = \frac{\zeta'(1+\alpha)}{\zeta(1+\alpha)} - \left(\frac{t}{2\pi}\right)^{-\alpha}\zeta(1-\alpha)A_{\{0\}}(-\alpha).$$

Now by (6.1), we see that

$$A_{\{\alpha\}}(0) = \prod_p \frac{(1-p^{-(1+\alpha)})}{(1-p^{-(1+\alpha)})} = 1$$

and so $A'_{\{\alpha\}}(0)=0$. Then (6.5) can be simplified to

$$\sum_{0<\gamma\leq T} \zeta\left(\frac{1}{2}+i\gamma+\alpha\right) = \frac{1}{2\pi}\int_1^T \left(\frac{\zeta'(1+\alpha)}{\zeta(1+\alpha)} - \left(\frac{t}{2\pi}\right)^{-\alpha}\zeta(1-\alpha)\right) dt + O\left(T^{1/2+\varepsilon}\right). \tag{6.6}$$

The Laurent expansion for $\frac{\zeta'(1+\alpha)}{\zeta(1+\alpha)}$ about $\alpha=0$ is given by

$$\frac{\zeta'(1+\alpha)}{\zeta(1+\alpha)} = -\frac{1}{\alpha} + \sum_{j=0}^{\infty} A_j\alpha^j,$$

the Laurent expansion for $-\zeta(1-\alpha)$ about $\alpha=0$ gives

$$-\zeta(1-\alpha) = \frac{1}{\alpha} - \sum_{j=0}^{\infty}\frac{\gamma_j}{j!}\alpha^j,$$

and the Taylor expansion of $(t/2\pi)^{-\alpha}$ about $\alpha=0$ gives

$$\left(\frac{t}{2\pi}\right)^{-\alpha} = \sum_{j=0}^{\infty}\frac{(-1)^j\alpha^jL^j}{j!},$$

where $L=\log(t/2\pi)$, the γ_j are the Stieltjes coefficients from the expansion of $\zeta(s)$ about $s=1$, and A_n is the n^{th} coefficient from the expansion of $\zeta'(s)/\zeta(s)$ about $s=1$.

Substitute these series into (6.6) and simplify to give

$$\begin{aligned}
&\sum_{0<\gamma\leq T} \zeta\left(\frac{1}{2}+i\gamma+\alpha\right) \\
&= \frac{1}{2\pi}\int_1^T \left(-\frac{1}{\alpha}+\sum_{j=0}^{\infty}A_j\alpha^j\right) + \left(\sum_{j=0}^{\infty}\frac{(-1)^j\alpha^jL^j}{j!}\right)\left(\frac{1}{\alpha}-\sum_{j=0}^{\infty}\frac{\gamma_j}{j!}\alpha^j\right)\, dt + O\left(T^{1/2+\varepsilon}\right) \\
&= \frac{1}{2\pi}\int_1^T \sum_{j=0}^{\infty}A_j\alpha^j + \sum_{j=1}^{\infty}\frac{(-1)^jL^j\alpha^{j-1}}{j!} + \sum_{j=0}^{\infty}\sum_{m=0}^{j}\frac{(-1)^{m+1}L^m\gamma_{j-m}\alpha^j}{m!(j-m)!}\, dt + O\left(T^{1/2+\varepsilon}\right).
\end{aligned}$$

For the general n^{th} derivative of $\zeta(s)$, where $n \in \mathbb{N}$, we have after Taylor expanding $\zeta(\rho+\alpha)$ about $\alpha = 0$, differentiating n times, setting $\alpha = 0$, and multiplying through by $n!$,

$$\sum_{0<\gamma\leq T} \zeta^{(n)}\left(\frac{1}{2}+i\gamma\right) = \frac{n!}{2\pi}\int_1^T A_n + \frac{(-1)^{n+1}L^{n+1}}{(n+1)!} + \sum_{m=0}^{n} \frac{(-1)^{m+1}L^m\gamma_{n-m}}{m!(n-m)!}\, dt + O\left(T^{1/2+\varepsilon}\right),$$

which is equivalent to Theorem 3.1 from Chapter 3 and from Hughes and Pearce-Crump [186].

6.2.4.2 *The second moment of $\zeta'(1/2+i\gamma)$ $(k=2)$*

To calculate the full asymptotic for the second moment of the first derivative of the Riemann zeta function, begin with Conjecture 6.3 with two shifts α, β to write

$$\begin{aligned}
&\sum_{0<\gamma\leq T} \zeta\left(\frac{1}{2}+i\gamma+\alpha\right)\zeta\left(\frac{1}{2}+i\gamma+\beta\right) \\
&= \frac{1}{2\pi}\int_1^T \Bigg(A'_{\{\alpha,\beta\}}(0) + \frac{\zeta'(1+\alpha)}{\zeta(1+\alpha)} - \left(\frac{t}{2\pi}\right)^{-\alpha}\zeta(1-\alpha)A_{\{0,\beta\}}(-\alpha)\frac{\zeta(1+\beta-\alpha)}{\zeta(1+\beta)} \\
&\qquad + \frac{\zeta'(1+\beta)}{\zeta(1+\beta)} - \left(\frac{t}{2\pi}\right)^{-\beta}\zeta(1-\beta)A_{\{\alpha,0\}}(-\beta)\frac{\zeta(1+\alpha-\beta)}{\zeta(1+\alpha)}\Bigg)\, dt \\
&\qquad + O\left(T^{1/2+\varepsilon}\right).
\end{aligned}$$

Note that by (6.1) we have that the arithmetic part can be written as

$$A_{\{\alpha,\beta\}}(\delta) = \prod_p \frac{1-p^{-(1+\alpha)}-p^{-(1+\beta)}+p^{-(2+\alpha+\beta+\delta)}}{\left(1-p^{-(1+\alpha)}\right)\left(1-p^{-(1+\beta)}\right)}.$$

By adding 'zero', we have

$$\begin{aligned}
A_{\{\alpha,\beta\}}(\delta) &= \prod_p \frac{1-p^{-(1+\alpha)}-p^{-(1+\beta)}+p^{-(2+\alpha+\beta)}}{\left(1-p^{-(1+\alpha)}\right)\left(1-p^{-(1+\beta)}\right)} + \prod_p \frac{p^{-(2+\alpha+\beta+\delta)}-p^{-(2+\alpha+\beta)}}{\left(1-p^{-(1+\alpha)}\right)\left(1-p^{-(1+\beta)}\right)} \\
&= 1 + \prod_p \frac{p^{-(2+\alpha+\beta+\delta)}-p^{-(2+\alpha+\beta)}}{\left(1-p^{-(1+\alpha)}\right)\left(1-p^{-(1+\beta)}\right)} \qquad (6.7)
\end{aligned}$$

which is the in a nicer form to work with.

We now employ a computer package to perform the expansions. We substitute the Laurent expansion for $\zeta(s)$ about $s=1$, which is where the various Stieltjes constants have come from.

Then for $L = \log \frac{t}{2\pi}$ and $\rho = 1/2 + i\gamma$ a non-trivial zero of the Riemann zeta function,

$$\sum_{0<\gamma\leq T} \zeta'\left(\frac{1}{2}+i\gamma\right)^2 =$$
$$\frac{1}{2\pi}\int_1^T \Bigg(\frac{1}{6}L^3 A^{(0,0,0)} + \frac{1}{2}L^2\left(2\gamma_0 A^{(0,0,0)} + A^{(0,0,1)} + A^{(0,1,0)}\right)$$
$$+\frac{1}{2}L\left(-8\gamma_1 A^{(0,0,0)} + 4\gamma_0 A^{(0,0,1)} + A^{(0,0,2)} + 4\gamma_0 A^{(0,1,0)} + 2A^{(0,1,1)} - A^{(0,2,0)}\right)$$
$$+\frac{1}{6}\Big(-12\gamma_0^3 A^{(0,0,0)} - 36\gamma_0\gamma_1 A^{(0,0,0)} + 6\gamma_2 A^{(0,0,0)} - 24\gamma_1 A^{(0,0,1)}$$
$$+6\gamma_0 A^{(0,0,2)} + A^{(0,0,3)} + 12\gamma_0 A^{(0,1,1)} + 3A^{(0,1,2)} - 3A^{(0,2,1)} + 6A^{(1,1,1)}$$
$$-12\gamma_1 A^{(0,1,0)} - 12\gamma_1 A^{(1,0,0)} + 6\gamma_0^2 A^{(0,1,0)} - 6\gamma_0 A^{(0,2,0)} + A^{(0,3,0)} - 3A^{(2,1,0)}$$
$$-6\gamma_0^2 A^{(1,0,0)} + 12\gamma_0 A^{(1,1,0)} - 3A^{(1,2,0)}\, dt\Big)\Bigg) + O\left(T^{1/2+\varepsilon}\right) \tag{6.8}$$

where the γ_m are the coefficients in the Laurent expansion of $\zeta(s)$ about $s = 1$ and the $A^{(i,j,k)}$ terms are various products over primes, where we are using the notation

$$A^{(i,j,k)} = \frac{\partial^i}{\partial\alpha^i}\frac{\partial^j}{\partial\beta^j}\frac{\partial^k}{\partial\delta^k}A_{\{\alpha,\beta\}}(\delta)\Bigg|_{\alpha=\beta=\delta=0}$$

for complex numbers (shifts) α, β, δ satisfying the conditions of Conjecture 6.3.

We now simplify this result to state a final version of the conjecture for this moment. Clearly, say from (6.7), if we do not differentiate with respect to δ and set $\delta = 0$, then the arithmetic piece equals 1. If we then differentiate with respect to α or β, and then set these equal to 0, these terms disappear. That is, for $i, j > 0$,

$$A^{(i,j,0)} = 0,$$

while if we don't differentiate at all (that is, $i = j = k = 0$) and set $\alpha, \beta, \delta = 0$, we have

$$A^{(0,0,0)} = 1.$$

It is also clear that the arithmetic piece is symmetric in the first two derivatives, so

$$A^{(i,j,k)} = A^{(j,i,k)}.$$

This means that whenever we see these terms, we can combine them together which is why the conjecture does not appear symmetric in i, j, k.

After using these rules for $A^{(i,j,k)}$, we form the conjecture for the second moment of the first derivative of the Riemann zeta function.

Conjecture. *Assume the Riemann Hypothesis. For $L = \log \frac{t}{2\pi}$ and $\rho = 1/2 + i\gamma$ a non-trivial zero of the Riemann zeta function,*

$$\sum_{0<\gamma\leq T} \zeta'\left(\frac{1}{2}+i\gamma\right)^2 =$$
$$\frac{1}{2\pi}\int_1^T \left(\frac{1}{6}L^3 + \frac{1}{2}L^2\left(2\gamma_0 + A^{(0,0,1)}\right) + \frac{1}{2}L\left(-8\gamma_1 + 4\gamma_0 A^{(0,0,1)} + A^{(0,0,2)} + 2A^{(0,1,1)}\right)\right.$$
$$+\frac{1}{6}\left(-12\gamma_0^3 - 36\gamma_0\gamma_1 + 6\gamma_2 - 24\gamma_1 A^{(0,0,1)} + 6\gamma_0 A^{(0,0,2)} + A^{(0,0,3)}\right.$$
$$\left.\left.+12\gamma_0 A^{(0,1,1)} + 3A^{(0,1,2)} - 3A^{(0,2,1)} + 6A^{(1,1,1)}\right)dt + O\left(T^{1/2+\varepsilon}\right)$$

where the γ_m are the coefficients in the Laurent expansion of $\zeta(s)$ about $s = 1$ and the $A^{(i,j,k)}$ are arithmetic terms that are various products and sums over primes.

We present some numerical evidence. To generate these numerics, we again use a computer package and describe how we have done so. Most of the calculations are standard so we just describe how to calculate the arithmetic pieces and so the full polynomial that appears in the integral version of this moment.

We begin by taking logarithms of the arithmetic pieces $A_{\{\alpha,\beta\}}(\delta)$ and expand it as a series about $\alpha, \beta, \delta = 0$, which we can do as they are all small by assumption. Note that since the highest derivative that we need to take is the third derivative for any of α, β, δ, we don't need to expand beyond the third powers. We then sum this expansion for the first 1000 prime numbers (note that for higher accuracy we could have done this calculation for more primes but at a higher computational cost - this would've generated better numerics and would be of future interest).

In doing these calculations, we have

$$\sum_{0<\gamma\leq T} \zeta'\left(\frac{1}{2}+i\gamma\right)^2 = \frac{1}{2\pi}\int_1^T \left(\frac{1}{6}L^3 - 0.03621L^2 + 2.12487L - 2.52789\right)dt + O\left(T^{1/2+\varepsilon}\right).$$

After integrating, we have

$$\sum_{0<\gamma\leq T} \zeta'\left(\frac{1}{2}+i\gamma\right)^2 = \frac{1}{6}\frac{T}{2\pi}\left(\log\frac{T}{2\pi}\right)^3 - 0.52037\frac{T}{2\pi}\left(\log\frac{T}{2\pi}\right)^2$$
$$+ 2.95321\frac{T}{2\pi}\left(\log\frac{T}{2\pi}\right) - 4.65238\frac{T}{2\pi} + O\left(T^{1/2+\varepsilon}\right).$$

We are now in a place to compare our theoretical conjecture with the true numerics of the $\sum_{0<\gamma\leq T}\zeta'(1/2+i\gamma)^2$, where we ignore the small imaginary part.

We begin by plotting the real part of the cumulative total of the sum $\sum_{0<\gamma\leq T}\zeta'(1/2+i\gamma)^2$ for the first 1,000,000 zeros, given in Figure 6.1. Numerically we can show that the imaginary part is small and so don't plot this in the following figures (which agrees with our conjecture only containing real terms in the asymptotic).

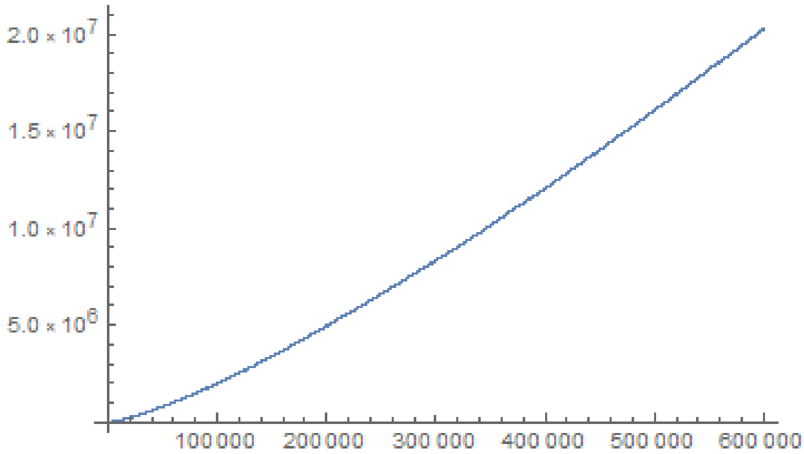

Figure 6.1: The real part of the true value of $\sum_{0<\gamma\leq T}\zeta'(1/2+i\gamma)^2$, for T up to the height of the 1,000,000$^{\text{th}}$ zero.

