Integral Moments of Quadratic Dirichlet L-functions: A Computational Perspective

by

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I hereby declare that I am the sole author of this thesis. This is a true copy of the thesis, including any required final revisions, as accepted by my examiners.

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Abstract

In recent years, the moments of L-functions has been a topic of growing interest in the field of analytic number theory. New techniques, including applications of Random Matrix Theory and multiple Dirichlet series, have lead to many well-posed theorems and conjectures for the moments of various L-functions. In this thesis, we theoretically and numerically examine the integral moments of quadratic Dirichlet L-functions. In particular, we exhibit and discuss the conjectures for the moments which result from the applications of Random Matrix Theory, number theoretic heuristics, and the theory of multiple Dirichlet series. In the case of the cubic moment, we further numerically investigate the possible existence of additional lower order main terms.

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Chapter 1

Introduction

Over the past 40 years, the utilization of Random Matrix Theory has lead to several advancements in the theory of L-functions. The marriage of these two theories was first conceived by Montgomery [**22**] in connection with his conjecture for the two-point correlations between the non-trivial zeros of the Riemann zeta function. Specifically, Montgomery realized the intimate connection such correlations held with the eigenvalues distributions of random unitary matrices. In recent years, correlations between the zeros of L-functions and the eigenvalues of random unitary matrices have become more prominent, rendering Random Matrix Theory a fundamental tool in today's study of L-functions. For example, in a paper of Conrey *et al* [**11**], random matrix theorems concerning the eigenvalue distributions of random unitary matrices were used to