In Figure 6.2 we have subtracted the main term, which shows a decrease in size of an order of magnitude, and also shows a sign change suggesting that we have the correct leading order behaviour.

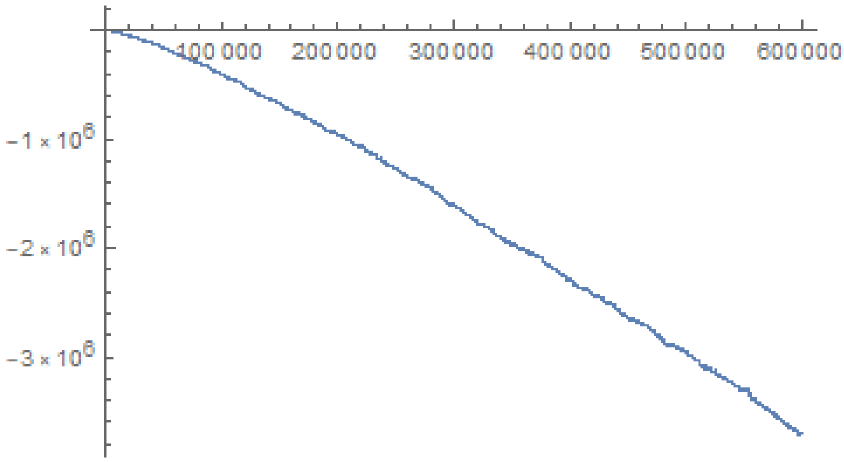

Figure 6.2: Difference in the real part of the actual value of $\sum_{0<\gamma\leq T}\zeta'(1/2+i\gamma)^2$ and the leading asymptotic result of the equation, for T up to the height of the 1,000,000$^{\text{th}}$ zero.

Finally, in Figure 6.3 we plot the sum over zeros minus all the remaining terms in the asymptotic expansion, leaving the error term. The arithmetic pieces are calculated for the first 1000 primes. Clearly there is excellent agreement, with a very small error compared with the original cumulative sum.

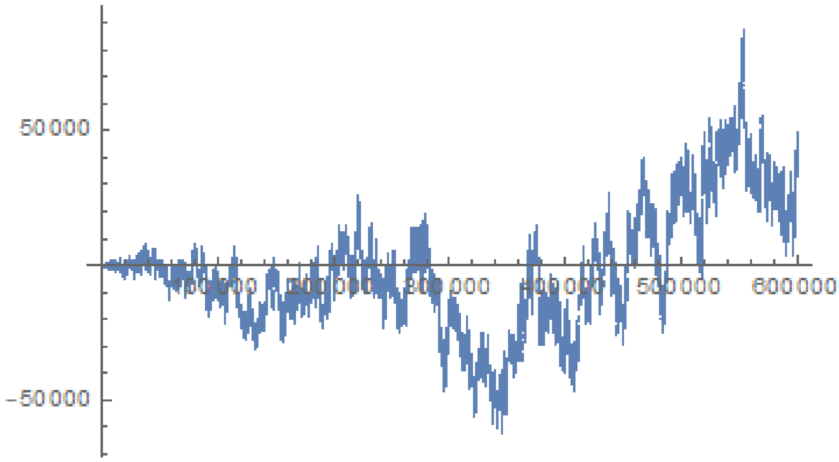

Figure 6.3: Difference in the real part of the actual value of $\sum_{0<\gamma\leq T}\zeta'(1/2+i\gamma)^2$ and the whole asymptotic result of the equation, for T up to the height of the 1,000,000$^{\text{th}}$ zero, showing the real error at each point.

Remark. As we have already remarked in this chapter, the error term here could plausibly be of size $O\left(T^{1-\delta}\right)$ for $0<\delta<1/2$, rather than of size $O\left(T^{1/2+\varepsilon}\right)$. While we do not rule out the possibility of the first option, as discussed earlier, we have settled on this second option, in keeping with the original statements of the recipe/Ratios Conjecture.

— 7 —

Moments of the Riemann zeta function at its local extrema

In this chapter we assume the Riemann Hypothesis, unless otherwise stated.

Recall that under the Riemann Hypothesis, Conrey and Ghosh [66] showed that

$$\sum_{0<\gamma\leq T} \max_{\gamma\leq t\leq\gamma^+} \left|\zeta\left(\frac{1}{2}+it\right)\right|^2 \sim \frac{e^2-5}{4\pi} T(\log T)^2 \tag{7.1}$$

as $T\to\infty$ where for each non-trivial zero $\rho = 1/2 + i\gamma$, let γ^+ denote the successive ordinate of a non-trivial zero of $\zeta(s)$.

In [183], Hughes, Lugmayer and Pearce-Crump calculated the full asymptotic expansion of (7.1), showing that under the Riemann Hypothesis, for K a positive integer, that

$$\begin{aligned}\sum_{0<\gamma\leq T} \max_{\gamma\leq t\leq\gamma^+} \left|\zeta\left(\frac{1}{2}+it\right)\right|^2 &= \frac{e^2-5}{2}\frac{T}{2\pi}\left(\log\frac{T}{2\pi}\right)^2 \\ &+ \left(5-e^2-10\gamma_0+2e^2\gamma_0\right)\frac{T}{2\pi}\log\frac{T}{2\pi} + \frac{T}{2\pi}\sum_{k=0}^{K}\frac{c_k}{(\log T/2\pi)^k} \\ &+ O_K\left(\frac{T}{(\log T)^{K+1}}\right)\end{aligned} \tag{7.2}$$

where γ_0 is Euler's constant and the other constants c_k are effectively computable constants.

Note that we can rewrite (7.1) and (7.2) in terms of the Hardy Z-function. Specifically, under the Riemann Hypothesis, we can rewrite the result of Conrey and Ghosh [66] as

$$\sum_{0<\lambda\leq T} Z(\lambda)^2 \sim \frac{e^2-5}{4\pi} T(\log T)^2 \tag{7.3}$$

as $T\to\infty$, where we recall that the points λ that are being summed over are the zeros of the derivative of the Hardy Z-function, described in Section 1.3.8.1, up to a height T.

In this section we combine some of the results presented in this thesis with these asymptotics, specifically equations (7.1) and (2.4), or rather the full asymptotic expansions given in (7.2) and Theorem 3.1. That is, under the Riemann Hypothesis, we calculate full asymptotics for the moments

$$\sum_{0<\lambda\leq T} \zeta^{(n)}\left(\frac{1}{2}+i\lambda\right)$$

where the sum is over the maxima of $|\zeta(s)|$ up to a height T, or equivalently, over those points λ such that $Z'(\lambda)=0$, where $Z(t)$ is the Hardy Z-function, up to a height T. This sum is considered for all non-negative integers n (specifically including the no derivative case which is non-trivial, compared with our previous sums over non-trivial zeros).

In addition, we also consider sums of the factor $\chi(s)$ from the non-symmetric functional equation for $\zeta(s)$ given in (1.1). These sums are considered both over the maxima of $|\zeta(s)|$ and over the non-trivial zeros of the Riemann zeta function.

We will also compare the results in this chapter with those from Chapter 3, specifically Theorem 3.1. In these comparisons we don't give many reasons beyond the obvious (that we are summing over different points/summing different functions), but the differences are worth pointing out explicitly in the remarks that follow the results. The actual, full reasons for these differences are of further interest and worth exploring.

The work presented in Section 7.1 has already appeared in print in [263]. Notation and cross-references have been updated for this thesis.

7.1 MOMENTS OF $\zeta(s)$, ITS DERIVATIVES, AND $\chi(s)$ AT THE LOCAL EXTREMA OF THE RIEMANN ZETA FUNCTION

We now state the results that are to be proved in this chapter. There are four main results that we prove (with one simple corollary).

The first two results (along with the corollary) involve moments of the derivatives of the Riemann zeta function, evaluated at the local extrema of the Riemann zeta function (recall, equivalently, at the zeros of the derivative of the Hardy Z-function). We split the cases of derivatives and no derivatives into two separate results, both for clarity of the results and as the proofs are slightly different. The no derivative case is non-trivial, compared with typical moments where the sums are over non-trivial zeros of the Riemann zeta function.

For the second pair of results, we evaluate the sum of the factor $\chi(s)$ from the functional equation (1.1) for $\zeta(s)$ over the local extrema of the Riemann zeta function and over the non-trivial zeros of the Riemann zeta function.

Theorem 7.1. *Assume the Riemann Hypothesis. Write $L = \log T/2\pi$. For λ defined by $Z'(\lambda) = 0$ and $K, n \geq 1$ positive integers, we have*

$$\sum_{0<\lambda\leq T} \zeta^{(n)}\left(\frac{1}{2}+i\lambda\right) = a_{n+1}\frac{T}{2\pi}L^{n+1} + \frac{T}{2\pi}\sum_{\ell=0}^{n} a_{n-\ell}L^{n-\ell} + \frac{T}{2\pi}\sum_{m=1}^{K}\frac{b_m}{L^m} + O\left(\frac{T}{L^{K+1}}\right),$$

as $T \to \infty$ where:

1. *The leading order coefficient is given by*

$$a_{n+1} = (-1)^n\left(\frac{e^2-2}{n+1} + (-1)^{n+1}\frac{n!}{2^{n+1}}\left(1 - e^2\sum_{k=0}^{n+1}\frac{(-2)^k}{k!}\right)\right).$$

2. *The subleading, non-negative logarithm power coefficients are given by*

$$\begin{aligned} a_{n-\ell} = (-1)^n \sum_{k=1}^{\infty} 2^k \sum_{j=0}^{n}\binom{n}{j}\Bigg[&\frac{c_{\ell+1}^{k,j}}{(k+j-\ell)!} + (k-n+j)\frac{c_{\ell}^{k,j}}{(k+j+1-\ell)!} \\ &+ (k-n+j)\sum_{m=0}^{\ell-1}(-1)^{\ell-m}(n-m)\ldots(n-\ell+1)\frac{c_m^{k,j}}{(k+j+1-m)!}\Bigg] \\ +(-1)^{n+1}\sum_{\ell=0}^{n}\binom{n}{\ell}(-1)^{\ell}\ell!&\left(-1+\sum_{m=0}^{\ell}\frac{1}{m!}\gamma_m\right), \end{aligned}$$

where if $\ell = 0$ the summation over m in the square brackets is empty, and where if $\ell = n$, the coefficient of L^0, that is to say a_0, has an extra contribution of $n!A_n$, where the A_n are the coefficients in the Laurent expansion of $\zeta'(s)/\zeta(s)$ about $s = 1$.

3. *The subleading, negative logarithm power coefficients are given by*

$$b_m = (-1)^n\sum_{k=1}^{\infty}2^k\sum_{j=0}^{n}\binom{n}{j}\beta_m^{k,j},$$

where for $1 \leq m \leq k+j-n$, we have

$$\beta_m^{k,j} = \frac{c_{m+n+1}^{k,j}}{(k+j-n-m)!} + \frac{(m-1)!}{k-n+j-1}\sum_{\ell=0}^{m-1}\binom{k-n+j}{\ell}c_{\ell+n+1}^{k,j}$$

and where for $m \leq k+j-n+1$, we have

$$\beta_m^{k,j} = \frac{(m-1)!}{k-n+j-1}\sum_{\ell=0}^{k+j-n}\binom{k-n+j}{\ell}c_{\ell+n+1}^{k,j}.$$

In these coefficients a_m, b_m, the $c_\ell^{k,j}$ are the Laurent series coefficients around $s = 1$ of

$$\left(\frac{\zeta'}{\zeta}(s)\right)'\left(-\frac{\zeta'}{\zeta}(s)\right)^{k-1}\zeta^{(j)}(s)\frac{1}{s} = \sum_{\ell=0}^{\infty}c_\ell^{k,j}(s-1)^{-k-j-2+\ell}.$$

An immediate corollary of Theorem 7.1 follows by setting $n = 1$. We state this result explicitly to compare it with (2.1) and Shanks' Conjecture.

Corollary 7.2. *Assume the Riemann Hypothesis. Write* $L = \log T/2\pi$*. For* λ *defined by* $Z'(\lambda) = 0$ *and* $K \geq 1$ *a positive integer, we have*

$$\sum_{0<\lambda\leq T} \zeta'\left(\frac{1}{2}+i\lambda\right) = -\frac{(e^2-3)}{4}\frac{T}{2\pi}L^2 + \frac{e^2-3+2\gamma_0}{2}\frac{T}{2\pi}L + \frac{3-e^2(1+2\gamma_0+2\gamma_1)}{2}\frac{T}{2\pi} + \frac{T}{2\pi}\sum_{m=1}^{K}\frac{c_m}{L^k} + O_K\left(\frac{T}{L^{K+1}}\right)$$

as $T \to \infty$*, where the other constants* c_m *are special cases of the coefficients* b_m *from Theorem 7.1 with* $n = 1$*.*

We may also prove the analogous result of Conrey and Ghosh in (7.1) from [66], with the modulus squared removed.

Theorem 7.3. *Assume the Riemann Hypothesis. Write* $L = \log T/2\pi$*. For* λ *defined by* $Z'(\lambda) = 0$ *and* $K \geq 1$ *a positive integer, we have*

$$\sum_{0<\lambda\leq T} \zeta\left(\frac{1}{2}+i\lambda\right) = \frac{e^2-3}{2}\frac{T}{2\pi}L + \frac{3-e^2-4\gamma_0}{2}\frac{T}{2\pi} + \frac{T}{2\pi}\sum_{m=1}^{K}\frac{d_m}{L^m} + O_K\left(\frac{T}{L^{K+1}}\right)$$

as $T \to \infty$*, where*

$$d_m = \sum_{k=m}^{\infty} 2^k \frac{c_{k,m+1}}{(k-m)!} + (m-1)!\sum_{k=1}^{\infty}\frac{2^k k}{(k-1)!}\sum_{\ell=0}^{\min\{m-1,k\}}\binom{k}{\ell}c_{k,\ell+1},$$

and where the $c_{k,\ell}$ *are the Laurent series coefficients around* $s = 1$ *of*

$$\left(\frac{\zeta'}{\zeta}(s)\right)'\left(-\frac{\zeta'}{\zeta}(s)\right)^{k-1}\zeta(s)\frac{1}{s} = \sum_{\ell=0}^{\infty} c_{k,\ell}(s-1)^{-k-2+\ell}.$$

We evaluate the sum of the factor $\chi(s)$ from the functional equation (1.1) for $\zeta(s)$ over the local extrema of $\zeta(s)$.

Theorem 7.4. *Assume the Riemann Hypothesis. Write* $L = \log T/2\pi$*. For* λ *defined by* $Z'(\lambda) = 0$ *and* $K \geq 1$ *a positive integer, we have*

$$\sum_{0<\lambda\leq T} \chi\left(\frac{1}{2}+i\lambda\right) = (e^2-2)\frac{T}{2\pi} - 4e^2\gamma_0\frac{T}{2\pi}\frac{1}{L} + \frac{T}{2\pi}\sum_{m=2}^{K}\frac{e_m}{L^m} + O_K\left(\frac{T}{L^{K+1}}\right)$$

as $T \to \infty$*, where*

$$e_m = \sum_{k=m}^{\infty} 2^k \frac{c_{k,m}}{(k-m)!} + (m-1)!\sum_{k=1}^{\infty}\frac{2^k}{(k-1)!}\sum_{\ell=0}^{\min\{m-1,k\}}\binom{k}{\ell}c_{k,\ell},$$

and where the $c_{k,\ell}$ *are the Laurent series coefficients around* $s = 1$ *of*

$$\left(\frac{\zeta'}{\zeta}(s)\right)' \left(-\frac{\zeta'}{\zeta}(s)\right)^{k-1} \frac{1}{s} = \sum_{\ell=0}^{\infty} c_{k,\ell}(s-1)^{-k-1+\ell}.$$

Remark. The infinite descending chain of powers of $\log T$ in the previous results where each function is summed over the relative extrema of zeta is due to a pole in the function that we consider near 1, given by

$$\beta_Z = 1 + 2/L + O\left(L^{-2}\right),$$

where $L = \log T/2\pi$.

We expect that we would be able to give these results with a power-saving error term of $O\left(T^{1/2+\varepsilon}\right)$ for all $\varepsilon > 0$ if we were able to find a closed form for the asymptotic as a function of β_Z.

As in [183], we have set aside the search for such a form for the time being.

With only minor adjustments to our proof of Theorem 7.4 (which we will specify in Section 7.1.7), we are also able to prove the following result. It is a special case of a result from [208], but here we give it with a power-saving error term.

Theorem 7.5. *Assume the Riemann Hypothesis. For* $\rho = 1/2 + i\gamma$ *a non-trivial zero of* $\zeta(s)$*, we have*

$$\sum_{0<\gamma\leq T} \chi\left(\frac{1}{2} + i\gamma\right) = -\frac{T}{2\pi} + O\left(T^{1/2+\varepsilon}\right)$$

as $T \to \infty$*, where* $\chi(s)$ *is the factor from the functional equation for* $\zeta(s)$ *given in* (1.1).

7.1.1 Remarks on the previous results

1. **Theorem 7.1**

   We compare the result from this theorem with that of Kaptan, Karabulut and Yıldırım [207] and Hughes and Pearce-Crump [186] on the Generalised Shank's conjecture. In that result, the average of $\zeta^{(n)}(s)$, summed over the non-trivial zeros of $\zeta(s)$, is clearly real and alternates between positive and negative as n increases.

   In the case of Theorem 7.1, the behaviour is reversed; the average of $\zeta^{(n)}(s)$, summed over the maxima of $|\zeta(s)|$, is real and alternates between negative and positive as n increases.

   It isn't immediately obvious from the leading order coefficient that this is the case, that is, that

$$(-1)^n \left(\frac{e^2-2}{n+1} + (-1)^{n+1}\frac{n!}{2^{n+1}}\left(1 - e^2\sum_{k=0}^{n+1}\frac{(-2)^k}{k!}\right)\right)$$

alternates. Begin by noting by Taylor's theorem with remainder that

$$e^{-2} = \sum_{k=0}^{n+1} \frac{(-2)^k}{k!} + O\left(\frac{1}{(n+2)!}\right)$$

so the coefficient of the leading order can be rewritten as

$$(-1)^n \left(\frac{e^2-2}{n+1} + (-1)^{n+1}\frac{n!}{2^{n+1}}\left(1 - e^2\left\{e^{-2} + O\left(\frac{1}{(n+2)!}\right)\right\}\right)\right)$$

and simplifying gives

$$(-1)^n \left(\frac{e^2-2}{n+1} + O\left(\frac{1}{n^2}\right)\right).$$

Since $e^2 - 2 > 0$, the alternating behaviour is then clear, but in reverse to the Generalised Shanks' Conjecture as n increases.

2. **Corollary 7.2**

As noted in the general n^{th} derivative case, while Shanks' conjecture is that $\zeta'(\rho)$ is positive and real on average, the same question with regards to $\zeta'(\lambda)$ is negative and real on average.

We plot the first few terms of the asymptotic against the real part of the true value of the sum in Figure 7.1. If we were to plot the imaginary part of the true value, we would find that it remains small (at most $\approx \pm 10$ in absolute value).

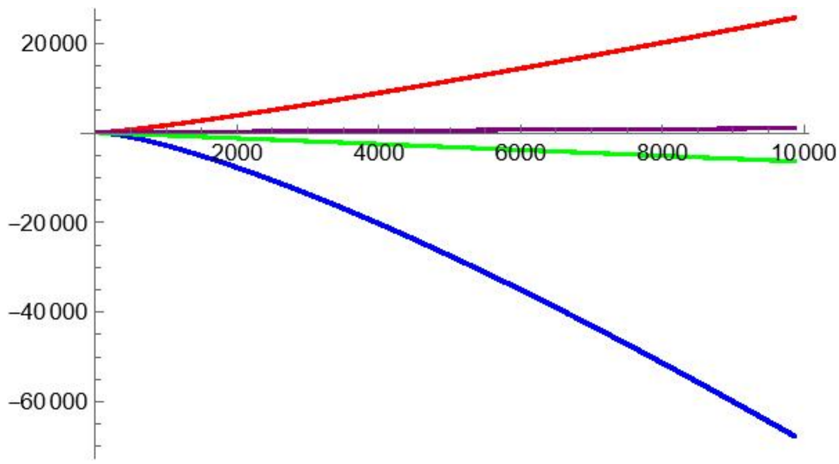

Figure 7.1: The real part of the sum $\sum_{0<\lambda\leq T} \zeta'(1/2 + i\lambda)$ with true value (blue), the true - leading (red), true - leading - subleading (green) and true - leading - subleading - subsubleading (purple) terms subtracted from the true value, for T up to the height of the 10,000$^{\text{th}}$ zero λ of $Z'(t)$.

3. **Theorem 7.3**

The result of Conrey and Ghosh in (7.1) has coefficient $(e^2 - 5)/2$ to leading order, with an extra power of a logarithm, compared with the $(e^2 - 3)/2$ here. The power of the logarithm can be explained by noting that we are taking a first moment in Theorem 7.3.

We plot the first few terms of the asymptotic against the real part of the true value of the sum in Figure 7.2. If we were to plot the imaginary part of the true value, we would find that it remains small (at most $\approx \pm 20$ in absolute value).

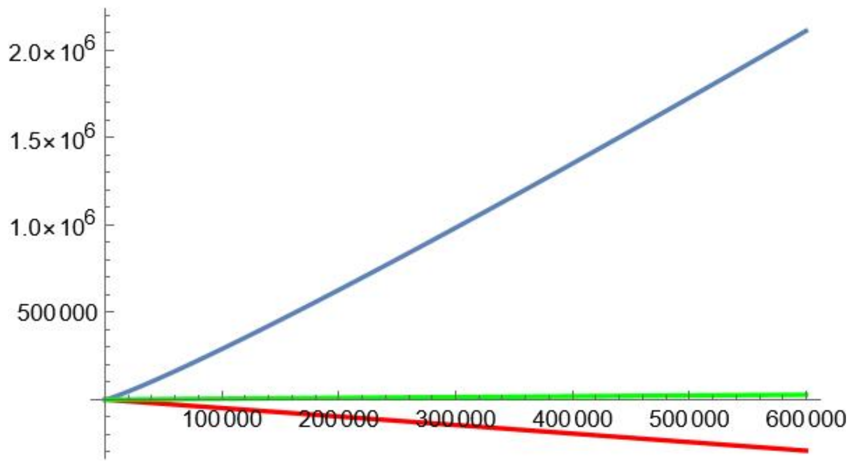

Figure 7.2: The real part of the sum $\sum_{0<\lambda\leq T} \zeta(1/2 + i\lambda)$ with true value (blue), the true - leading (red) and true - leading - subleading (green) terms subtracted from the true value, for T up to the height of the 1,000,000$^{\text{th}}$ zero λ of $Z'(t)$.

4. **Theorem 7.4**

   We plot the first few terms of the asymptotic against the real part of the true value of the sum in Figure 7.3. If we were to plot the imaginary part of the true value, we would find that it remains small (at most $\approx \pm 10$ in absolute value).

5. **Theorem 7.5**

   We assume the Riemann Hypothesis in proving this result but can make it unconditional by taking better care when calculating the error term.

   The behaviour is somewhat strange, however. Recall that the Gram points occur when $\theta(g_n) = n\pi$, and by the definition of the Riemann–Siegel function given in (1.28), we have

$$\chi\left(\frac{1}{2} + ig_n\right) = e^{-2i\theta(g_n)} = e^{-2in\pi} = 1,$$

   so

$$\sum_{0<\gamma\leq T} \chi\left(\frac{1}{2} + ig_n\right) = \frac{T}{2\pi}\log T + O(T).$$

   Given that a zero is expected to lie roughly in the middle of a Gram interval, it isn't overly surprising that the sum in Theorem 7.5 is negative, but this doesn't account

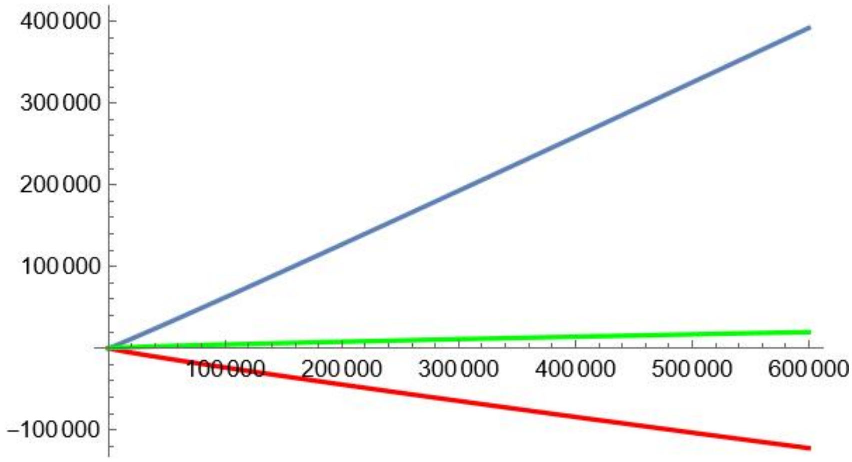

Figure 7.3: The real part of the sum $\sum_{0<\lambda\leq T}\chi(1/2+i\lambda)$ with true value (blue), the true - leading (red) and true - leading - subleading (green) terms subtracted from the true value, for T up to the height of the 1,000,000$^{\text{th}}$ zero λ of $Z'(t)$.

for the loss of the logarithm. Likewise, it then isn't overly surprising that the sum in Theorem 7.3 over λ is positive as we should expect these points to lie closer to the Gram points, but again doesn't account for the loss of the logarithm.

We plot the true value of the sum minus the main term of the asymptotic in Figure 7.4. As we can see, all that remains is clearly an error term. We have plotted both the real and imaginary parts as both are small and can be easily seen against each other, unlike in the previous figures where the imaginary parts are too small to be seen.

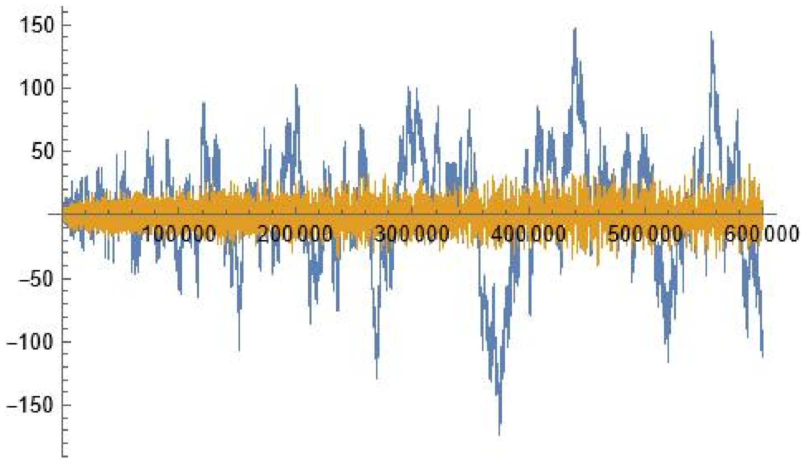

Figure 7.4: The real (blue) and imaginary (orange) part of $\sum_{0<\gamma\leq T}\chi(1/2+i\gamma)+\frac{T}{2\pi}$ for T up to the height of the 1,000,000$^{\text{th}}$ zero $1/2+i\gamma$ of $\zeta(s)$.

7.1.2 Overview of the proofs

In Section 7.1.3, we consider properties of the auxiliary function

$$Z_1(s) = \zeta'(s) - \frac{1}{2}\frac{\chi'}{\chi}(s)\zeta(s)$$

used in the proof, where $\chi(s)$ is the factor from the non-symmetrical form of the functional equation of the Riemann zeta function, given in (1.1). This function is zero at the extrema of the Riemann zeta function. We also list other useful lemmas in this section, including functional equations, stationary phase methods, and a moments result from Chapter 3 (and from [186]) on the average of derivatives of $\zeta(s)$, evaluated over the non-trivial zeros of $\zeta(s)$.

In Section 7.1.4, we prove Theorem 7.1. This involves using Cauchy's Theorem to write the sum over the extrema as an integral

$$\sum_{0<\lambda\leq T} \zeta^{(n)}\left(\frac{1}{2}+i\lambda\right) = \frac{1}{2\pi i}\int_{\mathcal{C}} \frac{Z_1'}{Z_1}(s)\zeta^{(n)}(s)\ ds$$

(up to a small error), where $\mathcal{C}$ is a contour we specify later that encloses the critical line up to a height T.

We begin by showing that only the left-hand side of the contour contributes to the asymptotic, with the rest going into a power-saving error term. The bulk of the argument then comes down to evaluating

$$\frac{1}{2\pi i}\int_{c+i}^{c+iT} \chi(1-s)\frac{Z_1'}{Z_1}(s)\zeta^{(n)}(1-s)\ ds$$

for some specific $c > 1$ defined in the proof.

We are able to write the logarithmic derivative of $Z_1(s)$ as a series of the form

$$\frac{Z_1'}{Z_1}(s) = \sum_{m=1}^{\infty}\frac{a(m,s)}{m^s}$$

which converges for some $c > 1$ with coefficients $a(n,s)$ given in Lemma 7.7. Using this and the Dirichlet series for the derivatives of $\zeta(s)$ allows us to apply the method of stationary phase to change this integral into a sum, given by

$$(-1)^n\left(\sum_{m_1m_2\leq T/2\pi}\Lambda(m_1)(\log m_1)^n - \sum_{k=1}^{\infty}2^k\sum_{j=0}^{n}\binom{n}{j}\sum_{m_1m_2\leq T/2\pi}\frac{(-1)^j(\log m_1)^j a_k(m_2)}{(\log m_1m_2)^{k-n+j}}\right)$$

up to a power-saving error term, where the coefficients $a_k(m)$ come from $a(m,s)$.

An application of Perron's formula turns the first sum back into an integral, which we can evaluate the residue of at the pole. Another application of Perron's formula turns the numerator of the inner sum of the second term into an integral that we evaluate the residue of at the pole, and complete the argument with partial summation and summing over $j =, 0, \dots, n$ and $k \geq 1$.

We then outline the proofs of Theorem 7.3 in Section 7.1.5, of Theorem 7.4 in Section 7.1.6, and of Theorem 7.5 in 7.1.7, leaving the full details of the proofs to the interested reader as they are similar to that of Theorem 7.1.

7.1.3 Preliminary Lemmas

Define the function $Z_1(s)$ by

$$Z_1(s) = \zeta'(s) - \frac{1}{2}\frac{\chi'}{\chi}(s)\zeta(s). \tag{7.4}$$

Note that by taking the logarithmic derivative of Hardy's Z function, we see that $Z_1(s)$ is zero exactly when $Z'(t) = 0$, that is, at an extrema of $|\zeta(s)|$ on the critical line.

The function $Z_1(s)$ satisfies various properties which were proved by Conrey and Ghosh [66] in their lemma. Note that only the properties we use in our proof are listed below. For a proof of this lemma, we refer the reader to their paper.

Lemma 7.6. *We have the following properties for $Z_1(s)$:*

1. $|Z_1(1/2 + it)| = |Z'(t)|$.
2. $Z_1(s)$ *satisfies the functional equation*

$$Z_1(s) = -\chi(s) Z_1(1-s)$$

   for all s, where $\chi(s)$ is the term in the functional equation for the Riemann zeta function, $\zeta(s) = \chi(s)\zeta(1-s)$.
3. *The number of zeros of $Z_1(t)$ up to a height T which lie off the critical line is bounded by* $\log T$.
4. *If* $Z_1(\beta_1 + i\gamma_1) = 0$ *then*

$$\left|\beta_1 - \frac{1}{2}\right| \leq \frac{1}{9}$$

   for γ_1 sufficiently large.

The logarithmic derivative of $Z_1(s)$ is given by

$$\frac{Z_1'}{Z_1}(s) = \frac{\chi'}{\chi}(s) - \frac{Z_1'}{Z_1}(1-s) \tag{7.5}$$

which follows directly from part (2) in Lemma 7.6.

For $s = \sigma + it$, where $|\sigma| \leq 2$, we have the following estimate for the logarithmic derivative for $\chi(s)$ given by

$$\frac{\chi'}{\chi}(s) = -\log\frac{t}{2\pi} + O\left(\frac{1}{t}\right), \tag{7.6}$$

(say for $t > 1$) which can be found in [66], for example. This enables us to rewrite the functional equation above as

$$\frac{Z_1'}{Z_1}(s) = -\log\frac{t}{2\pi} - \frac{Z_1'}{Z_1}(1-s) + O\left(\frac{1}{t}\right). \tag{7.7}$$

Lemma 7.7. *For $\Re(s) > 1$ and $t \geq 100$, we have*

$$\frac{Z_1'}{Z_1}(s) = \sum_{m=1}^{\infty}\frac{a(m,s)}{m^s} + O\left(\frac{1}{t\log t}\right)$$

where

$$a(m,s) = -\Lambda(m) + \sum_{k=1}^{\infty}\frac{1}{f(s)^k}a_k(m) \tag{7.8}$$

with

$$f(s) = -\frac{1}{2}\frac{\chi'}{\chi}(s) \tag{7.9}$$

and $a_k(m)$ is of the form

$$a_k(m) = \left((\Lambda\log) * \Lambda_{k-1}\right)(m), \tag{7.10}$$

where we use the notation Λ_k to denote

$$\underbrace{\Lambda * \Lambda * \Lambda * \cdots * \Lambda}_{k-1 \text{ convolutions}}$$

with the convention that $\Lambda_0(m)$ takes the value 1 if $m = 1$ and 0 otherwise, and where $\Lambda_1(m) = \Lambda(m)$ is the usual von Mangoldt function.

We give a variation of the proof given in [183].

Proof. Recall that we have defined the function $Z_1(s)$ in (7.4) by

$$Z_1(s) = \zeta'(s) + f(s)\zeta(s)$$

where $f(s)$ is given in (7.9). Differentiating this gives

$$Z_1'(s) = \zeta''(s) + f(s)\zeta'(s) + f'(s)\zeta(s).$$

Then

$$\frac{Z_1'}{Z_1}(s) = \frac{\zeta''(s) + f(s)\zeta'(s)}{\zeta'(s) + f(s)\zeta(s)} + f'(s)\frac{1}{\frac{\zeta'}{\zeta}(s) + f(s)}. \tag{7.11}$$

For $\Re(s) > 1$ with $t \geq 1$, the last term can be bounded by $O(1/t\log t)$ by noting that $f'(s) = O(1/t)$ (which follows from (7.6)), $f(s) = O(\log t)$ and $\zeta'(s)/\zeta(s) = O(\log\log t)$ (due to Littlewood [228], under the Riemann Hypothesis) in the region under consideration. Therefore we can write

$$\frac{Z_1'}{Z_1}(s) = \frac{\frac{\zeta''}{\zeta}(s) + f(s)\frac{\zeta'}{\zeta}(s)}{\frac{\zeta'}{\zeta}(s) + f(s)} + O\left(\frac{1}{t\log t}\right).$$

For s with sufficiently large real part, we can expand the denominator as a geometric series. This gives

$$\begin{aligned}\frac{1}{\frac{\zeta'}{\zeta}(s) + f(s)} &= \frac{1}{f(s)}\left(1 + \frac{1}{f(s)}\frac{\zeta'}{\zeta}(s)\right)^{-1} \\ &= \frac{1}{f(s)}\sum_{k=0}^{\infty}\frac{1}{f(s)^k}\left(-\frac{\zeta'}{\zeta}(s)\right)^k.\end{aligned}$$

This expansion will be valid so long as $\Re(s)$ is large enough so that $\left|\frac{1}{f(s)}\frac{\zeta'}{\zeta}(s)\right| \leq 1$. For example, we can take $\Re(s) > 1$ and $t \geq 100$.

Then we have

$$\begin{aligned}\frac{Z_1'}{Z_1}(s) &= \frac{1}{f(s)}\left(\frac{\zeta''}{\zeta}(s) + f(s)\frac{\zeta'}{\zeta}(s)\right)\sum_{k=0}^{\infty}\frac{1}{f(s)^k}\left(-\frac{\zeta'}{\zeta}(s)\right)^k + O\left(\frac{1}{t\log t}\right) \\ &= \sum_{n=1}^{\infty}\frac{a(n,s)}{n^s} + O\left(\frac{1}{t\log t}\right)\end{aligned} \tag{7.12}$$

where we calculate the coefficients $a(n,s)$ below.

By repeated use of the quotient rule, we may write

$$\frac{d}{ds}\left(\frac{\zeta^{(k)}}{\zeta}(s)\right) = \frac{\zeta^{(k+1)}}{\zeta}(s) - \frac{\zeta'}{\zeta}(s)\frac{\zeta^{(k)}}{\zeta}(s).$$

Rearranging this we have

$$\frac{\zeta^{(k+1)}}{\zeta}(s) = \frac{d}{ds}\left(\frac{\zeta^{(k)}}{\zeta}(s)\right) + \frac{\zeta'}{\zeta}(s)\frac{\zeta^{(k)}}{\zeta}(s).$$

The Dirichlet coefficients of these series then give us the recurrence relation for any non-negative integer k,

$$\Lambda^{(k+1)}(n) = \Lambda^{(k)}(n)\log(n) + (\Lambda^{(k)}(n) * \Lambda)(n), \tag{7.13}$$

for each $n \in \mathbb{N}$, where $\Lambda^{(1)}(n) = \Lambda(n)$ is the usual von Mangoldt function, that is, the coefficient from the Dirichlet series for $-\zeta'(s)/\zeta(s)$. (Note that this notation is not standard - see the remark at the end of this proof.)

Consider now the coefficient from each of the Dirichlet series in (7.12). For the terms on the right-hand side of that equation (ignoring the error term for now), we have

$$a(n,s)=\left(\frac{1}{f(s)}\Lambda^{(2)}(n)-\Lambda(n)\right)\sum_{k=0}^{\infty}\frac{1}{f(s)^k}\Lambda_k(n).$$

Now use the recurrence relation (7.13) with $k=1$ to write

$$\Lambda^{(2)}(n)=(\Lambda\log+\Lambda_2)(n).$$

Substitue this into the previous expression to obtain for each $n\in\mathbb{N}$,

$$\begin{aligned}
a(n,s)&=\left(\frac{1}{f(s)}(\Lambda\log+\Lambda_2)(n)-\Lambda(n)\right)\sum_{k=0}^{\infty}\frac{1}{f(s)^k}\Lambda_k(n)\\
&=\sum_{k=0}^{\infty}\frac{1}{f(s)^{k+1}}((\Lambda\log)*\Lambda_k)(n)+\sum_{k=0}^{\infty}\frac{1}{f(s)^{k+1}}(\Lambda_2*\Lambda_k)(n)-\sum_{k=0}^{\infty}\frac{1}{f(s)^k}(\Lambda*\Lambda_k)(n)\\
&=\sum_{k=1}^{\infty}\frac{1}{f(s)^{k+1}}((\Lambda\log)*\Lambda_k)(n)+\sum_{k=1}^{\infty}\frac{1}{f(s)^k}\Lambda_{k+1}(n)-\sum_{k=0}^{\infty}\frac{1}{f(s)^k}\Lambda_{k+1}(n)\\
&=\sum_{k=1}^{\infty}\frac{1}{f(s)^{k+1}}((\Lambda\log)*\Lambda_k)(n)+\sum_{k=0}^{\infty}\frac{1}{f(s)^k}\Lambda_{k+1}(n)-\Lambda(n)-\sum_{k=0}^{\infty}\frac{1}{f(s)^k}\Lambda_{k+1}(n)\\
&=\sum_{k=0}^{\infty}\frac{1}{f(s)^k}((\Lambda\log)*\Lambda_{k-1})(n)-\Lambda(n),
\end{aligned}$$

completing the proof of the Lemma. □

Remark. Note that while we can only use the expansion in this Lemma for $t\ge 100$, in the proofs of our results in later sections we will ignore this slight technicality as using the result for $t\ge 1$ in our applications will only introduce an error of $O(1)$, which is well within our other error terms.

Remark. As our notation Λ_k is used for $(k-1)$-convolutions, we use non-standard notation

$$\frac{\zeta^{(k)}}{\zeta}(s)=\sum_{n=1}^{\infty}\frac{\Lambda^{(k)}(n)}{n^s}.$$

Typically in the literature, $\Lambda_k(n)$ is used here but we have already used it in a different meaning in this section, and want to stay consistent with the notation in [183]. Since this proof is the only place in this section that we use this convention, we don't worry about any confusion or conflicts and remind the reader that we are using Λ_k to denote $(k-1)$-convolutions.

We will be applying the method of stationary phase at various points throughout our argument. The following version of this result can be found in [208], and is based on a similar result due to Gonek [143] where he took k in the following lemma to be a non-negative integer, which we have previously stated in this thesis as Lemma 3.10.

Lemma 7.8. *Let $\{b_m\}_{m=1}^{\infty}$ be a sequence of complex numbers such that for any $\varepsilon > 0$, $b_m \ll m^{\varepsilon}$. Let $c > 1$ and suppose $|k| = o(\log T)$ as $T \to \infty$. Then for T sufficiently large,*

$$\frac{1}{2\pi}\int_0^T \chi(1-c-it)\left(\log\frac{t}{2\pi}\right)^k\left(\sum_{m=1}^{\infty} b_m m^{-c-it}\right)dt = \sum_{m\leq \frac{T}{2\pi}} b_m(\log m)^k + O\left(T^{c-1/2}(\log T)^k\right).$$

The last result we need is from the proof of the main result from Chapter 3, and from Hughes and Pearce-Crump [186]. This equation is stated in this thesis as (3.10), and involves calculating the sum

$$\sum_{m_1 m_2 \leq T/2\pi} \Lambda(m_1)(\log m_1)^n.$$

This result is unconditional in that section, but as we are assuming the Riemann Hypothesis here, we will also assume it here (note that this only affects the error term coming from this sum).

7.1.4 Proof Theorem 7.1

7.1.4.1 Initial Manipulations

We note that the beginning of the proofs of Theorems 7.1, 7.3, and 7.4 start in a similar way to that of Conrey and Ghosh [66], and of Hughes, Lugmayer and Pearce-Crump [183]. We repeat it here for completeness sake but skip over the details in the later cases.

Under the Riemann Hypothesis, we know that the zeros λ of $Z'(t)$ interlace those of $Z(t)$, and so the set of points where $|\zeta(1/2 + it)|$ achieves its local maximum are exactly the points where $Z'(t) = 0$.

Let $\rho_1 = \beta_1 + i\gamma_1$ be the zeros of $Z_1(s)$. By part (3) of Lemma 7.6, $Z_1(s)$ has $O(\log T)$ zeros off the critical line (that is, $\beta_1 \neq 1/2$). At the zeros off the critical line, we may use part (4) of Lemma 7.6 together with the Lindelöf bounds on $\zeta(s)$ and its derivatives to obtain

$$\sum_{\substack{0<\gamma_1\leq T\\ \beta_1\neq 1/2}} \zeta^{(n)}(\rho_1) \ll T^{1/9+\varepsilon}\log T \ll T^{1/9+\varepsilon}$$

for any integer $n \geq 0$.

Therefore, we have

$$\sum_{0<\lambda\leq T} \zeta^{(n)}\left(\frac{1}{2}+i\lambda\right) = \sum_{\substack{0<\gamma_1\leq T\\ \beta_1=1/2}} \zeta^{(n)}\left(\frac{1}{2}+i\gamma_1\right).$$

We can write this as an integral using Cauchy's theorem,

$$\begin{aligned}\frac{1}{2\pi i}\int_{\mathcal{C}}\frac{Z_1'}{Z_1}(s)\zeta^{(n)}(s)\ ds &= \sum_{0<\gamma_1\le T}\zeta^{(n)}(\rho_1)\\ &= \sum_{\substack{0<\gamma_1\le T\\ \beta_1=1/2}}\zeta^{(n)}\left(\frac{1}{2}+i\gamma_1\right)+O\left(T^{1/9+\varepsilon}\right) \qquad (7.14)\end{aligned}$$

where $\mathcal{C}$ is a positively oriented contour with vertices $c+i$, $c+iT$, $1-c+iT$, and $1-c+i$, where $c=1+1/\log T$. We may assume, without loss of generality, that the distance from the contour to any zero ρ_1 of $Z_1(s)$ is uniformly $\gg 1/\log T$.

We split the integral as

$$\begin{aligned}&\frac{1}{2\pi i}\left(\int_{c+i}^{c+iT}+\int_{c+iT}^{1-c+iT}+\int_{1-c+iT}^{1-c+i}+\int_{1-c+i}^{c+i}\right)\frac{Z_1'}{Z_1}(s)\zeta^{(n)}(s)\ ds\\ &= S^R+S^T+S^L+S^B,\end{aligned}$$

say. We will first bound S^B, S^T, S^R trivially within error term, and show that the leading contributions to the asymptotic will then come from S^L. Consider each of these integrals in turn.

First note that the integral S^B, which is the integral along the bottom of the contour, is $O(1)$.

For the integral S^T, which is the integral along the top of the contour, we may use the bound proved in [183] that states if $|T-\rho_1|\gg 1/\log T$ for all zeros ρ_1 of Z_1 (which we are in this proof), we have

$$\frac{Z_1'}{Z_1}(\sigma+iT)\ll(\log T)^2$$

uniformly for $-1<\sigma\le 2$. Combining the Lindelöf bounds on $\zeta(s)$ and its derivatives with this shows that the integral along the top of the contour is $O\left(T^{1/2+\varepsilon}\right)$.

Next note that for the integral S^R, which is the integral along the right-hand vertical side of the contour, we have $c>1$ which is past the abscissa of convergence for $\zeta^{(n)}(s)$ and $Z_1(s)$ as given in (7.4). Then

$$S^R=\frac{1}{2\pi}\int_0^T\frac{Z_1'}{Z_1}(c+it)\zeta^{(n)}(c+it)\ dt\ll T^{\varepsilon}.$$

Note then that S^B, S^T, S^R are all within an error term of $O\left(T^{1/2+\varepsilon}\right)$. All that remains is to evaluate S^L. Observe that

$$S^L=\frac{1}{2\pi i}\int_{1-c+iT}^{1-c+i}\frac{Z_1'}{Z_1}(s)\zeta^{(n)}(s)\ ds=-\frac{1}{2\pi i}\int_{c-iT}^{c-i}\frac{Z_1'}{Z_1}(1-s)\zeta^{(n)}(1-s)\ ds=-\overline{I},$$

where

$$I=\frac{1}{2\pi i}\int_{c+i}^{c+iT}\frac{Z_1'}{Z_1}(1-s)\zeta^{(n)}(1-s)\ ds. \qquad (7.15)$$

Overall, we have

$$\sum_{0<\lambda\le T} \zeta^{(n)}\left(\frac{1}{2}+i\lambda\right) = -\overline{I} + O\left(T^{1/2+\varepsilon}\right).$$

7.1.4.2 Deriving the main terms

To begin manipulating I into a form that we can evaluate, we use the logarithmic derivative of the functional equation for $Z_1(s)$ given in (7.5). We will also use for functional equation for the derivatives of $\zeta(1-s)$ given in Lemma 3.5. Substituting these two expressions into (7.15) gives

$$\begin{aligned} I = &\frac{1}{2\pi i}\int_{c+i}^{c+iT}\left(-\log\frac{t}{2\pi}\right)(-1)^n\chi(1-s)\sum_{j=0}^{n}\binom{n}{j}\left(\log\frac{t}{2\pi}\right)^{n-j}\zeta^{(j)}(s)\ ds \\ &+\frac{1}{2\pi i}\int_{c+i}^{c+iT}\left(-\frac{Z_1'}{Z_1}(s)\right)(-1)^n\chi(1-s)\sum_{j=0}^{n}\binom{n}{j}\left(\log\frac{t}{2\pi}\right)^{n-j}\zeta^{(j)}(s)\ ds + O\left(T^{1/2+\varepsilon}\right). \end{aligned}$$

Simplifying slightly gives

$$\begin{aligned} I &= \frac{(-1)^{n+1}}{2\pi i}\int_{c+i}^{c+iT}\chi(1-s)\sum_{j=0}^{n}\binom{n}{j}\left(\log\frac{t}{2\pi}\right)^{n-j+1}\zeta^{(j)}(s)\ ds \\ &\quad + \frac{(-1)^{n+1}}{2\pi i}\int_{c+i}^{c+iT}\chi(1-s)\sum_{j=0}^{n}\binom{n}{j}\left(\log\frac{t}{2\pi}\right)^{n-j}\zeta^{(j)}(s)\frac{Z_1'}{Z_1}(s)\ ds + O\left(T^{1/2+\varepsilon}\right) \\ &= I_1 + I_2 + O\left(T^{1/2+\varepsilon}\right), \end{aligned}$$

say.

7.1.4.3 The integral I_1

First consider I_1. We want to apply Lemma 7.8 here to extract terms for the asymptotic. To do this we begin by switching the order of integration and summation and substitute the Dirichlet series for $\zeta^{(j)}(s)$ to obtain

$$I_1 = (-1)^{n+1}\sum_{j=0}^{n}\binom{n}{j}\left[\frac{1}{2\pi i}\int_{c+i}^{c+iT}\chi(1-s)\left(\log\frac{t}{2\pi}\right)^{n-j+1}\sum_{m=1}^{\infty}\frac{(-1)^j(\log m)^j}{m^s}\ ds\right]$$

Now apply Lemma 7.8 to the integral, obtaining

$$I_1 = (-1)^{n+1}\sum_{j=0}^{n}\binom{n}{j}\left[\sum_{m\le T/2\pi}(\log m)^{n-j+1}(-1)^j\log(m)^j\right] + O\left(T^{1/2+\varepsilon}\right).$$

Simplifying this gives

$$I_1 = (-1)^{n+1}\sum_{j=0}^{n}\binom{n}{j}(-1)^j\left[\sum_{m\le T/2\pi}(\log m)^{n+1}\right] + O\left(T^{1/2+\varepsilon}\right).$$

Now by the Binomial Theorem, this summation over j equals zero for $n > 0$ and equals 1 if $n = 0$. Hence in the case $n = 0$, we have a contribution of

$$I_1 = -\sum_{m \le T/2\pi} \log m + O\left(T^{1/2+\varepsilon}\right).$$

By standard methods, we have

$$I_1 = -\frac{T}{2\pi}\log\frac{T}{2\pi} + \frac{T}{2\pi} + O\left(T^{1/2+\varepsilon}\right).$$

and so we have proved the following result.

Lemma 7.9. *For n a non-negative integer, the integral I_1 satisfies*

$$I_1 = \begin{cases} -\frac{T}{2\pi}\log\frac{T}{2\pi} + \frac{T}{2\pi} + O\left(T^{1/2+\varepsilon}\right) & \text{if } n=0 \\ O\left(T^{1/2+\varepsilon}\right) & \text{if } n>0. \end{cases}$$

7.1.4.4 The integral I_2

Similarly to when we evaluated the integral I_1, we want to apply stationary phase calculations to extract terms for the asymptotic from I_2. To do this we begin by switching the order of integration and summation and substitute the Dirichlet series for $\zeta^{(j)}(s)$ and the series for the logarithmic derivative of $Z_1(s)$ to obtain

$$\begin{aligned} I_2 =& (-1)^{n+1}\sum_{j=0}^{n}\binom{n}{j} \\ &\times\left[\frac{1}{2\pi i}\int_{c+i}^{c+iT}\chi(1-s)\left(\log\frac{t}{2\pi}\right)^{n-j}\sum_{m_1=1}^{\infty}\frac{(-1)^j(\log m_1)^j}{m_1^s}\sum_{m_2=1}^{\infty}\frac{(-\Lambda(m_2))}{m_2^s}\,ds\right] \\ &+\sum_{k=1}^{\infty}(-1)^{n+1}\sum_{j=0}^{n}\binom{n}{j} \\ &\times\left[\frac{1}{2\pi i}\int_{c+i}^{c+iT}\chi(1-s)\frac{1}{f(s)^k}\left(\log\frac{t}{2\pi}\right)^{n-j}\sum_{m_1=1}^{\infty}\frac{(-1)^j(\log m_1)^j}{m_1^s}\sum_{m_2=1}^{\infty}\frac{a_k(m_2))}{m_2^s}\,ds\right] \\ &= I_{2,1} + I_{2,2}, \end{aligned}$$

say, where we split the initial term of $Z_1'(s)/Z_1(s)$ from the rest as $I_{2,1}$ follows directly from stationary phase methods, while $I_{2,2}$ has a more involved argument.

For $I_{2,1}$ we may use Lemma 7.8 to write

$$I_{2,1} = (-1)^{n+1}\sum_{j=0}^{n}\binom{n}{j}\left[\sum_{m_1 m_2 \le T/2\pi}(-1)^j(\log m_1)^j(-\Lambda(m_2))(\log m_1 m_2)^{n-j}\right] + O\left(T^{1/2+\varepsilon}\right).$$

Switching the order of summation, expanding the logarithms, and performing some basic algebraic manipulations allows us to rewrite this as

$$I_{2,1} = (-1)^n \sum_{m_1 m_2 \leq T/2\pi} \Lambda(m_1)(\log m_1)^n + O\left(T^{1/2+\varepsilon}\right).$$

We note that this calculation was preformed in Hughes and Pearce-Crump [186], and is effectively given as the negative of the result of Theorem 3.1. That is,

$$\begin{aligned} I_{2,1} = (-1)^n \frac{1}{n+1} \frac{T}{2\pi} \left(\log \frac{T}{2\pi}\right)^{n+1} \\ + (-1)^n \sum_{k=0}^{n} \binom{n}{k} (-1)^k k! \left(-1 + \sum_{j=0}^{k} \frac{1}{j!}\gamma_j\right) \frac{T}{2\pi} \left(\log \frac{T}{2\pi}\right)^{n-k} \\ - n! A_n \frac{T}{2\pi} + O\left(T^{1/2+\varepsilon}\right) \end{aligned} \tag{7.16}$$

where we remind the reader that the γ_j are the coefficients from the Laurent expansion of $\zeta(s)$ about $s = 1$ and the A_n are the coefficients from the Laurent expansion of $\zeta'(s)/\zeta(s)$ about $s = 1$.

Finally we need to evaluate $I_{2,2}$. By (7.6) and (7.9), we can write

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

and so

$$\frac{1}{f(s)^k} = \frac{2^k}{(\log t/2\pi)^k}\left(1 + O\left(\frac{1}{t\log t}\right)\right)^{-k} = \frac{2^k}{(\log t/2\pi)^k}\left(1 + O\left(\frac{k}{t\log t}\right)\right).$$

Then

$$\begin{aligned} I_{2,2} &= \sum_{k=1}^{\infty} (-1)^{n+1} \sum_{j=0}^{n} \binom{n}{j} \\ &\quad \times \frac{1}{2\pi i}\int_{c+i}^{c+iT} \chi(1-s) \frac{2^k}{(\log t/2\pi)^k}\left(1 + O\left(\frac{k}{t\log t}\right)\right) \\ &\quad \times \left(\log \frac{t}{2\pi}\right)^{n-j} \sum_{m_1=1}^{\infty} \frac{(-1)^j (\log m_1)^j}{m_1^s} \sum_{m_2=1}^{\infty} \frac{a_k(m_2))}{m_2^s}\, ds \\ &= \sum_{k=1}^{\infty} (-1)^{n+1} \sum_{j=0}^{n} \binom{n}{j} \\ &\quad \times \frac{1}{2\pi i}\int_{c+i}^{c+iT} \chi(1-s) \frac{2^k}{(\log t/2\pi)^k}\left(\log \frac{t}{2\pi}\right)^{n-j} \\ &\quad \times \sum_{m_1=1}^{\infty} \frac{(-1)^j (\log m_1)^j}{m_1^s} \sum_{m_2=1}^{\infty} \frac{a_k(m_2)}{m_2^s}\, ds + O\left(T^{1/2+\varepsilon}\right). \end{aligned}$$

After these initial manipulations performed above, we may apply Lemma 7.8. This gives

$$I_{2,2} = (-1)^{n+1} \sum_{k=1}^{\infty} 2^k \sum_{j=0}^{n} \binom{n}{j} \left[\sum_{m_1 m_2 \le T/2\pi} \frac{(-1)^j (\log m_1)^j a_k(m_2) (\log m_1 m_2)^{n-j}}{(\log m_1 m_2)^k} \right] + O\left(T^{1/2+\varepsilon}\right). \tag{7.17}$$

Remark. Now we note that we could repeat our trick that we used when switching the order of summation and expanding the logarithm when we evaluated $I_{2,1}$. However it is then unclear what the correct Dirichlet series is to use in the upcoming Perron argument. Instead we take the approach of cancelling the appropriate powers of the logarithm, and work with $I_{2,2}$ in this form.

Switching the order of summation in $I_{2,2}$ gives

$$I_{2,2} = (-1)^{n+1} \sum_{k=1}^{\infty} 2^k \sum_{j=0}^{n} \binom{n}{j} \left[\sum_{m_1 m_2 \le T/2\pi} \frac{(-1)^j (\log m_1)^j a_k(m_2)}{(\log m_1 m_2)^{k-n+j}} \right] + O\left(T^{1/2+\varepsilon}\right) \tag{7.18}$$

To evaluate $I_{2,2}$, we begin with evaluating the numerator of the inner sum. After calculating the sum of the numerator of the inner sum, we can preform partial summation to reinsert the logarithm in the denominator of the inner sum, and then sum over j and k.

Lemma 7.10. *Let*

$$A_{k,j}(x) = \sum_{m \le x} \alpha_{k,j}(m),$$

where

$$\alpha_{k,j}(m) = \sum_{m_1 m_2 = m} (-1)^j (\log m_1)^j a_k(m_2)$$

and where $a_k(m_2)$ is given in (7.10)*. This sum can also be written as*

$$A_{k,j}(x) = \sum_{1 \le m n_1 n_2 \dots n_k \le x} (-1)^j (\log m)^j \log(n_1) \Lambda(n_1) \Lambda(n_2) \dots \Lambda(n_k).$$

Then for large x,

$$A_{k,j}(x) = x \sum_{\ell=0}^{k+j+1} \frac{c_\ell^{k,j}}{(k+j+1-\ell)!} (\log x)^{k+j+1-\ell} + O\left(x^{1/2+\varepsilon}\right)$$

where the $c_\ell^{k,j}$ are the Laurent series coefficients around $s=1$ of

$$\left(\frac{\zeta'}{\zeta}(s)\right)' \left(-\frac{\zeta'}{\zeta}(s)\right)^{k-1} \zeta^{(j)}(s) \frac{1}{s} = \sum_{\ell=0}^{\infty} c_\ell^{k,j} (s-1)^{-k-j-2+\ell}.$$

Remark. A long but straightforward calculation tells us what the coefficients $c_\ell^{k,j}$ equal. The leading coefficient is when $\ell = 0$ and is given by

$$c_0^{k,j} = (-1)^j j!$$

for all $j \geq 0$. When $\ell = 1$, the subleading coefficients are given by

$$c_1^{k,j} = \begin{cases} -1 + \gamma_0 + (1-k)\gamma_0 & \text{if } j = 0 \\ (-1)^j j!(-1 + (1-k)\gamma_0) & \text{for all } j \geq 1. \end{cases}$$

Remark. The superscripts on the coefficients $c_\ell^{k,j}$ is to indicate that the terms depend on both k and j.

Proof. We begin by applying Perron's formula to $A_{k,j}(x)$, that is, we have

$$A_{k,j}(x) = \frac{1}{2\pi i}\int_{3/2-iR}^{3/2+iR} \left(\frac{\zeta'}{\zeta}(s)\right)' \left(-\frac{\zeta'}{\zeta}(s)\right)^{k-1} \zeta^{(j)}(s)\frac{x^s}{s}\, ds + O\left(\frac{x^{3/2+\varepsilon}}{R}\right)$$

Note that the integrand has a pole of order $k + j + 2$ at $s = 1$. We shift past the pole at $s = 1$ to the line $\Re(s) = 1/2 + \varepsilon$, and evaluate the residue at $s = 1$. Therefore, up to a power-saving error, $A_{k,j}(x)$ will equal the residue of the integrand around that point. That is,

$$A_{k,j}(x) = x\sum_{\ell=0}^{k+j+1} b_\ell^{k,j}(\log x)^{k+j+1-\ell} + O\left(R^\varepsilon x^{1/2+\varepsilon}\right) + O\left(\frac{x^{3/2+\varepsilon}}{R}\right)$$

for some constants $b_\ell^{k,j}$. We have started the sum at the largest power of $\log x$ as this simplifies future calculations. Choosing $R = x$ optimises the error terms, giving an error of $O(x^{1/2+\varepsilon})$.

To evaluate the residue, we use the various Laurent expansions about $s = 1$ in the various terms in the integrand. The expansions we need are

$$\begin{aligned}
\left(\frac{\zeta'}{\zeta}(s)\right)' &= \frac{1}{(s-1)^2} + \left(-2\gamma_1 - \gamma_0^2\right) + \left(6\gamma_0\gamma_1 + 3\gamma_2 + 2\gamma_0^3\right)(s-1) + \ldots \\
\left(-\frac{\zeta'}{\zeta}(s)\right)^{k-1} &= \frac{1}{(s-1)^{k-1}} + \frac{(1-k)\gamma_0}{(s-1)^{k-2}} + \frac{\frac{1}{2}k(k-1)\gamma_0^2 + 2(k-1)\gamma_1}{(s-1)^{k-3}} + \ldots \\
\zeta^{(j)}(s) &= \frac{(-1)^j j!}{(s-1)^{j+1}} + (-1)^j\gamma_j + (-1)^{j+1}\gamma_{j+1}(s-1) + \ldots \\
\frac{1}{s} &= 1 - (s-1) + (s-1)^2 + ...
\end{aligned}$$

where the Stieltjes constants are from the Laurent expansion of $\zeta(s)$ about $s = 1$.

Combining these Laurent expansions allows us to write

$$\left(\frac{\zeta'}{\zeta}(s)\right)'\left(-\frac{\zeta'}{\zeta}(s)\right)^{k-1}\zeta^{(j)}(s)\frac{1}{s}=\sum_{\ell=0}^{\infty}c_\ell^{k,j}(s-1)^{-k-j-2+\ell}$$

where we have explicitly given the first few values of $c_\ell^{k,j}$ in the remark following the statement of the lemma.

The residue is the coefficient of $1/(s-1)$ which will come from combining these terms with the x^s in the integrand (which is the only term that contains an x). Its expansion about $s=1$ is

$$x^s=x\left(1+(s-1)\log x+\frac{(s-1)^2}{2!}(\log x)^2+\ldots+\frac{(s-1)^k}{k!}(\log x)^k+\ldots\right)$$

so the coefficient of $(\log x)^{k+j+1-\ell}$ in the $(s-1)^{-1}$ term equals

$$b_\ell^{k,j}=\frac{c_\ell^{k,j}}{(k+j+1-\ell)!}$$

and such a combination is possible for ℓ between 0 and $k+j+1$. □

To complete the proof of Theorem 7.1, we want to use the asymptotic from Lemma 7.10 in (7.18) and use partial summation to reinsert the logarithm in the denominator of the inner sum in (7.17).

This means that we need to calculate

$$I_{2,2}=(-1)^{n+1}\sum_{k=1}^{\infty}2^k\sum_{j=0}^{n}\binom{n}{j}\left[A_k\left(\frac{T}{2\pi}\right)f\left(\frac{T}{2\pi}\right)-\int_2^{T/2\pi}A_k(x)f'(x)\,dx\right]+O\left(T^{1/2+\varepsilon}\right)$$

with $f(x)=1/(\log x)^{k-n+j}$, so that $f'(x)=-(k-n+j)/(x(\log x)^{k-n+j+1})$, and with $A_{k,j}(x)$ as in Lemma 7.10.

Note that while we want to sum the inner sum in $I_{2,2}$ over all positive integers m_1,m_2 such that $1\le m_1m_2\le T/2\pi$, this introduces a problem with the logarithms appearing in the denominator. Instead we will sum from 2 to avoid this problem, at the cost of a $O(1)$ error which we ignore as it is smaller than our largest error.

Writing $L=\log T/2\pi$, by partial summation we have

$$\begin{aligned}I_{2,2}=(-1)^{n+1}\sum_{k=1}^{\infty}2^k\sum_{j=0}^{n}\binom{n}{j}&\\ \Bigg[\left(\frac{T}{2\pi}\right)\sum_{\ell=0}^{k+j+1}\frac{c_\ell^{k,j}}{(k+j+1-\ell)!}L^{n+1-\ell}&\\ +(k-n+j)\sum_{\ell=0}^{k+j+1}\frac{c_\ell^{k,j}}{(k+j+1-\ell)!}\int_2^{T/2\pi}(\log x)^{n-\ell}\,dx\Bigg]&\\ +O\left(T^{1/2+\varepsilon}\right).&\end{aligned}\tag{7.19}$$

Lemma 7.11. *Writing $L = \log T/2\pi$, for any integer $K \geq 1$, we have*

$$\begin{aligned}
I_{2,2} = (-1)^{n+1}\frac{T}{2\pi}\sum_{k=1}^{\infty}2^k\sum_{j=0}^{n}\binom{n}{j}\Bigg(L^{n+1}\frac{c_0^{k,j}}{(k+j+1)!}\\
+\sum_{\ell=0}^{n}L^{n-\ell}\Bigg[\frac{c_{\ell+1}^{k,j}}{(k+j-\ell)!}+(k-n+j)\frac{c_{\ell}^{k,j}}{(k+j+1-\ell)!}\\
+(k-n+j)\sum_{m=0}^{\ell-1}(-1)^{\ell-m}(n-m)\dots(n-\ell+1)\frac{c_m^{k,j}}{(k+j+1-m)!}\Bigg]\Bigg)\\
+(-1)^{n+1}\frac{T}{2\pi}\sum_{m=1}^{K}\frac{1}{L^m}\sum_{k=1}^{\infty}2^k\sum_{j=0}^{n}\binom{n}{j}\beta_m^{k,j}+O\left(\frac{T}{L^{K+1}}\right),
\end{aligned}$$

where for $1 \leq m \leq k+j-n$, we have

$$\beta_m^{k,j} = \frac{c_{m+n+1}^{k,j}}{(k+j-n-m)!}+\frac{(m-1)!}{k-n+j-1}\sum_{\ell=0}^{m-1}\binom{k-n+j}{\ell}c_{\ell+n+1}^{k,j}$$

and where for $m \leq k+j-n+1$, we have

$$\beta_m^{k,j} = \frac{(m-1)!}{k-n+j-1}\sum_{\ell=0}^{k+j-n}\binom{k-n+j}{\ell}c_{\ell+n+1}^{k,j},$$

where the constants $c_\ell^{k,j}$ are given in Lemma 7.10.

Proof. We begin by noting from (7.19) that we can obtain the leading order, that is, the L^{n+1}, from the first sum within the square brackets by setting $\ell = 0$. There are then positive and negative powers of L^n which come from both sums in the square brackets.

We begin by splitting the sums into those that contribute to non-negative powers of L, and those that contribute to negative powers of L. This is because we can evaluate the positive powers exactly, while the negative powers are slightly more complicated. The positive powers occur for $\ell \leq n+1$ in the first sum, and $\ell \leq n$ in the second sum from the square brackets. This splitting gives

$$
\begin{aligned}
I_{2,2} = (-1)^{n+1} \sum_{k=1}^{\infty} 2^k \sum_{j=0}^{n} \binom{n}{j} \\
&\left[\left(\frac{T}{2\pi} \sum_{\ell=0}^{n+1} \frac{c_\ell^{k,j}}{(k+j+1-\ell)!} L^{n+1-\ell} \right.\right. \\
&\qquad \left. + (k-n+j) \sum_{\ell=0}^{n} \frac{c_\ell^{k,j}}{(k+j+1-\ell)!} \int_2^{T/2\pi} (\log x)^{n-\ell}\, dx \right) \\
&+ \left(\frac{T}{2\pi} \sum_{\ell=n+2}^{k+j+1} \frac{c_\ell^{k,j}}{(k+j+1-\ell)!} L^{n+1-\ell} \right. \\
&\qquad \left.\left. + (k-n+j) \sum_{\ell=n+1}^{k+j+1} \frac{c_\ell^{k,j}}{(k+j+1-\ell)!} \int_2^{T/2\pi} (\log x)^{n-\ell}\, dx \right) \right] \\
&\qquad + O\left(T^{1/2+\varepsilon}\right)
\end{aligned}
$$

For ease of notation, we write the sum $I_{2,2}$ as

$$
I_{2,2} = (-1)^{n+1} \sum_{k=1}^{\infty} 2^k \sum_{j=0}^{n} \binom{n}{j} [J_1 + J_2] + O\left(T^{1/2+\varepsilon}\right),
$$

say, where both J_1 and J_2 depend on k and j, and the J_1 sum is for the non-negative powers of the logarithm, and the J_2 sum is for the negative powers of the logarithm.

We now consider the two sums J_1 and J_2 in turn.

Consider J_1 first. Recall that for $m \geq 0$, we have

$$
\int_2^{T/2\pi} (\log x)^m\, dx = \frac{T}{2\pi} \sum_{r=0}^{m} (-1)^r \frac{m!}{(m-r)!} L^{m-r} + O(1).
$$

Then using this (and ignoring the error term as it is consumed by larger error terms that we have already seen in this proof), we have

$$
\begin{aligned}
J_1 = \frac{T}{2\pi} &\left[\sum_{\ell=0}^{n+1} \frac{c_\ell^{k,j}}{(k+j+1-\ell)!} L^{n+1-\ell} \right. \\
&\left. + (k-n+j) \sum_{\ell=0}^{n} \frac{c_\ell^{k,j}}{(k+j+1-\ell)!} \left(\sum_{r=0}^{n-\ell} (-1)^r \frac{(n-\ell)!}{(n-\ell-r)!} L^{n-\ell-r} \right) \right].
\end{aligned}
$$

We first note that we can extract the leading order behaviour from the first sum, and reindex the remaining terms in the first sum to obtain

$$\begin{aligned} J_1 = \frac{T}{2\pi} L^{n+1} \frac{c_0^{k,j}}{(k+j+1)!} \\ &+ \frac{T}{2\pi} \left[\sum_{\ell=0}^{n} \frac{c_{\ell+1}^{k,j}}{(k+j-\ell)!} L^{n-\ell} \right. \\ &\left. +(k-n+j) \sum_{\ell=0}^{n} \frac{c_\ell^{k,j}}{(k+j+1-\ell)!} \left(\sum_{r=0}^{n-\ell} (-1)^r \frac{(n-\ell)!}{(n-\ell-r)!} L^{n-\ell-r} \right) \right]. \end{aligned}$$

We now reorder the second summation to write

$$\begin{aligned} J_1 = \frac{T}{2\pi} L^{n+1} \frac{c_0^{k,j}}{(k+j+1)!} \\ &+ \frac{T}{2\pi} \sum_{\ell=0}^{n} \left[\frac{c_{\ell+1}^{k,j}}{(k+j-\ell)!} + (k-n+j) \frac{c_\ell^{k,j}}{(k+j+1-\ell)!} \right. \\ &\left. +(k-n+j) \sum_{m=0}^{\ell-1} (-1)^{\ell-m} (n-m) \dots (n-\ell+1) \frac{c_m^{k,j}}{(k+j+1-m)!} \right] L^{n-\ell} \end{aligned}$$

where if $\ell = 0$ the last sum is empty.

We now calculate the contribution from J_2. By a simple relabelling, we have

$$\begin{aligned} J_2 = \frac{T}{2\pi} \sum_{\ell=1}^{k+j+1} \frac{c_{\ell+n+1}^{k,j}}{(k+j-n-\ell)!} L^{-\ell} \\ &+ (k-n+j) \sum_{\ell=1}^{k+j+1-n} \frac{c_{\ell+n}^{k,j}}{(k+j+1-n-\ell)!} \int_2^{T/2\pi} (\log x)^{-\ell} \, dx, \end{aligned}$$

so both of our sums in J_2 start from $\ell = 1$.

Next we note that in the remaining integrals, all of the powers of $\log x$ are negative, so evaluate to an infinite chain of descending powers of L. For example, for $1 \le m \le M$, we have

$$\begin{aligned} \int_2^{T/2\pi} \frac{1}{(\log x)^m} \, dx &= \frac{T}{2\pi} \frac{1}{L^m} + m \int_2^{T/2\pi} \frac{1}{(\log x)^{m+1}} \, dt + O(1) \\ &= \frac{T}{2\pi} \sum_{r=m}^{M} \frac{(r-1)!}{(m-1)!} \frac{1}{L^r} + O\left(\frac{T}{L^{M+1}} \right). \end{aligned}$$

We write $\beta_m^{k,j}$ for the coefficient of L^{-m} and split into two cases.

If $m \le k+j-n$, then there will be a contribution from the first sum in J_2 when $m = \ell$ and from all integrals in the second sum for $\ell = 1, \dots, m$. We have

$$\beta_m^{k,j} = \frac{c_{m+n+1}^{k,j}}{(k+j-n-m)!} + (k-n+j) \sum_{\ell=1}^{m} \frac{c_{\ell+n}^{k,j}}{(k+j+1-n-\ell)!} \frac{(m-1)!}{(\ell-1)!}.$$

Using the fact

$$\frac{(k-n+j)}{(k+j+1-n-\ell)!(\ell-1)!} = \binom{k-n+j}{\ell-1}\frac{1}{k-n+j-1},$$

this simplifies to

$$\beta_m^{k,j} = \frac{c_{m+n+1}^{k,j}}{(k+j-n-m)!} + \frac{(m-1)!}{k-n+j-1}\sum_{\ell=1}^{m}\binom{k-n+j}{\ell-1}c_{\ell+n}^{k,j}.$$

If $m \geq k+j-n+1$, then there will only be a contribution coming from the second sum of J_2, but every term in that sum contributes. We have

$$\beta_m^{k,j} = \frac{(m-1)!}{k-n+j-1}\sum_{\ell=1}^{k+j+1-n}\binom{k-n+j}{\ell-1}c_{\ell+n}^{k,j}.$$

After a trivial relabelling for both versions of $\beta_m^{k,j}$, we have the statement of the lemma. □

We can see that we have

$$I_{2,2} = \mathfrak{a}_{n+1}\frac{T}{2\pi}L^{n+1} + \frac{T}{2\pi}\sum_{\ell=0}^{n}\mathfrak{a}_{n-\ell}L^{n-\ell} + \frac{T}{2\pi}\sum_{m=1}^{K}\frac{\mathfrak{b}_m}{L^m} + O\left(\frac{T}{L^{K+1}}\right),$$

where the leading order coefficient is given by

$$\mathfrak{a}_{n+1} = (-1)^{n+1}\sum_{k=1}^{\infty}2^k\sum_{j=0}^{n}\binom{n}{j}\frac{c_0^{k,j}}{(k+j+1)!},$$

the subleading, non-negative logarithm power coefficients are given by

$$\mathfrak{a}_{n-\ell} = (-1)^{n+1}\sum_{k=1}^{\infty}2^k\sum_{j=0}^{n}\binom{n}{j}\Bigg[\frac{c_{\ell+1}^{k,j}}{(k+j-\ell)!} + (k-n+j)\frac{c_\ell^{k,j}}{(k+j+1-\ell)!} + (k-n+j)\sum_{m=0}^{\ell-1}(-1)^{\ell-m}(n-m)\ldots(n-\ell+1)\frac{c_m^{k,j}}{(k+j+1-m)!}\Bigg],$$

and the subleading, negative logarithm power coefficients are given by

$$\mathfrak{b}_m = (-1)^{n+1}\sum_{k=1}^{\infty}2^k\sum_{j=0}^{n}\binom{n}{j}\beta_m^{k,j},$$

where for $1 \leq m \leq k+j-n$, we have

$$\beta_m^{k,j} = \frac{c_{m+n+1}^{k,j}}{(k+j-n-m)!} + \frac{(m-1)!}{k-n+j-1}\sum_{\ell=0}^{m-1}\binom{k-n+j}{\ell}c_{\ell+n+1}^{k,j}$$

and where for $m \leq k+j-n+1$, we have

$$\beta_m^{k,j} = \frac{(m-1)!}{k-n+j-1}\sum_{\ell=0}^{k+j-n}\binom{k-n+j}{\ell}c_{\ell+n+1}^{k,j},$$

where the constants $c_\ell^{k,j}$ are given in Lemma 7.10.

By Lemma 7.11 we can see that to complete calculating $I_{2,2}$, all we need to do is sum over $j = 0, \ldots, n$ and over $k \geq 1$.

In the remark following Lemma 7.10 we calculated $c_0^{k,j}$ and $c_1^{k,j}$ explicitly, and so we could calculate the leading and subleading terms in $I_{2,2}$, using our result for J_1.

In this case, to leading order we would have

$$(-1)^{n+1}\frac{T}{2\pi}L^{n+1}\sum_{k=1}^{\infty}2^k\sum_{j=0}^{n}\binom{n}{j}\frac{c_0^{k,j}}{(k+j+1)!}.$$

Substitute the value of $c_0^{k,j}$ from Lemma 7.10 to obtain

$$\begin{aligned}&(-1)^{n+1}\frac{T}{2\pi}\left(\log\frac{T}{2\pi}\right)^{n+1}\sum_{k=1}^{\infty}2^k\sum_{j=0}^{n}\binom{n}{j}\frac{(-1)^j j!}{(k+j+1)!}\\ =&(-1)^{n+1}\frac{T}{2\pi}\left(\log\frac{T}{2\pi}\right)^{n+1}\sum_{k=1}^{\infty}\left(\frac{2^k}{k!(k+n+1)}\right),\end{aligned}$$

where the second line follows after summing over j. Now we need to sum over k. For this sum we obtain

$$\begin{aligned}\sum_{k=1}^{\infty}\frac{2^k}{k!(k+n+1)} &= \frac{e^2-1}{n+1}+(-1)^{n+1}\left(\frac{\Gamma(n+2)-\Gamma(n+2,-2)}{2^{n+1}(n+1)}\right)\\ &= \frac{e^2-1}{n+1}+(-1)^{n+1}\frac{n!}{2^{n+1}}\left(1-e^2\sum_{k=0}^{n+1}\frac{(-2)^k}{k!}\right)\end{aligned}$$

where we have used the incomplete gamma function in simplifying the expressions above, which for integer n is given by

$$\Gamma(n,x) = (n-1)!e^{-x}\sum_{k=0}^{n-1}\frac{x^k}{k!}.$$

This means that to leading order, we have

$$I_{2,2} \sim (-1)^{n+1}\left(\frac{e^2-1}{n+1}+(-1)^{n+1}\frac{n!}{2^{n+1}}\left(1-e^2\sum_{k=0}^{n+1}\frac{(-2)^k}{k!}\right)\right)\frac{T}{2\pi}\left(\log\frac{T}{2\pi}\right)^{n+1}.$$

In a similar way, we can calculate the subleading behaviour, and show that this contributes

$$(-1)^{n+1}\frac{T}{2\pi}L^n\left(1-(1+e^2)\gamma_0+(-1)^{n+1}\frac{(n+1)!}{2^{n+1}}(-1+2\gamma_0)\left(1-e^2\sum_{k=0}^{n}\frac{(-2)^k}{k!}\right)\right).$$

to the asymptotic.

Further calculations from Lemma 7.10 would give rise to more lower order terms in the obvious way.

We then recombine $I_{2,2}$ here with I_1 from Lemma 7.9 and with $I_{2,1}$ from (7.16), which gives I.

Finally, recall that

$$\sum_{0<\lambda\leq T} \zeta^{(n)}\left(\frac{1}{2}+i\lambda\right) = -\overline{I} + O\left(T^{1/2+\varepsilon}\right)$$

to obtain the asymptotic, proving Theorem 7.1.

7.1.5 Outline of the proof of Theorem 7.3

We begin by noting that the proof of Theorem 7.3 follows in a similar way to that of Theorem 7.1. We sketch the differences below but leave the full details to the interested reader.

The initial steps remain the same in the case $n = 0$ as in the proof of Theorem 7.1. We are able to write

$$\sum_{0<\lambda\leq T} \zeta\left(\frac{1}{2}+i\lambda\right) = -\overline{I} + O\left(T^{1/2+\varepsilon}\right)$$

where

$$I = \frac{1}{2\pi i}\int_{c+i}^{c+iT} \frac{Z_1'}{Z_1}(1-s)\zeta(1-s)\ ds,$$

where $c = 1 + 1/\log T$.

To begin manipulating I into a form that we can evaluate, we use the logarithmic derivative of the functional equation for $Z_1(s)$, given in (7.5), and the functional equation for $\zeta(s)$, given in (1.1). Then

$$\begin{aligned} I &= \frac{1}{2\pi i}\int_{c+i}^{c+iT} \frac{Z_1'}{Z_1}(1-s)\zeta(1-s)\ ds \\ &= -\frac{1}{2\pi i}\int_{c+i}^{c+iT} \log\frac{t}{2\pi}\chi(1-s)\zeta(s)\ ds - \frac{1}{2\pi i}\int_{c+i}^{c+iT} \frac{Z_1'}{Z_1}(s)\chi(1-s)\zeta(s)\ ds + O\left(T^{1/2+\varepsilon}\right) \\ &= I_1 + I_2 + O\left(T^{1/2+\varepsilon}\right), \end{aligned}$$

say.

Then by Lemma 7.9, we have

$$I_1 = -\frac{T}{2\pi}\log\frac{T}{2\pi} + \frac{T}{2\pi} + O\left(T^{1/2+\varepsilon}\right). \tag{7.20}$$

For I_2, we have

$$\begin{aligned}
I_2 &= -\frac{1}{2\pi i}\int_{c+i}^{c+iT} \frac{Z_1'}{Z_1}(s)\chi(1-s)\zeta(s)\, ds \\
&= \frac{1}{2\pi i}\int_{c+i}^{c+iT} \chi(1-s)\sum_{n=1}^{\infty}\frac{\Lambda(n)}{n^s}\sum_{m=1}^{\infty}\frac{1}{m^s}\, ds \\
&\quad -\sum_{k=1}^{\infty}\frac{1}{2\pi i}\int_{c+i}^{c+iT} \chi(1-s)\frac{1}{f(s)^k}\sum_{n=1}^{\infty}\frac{a_k(n)}{n^s}\sum_{m=1}^{\infty}\frac{1}{m^s}\, ds \\
&= I_{2,1} + I_{2,2},
\end{aligned}$$

say.

Then $I_{2,1}$ can be evaluated through a simple application of Lemma 7.8 and Perron's theorem, giving

$$I_{2,1} = \frac{T}{2\pi}\log\frac{T}{2\pi} - \frac{T}{2\pi} + O\left(T^{1/2+\varepsilon}\right). \tag{7.21}$$

Combining I_1 from (7.20) and $I_{2,1}$ from (7.21) gives a contribution of $O\left(T^{1/2+\varepsilon}\right)$ to the asymptotic.

Finally, to evaluate $I_{2,2}$, we have after using Lemma 7.8

$$\begin{aligned}
I_{2,2} &= -\sum_{k=1}^{\infty}\frac{1}{2\pi i}\int_{c+i}^{c+iT} \chi(1-s)\frac{1}{f(s)^k}\sum_{n=1}^{\infty}\frac{a_k(n)}{n^s}\sum_{m=1}^{\infty}\frac{1}{m^s}\, ds \\
&= -\sum_{k=1}^{\infty} 2^k \sum_{nm\le T/2\pi}\frac{a_k(n)}{(\log nm)^k} + O\left(T^{1/2+\varepsilon}\right) + O\left(T^{1/2+\varepsilon}\right).
\end{aligned}$$

As in the proof of Theorem 7.1, we evaluate the numerator of the inner sum in the previous line via Perron. This is actually a special case of Lemma 7.10 in the case $j=0$, so we have the following result.

Lemma 7.12. *Let*

$$A_k(x) = \sum_{mn\le x} a_k(n),$$

where $a_k(n)$ is given in (7.10)*. This sum can also be written as*

$$A_k(x) = \sum_{1\le mn_1n_2\ldots n_k\le x} \log(n_1)\Lambda(n_1)\Lambda(n_2)\ldots\Lambda(n_k).$$

Then for large x,

$$A_k(x) = x\sum_{\ell=0}^{k+1}\frac{c_{k,\ell}}{(k+1-\ell)!}(\log x)^{k+1-\ell} + O\left(x^{1/2+\varepsilon}\right)$$

where the $c_{k,\ell}$ are the Laurent series coefficients around $s=1$ of

$$\left(\frac{\zeta'}{\zeta}(s)\right)'\left(-\frac{\zeta'}{\zeta}(s)\right)^{k-1}\zeta(s)\frac{1}{s} = \sum_{\ell=0}^{\infty} c_{k,\ell}(s-1)^{-k-2+\ell}.$$

Remark. A long but straightforward calculation tells us what the coefficients $c_{k,\ell}$ equal. The leading coefficient is when $\ell = 0$ and is given by

$$c_{k,0} = 1.$$

When $\ell = 1$, the subleading coefficient is given by

$$c_{k,1} = -1 + \gamma_0 + (1-k)\gamma_0.$$

Next we use partial summation to calculate

$$\sum_{nm \le T/2\pi} \frac{a_k(n)}{(\log nm)^k} = A_k\left(\frac{T}{2\pi}\right) f\left(\frac{T}{2\pi}\right) - \int_2^{T/2\pi} A_k(x) f'(x)\, dx,$$

in the case $f(x) = 1/(\log x)^k$ (so $f'(x) = -k/(x(\log x)^{k+1})$). Then using $A_k(x)$ from Lemma 7.12, we have with $L = \log T/2\pi$,

$$\sum_{nm \le T/2\pi} \frac{a_k(n)}{(\log nm)^k} = \\ \frac{T}{2\pi} \sum_{\ell=0}^{k+1} \frac{c_{k,\ell}}{(k+1-\ell)!} L^{1-\ell} + k \sum_{\ell=0}^{k+1} \frac{c_{k,\ell}}{(k+1-\ell)!} \int_2^{T/2\pi} (\log x)^{-\ell}\, dx + O\left(T^{1/2+\varepsilon}\right).$$

As before, we extract the non-negative powers of the logarithm and calculate the coefficients of the negative powers as we clearly have an infinite chain of decreasing powers of the logarithm. This gives

$$\sum_{nm \le T/2\pi} \frac{a_k(n)}{(\log nm)^k} = \frac{T}{2\pi} \frac{c_{k,0}}{(k+1)!} L + \frac{T}{2\pi} \frac{c_{k,1}}{k!} + \frac{T}{2\pi} k \frac{c_{k,0}}{(k+1)!} \\ + \frac{T}{2\pi} \sum_{\ell=2}^{k+1} \frac{c_{k,\ell}}{(k+1-\ell)!} L^{1-\ell} + k \sum_{\ell=1}^{k+1} \frac{c_{k,\ell}}{(k+1-\ell)!} \int_2^{T/2\pi} (\log x)^{-\ell}\, dx + O\left(T^{1/2+\varepsilon}\right).$$

For the negative powers of the logarithm, we reindex so both sums start at $\ell = 1$ to give

$$\frac{T}{2\pi} \sum_{\ell=1}^{k} \frac{c_{k,\ell+1}}{(k-\ell)!} L^{-\ell} + k \sum_{\ell=1}^{k+1} \frac{c_{k,\ell}}{(k+1-\ell)!} \int_2^{T/2\pi} (\log x)^{-\ell}\, dx.$$

Recall that for $1 \le m \le M$, we have

$$\int_2^{T/2\pi} \frac{1}{(\log x)^m}\, dx = \frac{T}{2\pi} \frac{1}{L^m} + m \int_2^{T/2\pi} \frac{1}{(\log x)^{m+1}}\, dt + O(1) \\ = \frac{T}{2\pi} \sum_{r=m}^{M} \frac{(r-1)!}{(m-1)!} \frac{1}{L^r} + O\left(\frac{T}{L^{M+1}}\right).$$

We now write $\beta_m^{k,\ell}$ for the coefficient of L^{-m}. In an analogous way to to the proof of Theorem 7.1, we have for $m \leq k$,

$$\beta_m^{k,j} = \frac{c_{k,m+1}}{(k-m)!} + k\frac{(m-1)!}{(k-1)!}\sum_{\ell=0}^{m-1}\binom{k}{\ell}c_{k,\ell+1}$$

and where for $m \leq k+j-n+1$, we have

$$\beta_m^{k,j} = k\frac{(m-1)!}{(k-1)!}\sum_{\ell=0}^{k}\binom{k}{\ell}c_{k,\ell+1},$$

where the constants $c_{k,\ell}$ are given in Lemma 7.12.

In order to complete the proof, we multiply through by -2^k, and sum over all $k \geq 1$ to obtain $I_{2,2}$. Since the combination from the rest of the calculation only contributes to the error term, we have evaluated I and so the sum in question.

Note that since we have a simple form for $c_{k,0}$ and $c_{k,1}$, we can easily calculate the leading and subleading behaviour explicitly, giving for K a positive integer

$$\sum_{0<\lambda\leq T}\zeta\left(\frac{1}{2}+i\lambda\right) = \frac{e^2-3}{2}\frac{T}{2\pi}L + \frac{3-e^2-4\gamma_0}{2}\frac{T}{2\pi} + \frac{T}{2\pi}\sum_{m=1}^{K}\frac{d_m}{L^m} + O_K\left(\frac{T}{L^{K+1}}\right)$$

as $T \to \infty$, where

$$d_m = \sum_{k=1}^{\infty} 2^k \beta_m^{k,\ell},$$

with the $\beta_m^{k,\ell}$ as above.

7.1.6 Proof Theorem 7.4

The main steps in the proof of Theorem 7.4 follow in a similar way to Theorem 7.1. We sketch the steps here for completeness sake.

Under the Riemann Hypothesis we can show that all the zeros off the critical line only contribute to the error term in our asymptotic with a similar justification to the proof of Theorem 7.1. Recall $\chi(s) \ll T^{1/2-\sigma}$ for $s = \sigma + it$ with $|t| \ll T$. Write $\rho_1 = \beta_1 + i\gamma_1$ for a zero of $Z_1(s)$. By part (3) of Lemma 7.6, $Z_1(s)$ has $O(\log T)$ zeros off the critical line (that is, $\beta_1 \neq 1/2$). At the zeros off the critical line, we may use part (4) of Lemma 7.6 to obtain

$$\sum_{\substack{0<\gamma_1\leq T\\ \beta_1\neq 1/2}}\chi(\rho_1) \ll T^{1/9}\log T \ll T^{1/9+\varepsilon}.$$

Therefore, we have

$$\sum_{0<\lambda\leq T}\chi\left(\frac{1}{2}+i\lambda\right) = \sum_{\substack{0<\gamma_1\leq T\\ \beta_1=1/2}}\chi\left(\frac{1}{2}+i\gamma_1\right).$$

We can write this as an integral using Cauchy's theorem,

$$\frac{1}{2\pi i}\int_{\mathcal{C}}\frac{Z_1'}{Z_1}(s)\chi(s)\ ds = \sum_{0<\gamma_1\leq T}\chi(\rho_1)$$
$$= \sum_{\substack{0<\gamma_1\leq T\\ \beta_1=1/2}}\chi\left(\frac{1}{2}+i\gamma_1\right)+O\left(T^{1/9+\varepsilon}\right) \tag{7.22}$$

where $\mathcal{C}$ is a positively oriented contour with vertices $c+i$, $c+iT$, $1-c+iT$, and $1-c+i$, where $c = 1+1/\log T$. We may assume, without loss of generality, that the distance from the contour to any zero ρ_1 of $Z_1(s)$ is uniformly $\gg 1/\log T$.

We split the integral as

$$\frac{1}{2\pi i}\left(\int_{c+i}^{c+iT}+\int_{c+iT}^{1-c+iT}+\int_{1-c+iT}^{1-c+i}+\int_{1-c+i}^{c+i}\right)\frac{Z_1'}{Z_1}(s)\chi(s)\ ds$$
$$= S^R+S^T+S^L+S^B,$$

say. Note that S^B, S^T, S^R are all trivially bounded within error term in a similar way to the proof of Theorem 7.1, using the bound $\chi(s) \ll T^{1/2-\sigma}$ where appropriate. This shows that the leading contributions to the asymptotic will then come from S^L.

Since S^B, S^T, S^R are all within an error term of $O\left(T^{1/2+\varepsilon}\right)$, all that remains is to evaluate S^L. Note that

$$S^L = \frac{1}{2\pi i}\int_{1-c+iT}^{1-c+i}\frac{Z_1'}{Z_1}(s)\chi(s)\ ds = -\frac{1}{2\pi i}\int_{c-iT}^{c-i}\frac{Z_1'}{Z_1}(1-s)\chi(1-s)\ ds = -\overline{I},$$

where

$$I = \frac{1}{2\pi i}\int_{c+i}^{c+iT}\frac{Z_1'}{Z_1}(1-s)\chi(1-s)\ ds. \tag{7.23}$$

Overall, we have

$$\sum_{0<\lambda\leq T}\chi\left(\frac{1}{2}+i\lambda\right) = -\overline{I}+O\left(T^{1/2+\varepsilon}\right).$$

Using the version of the functional equation for $Z_1'(s)/Z_1(s)$ given in (7.7), we have

$$I = \frac{1}{2\pi i}\int_{c+i}^{c+iT}\left(-\log\frac{t}{2\pi}\right)\chi(1-s)\ ds$$
$$+\frac{1}{2\pi i}\int_{c+i}^{c+iT}\left(-\frac{Z_1'}{Z_1}(s)\right)\chi(1-s)\ ds+O\left(T^{1/2+\varepsilon}\right)$$
$$= I_1+I_2+O\left(T^{1/2+\varepsilon}\right),$$

say.

Then I_1 doesn't contribute to anything beyond an error term, so we split I_2 as before to write

$$I_2 = \frac{1}{2\pi i}\int_{c+i}^{c+iT}\left(\sum_{n=1}^{\infty}\frac{\Lambda(n)}{n^s}\right)\chi(1-s)\;ds \\ -\sum_{k=1}^{\infty}\frac{1}{2\pi i}\int_{c+i}^{c+iT}\chi(1-s)\frac{1}{f(s)^k}\sum_{n=1}^{\infty}\frac{a_k(n)}{n^s}\;ds + O\left(T^{1/2+\varepsilon}\right) \\ = I_{2,1} + I_{2,2} + O\left(T^{1/2+\varepsilon}\right).$$

Then applying Lemma 7.8 to $I_{2,1}$ we have

$$I_{2,1} = \sum_{n\le T/2\pi}\Lambda(n) + O\left(T^{1/2+\varepsilon}\right).$$

By Perron/the Prime Number Theorem, we have

$$I_{2,1} = \frac{T}{2\pi} + O\left(T^{1/2+\varepsilon}\right). \tag{7.24}$$

Finally, applying Lemma 7.8 to $I_{2,2}$ gives

$$I_{2,2} = -\sum_{k=1}^{\infty}2^k\sum_{n\le T/2\pi}\frac{a_k(n)}{(\log n)^k} + O\left(T^{1/2+\varepsilon}\right).$$

As in the proof of Theorem 7.1, we evaluate the numerator of the inner sum in the previous line via Perron.

Lemma 7.13. *Let*

$$A_k(x) = \sum_{n\le x}a_k(n),$$

where $a_k(n)$ is given in (7.10)*. This sum can also be written as*

$$A_k(x) = \sum_{1\le n_1n_2\ldots n_k\le x}\log(n_1)\Lambda(n_1)\Lambda(n_2)\ldots\Lambda(n_k).$$

Then for large x,

$$A_k(x) = x\sum_{\ell=0}^{k}\frac{c_{k,\ell}}{(k-\ell)!}(\log x)^{k-\ell} + O\left(x^{1/2+\varepsilon}\right)$$

where the $c_{k,\ell}$ are the Laurent series coefficients around $s=1$ of

$$\left(\frac{\zeta'}{\zeta}(s)\right)'\left(-\frac{\zeta'}{\zeta}(s)\right)^{k-1}\frac{1}{s} = \sum_{\ell=0}^{\infty}c_{k,\ell}(s-1)^{-k-1+\ell}.$$

Remark. A long but straightforward calculation tells us what the coefficients $c_{k,\ell}$ equal. The leading coefficient is when $\ell = 0$ and is given by

$$c_{k,0} = 1.$$

When $\ell = 1$, the subleading coefficient is given by

$$c_{k,1} = -1 + \gamma_0 - k\gamma_0.$$

Next we use partial summation to calculate

$$\sum_{n \le T/2\pi} \frac{a_k(n)}{(\log n)^k} = A_k\left(\frac{T}{2\pi}\right) f\left(\frac{T}{2\pi}\right) - \int_2^{T/2\pi} A_k(x) f'(x)\, dx,$$

in the case $f(x) = 1/(\log x)^k$ (so $f'(x) = -k/(x(\log x)^{k+1})$). Then using $A_k(x)$ from Lemma 7.13, we have with $L = \log T/2\pi$,

$$\sum_{n \le T/2\pi} \frac{a_k(n)}{(\log n)^k} = \\ \frac{T}{2\pi}\sum_{\ell=0}^{k} \frac{c_{k,\ell}}{(k-\ell)!} L^{-\ell} + k\sum_{\ell=0}^{k} \frac{c_{k,\ell}}{(k-\ell)!}\int_2^{T/2\pi} (\log x)^{-1-\ell}\, dx + O\left(T^{1/2+\varepsilon}\right).$$

As before, we extract the non-negative powers of the logarithm and calculate the coefficients of the negative powers as we clearly have an infinite chain of decreasing powers of the logarithm. This gives

$$\sum_{n \le T/2\pi} \frac{a_k(n)}{(\log n)^k} = \frac{T}{2\pi}\frac{c_{k,0}}{k!} L \\ + \frac{T}{2\pi}\sum_{\ell=1}^{k} \frac{c_{k,\ell}}{(k-\ell)!} L^{-\ell} + k\sum_{\ell=0}^{k} \frac{c_{k,\ell}}{(k-\ell)!}\int_2^{T/2\pi} (\log x)^{-1-\ell}\, dx + O\left(T^{1/2+\varepsilon}\right).$$

For the negative powers of the logarithm, we reindex so both sums start at $\ell = 1$ to give

$$\frac{T}{2\pi}\sum_{\ell=1}^{k} \frac{c_{k,\ell}}{(k-\ell)!} L^{-\ell} + k\sum_{\ell=1}^{k+1} \frac{c_{k,\ell-1}}{(k+1-\ell)!}\int_2^{T/2\pi} (\log x)^{-\ell}\, dx.$$

Recall that for $1 \le m \le M$, we have

$$\begin{aligned}\int_2^{T/2\pi} \frac{1}{(\log x)^m}\, dx &= \frac{T}{2\pi}\frac{1}{L^m} + m\int_2^{T/2\pi} \frac{1}{(\log x)^{m+1}}\, dt + O(1) \\ &= \frac{T}{2\pi}\sum_{r=m}^{M} \frac{(r-1)!}{(m-1)!}\frac{1}{L^r} + O\left(\frac{T}{L^{M+1}}\right).\end{aligned}$$

We now write $\beta_m^{k,\ell}$ for the coefficient of L^{-m}. In an analogous way to to the proof of Theorem 7.1, we have for $m \le k$,

$$\beta_m^{k,j} = \frac{c_{k,m}}{(k-m)!} + \frac{(m-1)!}{(k-1)!}\sum_{\ell=0}^{m-1}\binom{k}{\ell}c_{k,\ell}$$

and where for $m \le k+j-n+1$, we have

$$\beta_m^{k,j} = \frac{(m-1)!}{(k-1)!}\sum_{\ell=0}^{k}\binom{k}{\ell}c_{k,\ell},$$

where the constants $c_{k,\ell}$ are given in Lemma 7.13.

In order to complete the proof, we multiply through by -2^k, and sum over all $k \ge 1$ to obtain $I_{2,2}$. Once we add in the contribution from $I_{2,1}$ given in (7.24), we have evaluated I and so the sum in question.

Note that since we have a simple form for $c_{k,0}$ and $c_{k,1}$, we can easily calculate the leading and subleading behaviour explicitly, giving for K a positive integer

$$\sum_{0<\lambda\le T}\chi\left(\frac{1}{2}+i\lambda\right) = (e^2-2)\frac{T}{2\pi} - 4e^2\gamma_0\frac{T}{2\pi}\frac{1}{L} + \frac{T}{2\pi}\sum_{m=2}^{K}\frac{e_m}{L^m} + O_K\left(\frac{T}{L^{K+1}}\right)$$

as $T \to \infty$, where

$$e_m = \sum_{k=1}^{\infty} 2^k \beta_m^{k,\ell},$$

with the $\beta_m^{k,\ell}$ as above.

7.1.7 Outline of the proof of Theorem 7.5

The proof of Theorem 7.5 is very similar to that of Theorem 7.4. We just sketch out the main steps here. Note that this result can be made unconditional but we assume the Riemann Hypothesis to make the error terms trivial to deal with.

We begin by using Cauchy's theorem to write

$$\sum_{0<\gamma\le T}\chi\left(\frac{1}{2}+i\gamma\right) = \frac{1}{2\pi i}\int_{\mathcal{C}}\frac{\zeta'}{\zeta}(s)\chi(s)\, ds,$$

where $\mathcal{C}$ is a positively oriented contour with vertices $c+i$, $c+iT$, $1-c+iT$, and $1-c+i$, where $c = 1+1/\log T$. We may assume, without loss of generality, that the distance from the contour to any zero of $\zeta(s)$ is uniformly $\gg 1/\log T$.

Note that the integrals along the bottom, top and right-hand side of the contour are bounded by $O\left(T^{1/2+\varepsilon}\right)$, using the bound $\chi(s) \ll T^{1/2-\sigma}$ for $s=\sigma+it$ with $|t| \ll T$. As before, the only contribution comes from the left-hand side of the contour, and as before, we have

$$\frac{1}{2\pi i}\int_{1-c+iT}^{1-c+i}\frac{\zeta}{\zeta}(s)\chi(s)\ ds=-\frac{1}{2\pi i}\int_{c-iT}^{c-i}\frac{\zeta}{\zeta}(1-s)\chi(1-s)\ ds=-\overline{I},$$

where

$$I=\frac{1}{2\pi i}\int_{c+i}^{c+iT}\frac{\zeta}{\zeta}(1-s)\chi(1-s)\ ds.$$

Overall, we have

$$\sum_{0<\gamma\leq T}\chi\left(\frac{1}{2}+i\gamma\right)=-\overline{I}+O\left(T^{1/2+\varepsilon}\right).$$

Next we need the functional equation for $\zeta'(s)/\zeta(s)$, which can be derived easily from either the functional equation for $\zeta(s)$ in (1.1), or Lemma 3.5. This gives

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

Substituting this into I gives

$$\begin{aligned}I=-\frac{1}{2\pi i}\int_{c+i}^{c+iT}&\log\frac{t}{2\pi}\chi(1-s)\ ds\\&-\frac{1}{2\pi i}\int_{c+i}^{c+iT}\frac{\zeta'}{\zeta}(s)\chi(1-s)\ ds+O\left(T^{1/2+\varepsilon}\right)\\&=I_1+I_2+O\left(T^{1/2+\varepsilon}\right).\end{aligned}$$

Clearly I_1 doesn't contribute to the asymptotic, so consider I_2. Then by Lemma 7.8

$$I_2=\sum_{n\leq T/2\pi}\Lambda(n)+O\left(T^{1/2+\varepsilon}\right).$$

Then by Perron/the Prime Number Theorem,

$$I_2=\frac{T}{2\pi}+O\left(T^{1/2+\varepsilon}\right).$$

The result then follows by working back up the proof.

Remark. We could see this result directly from the proof of Theorem 7.4, noticing that the logarithmic derivative of $\zeta(s)$ is included in that of $Z_1(s)$, and making the obvious changes to the proof. We have included the basic steps above for clarity.

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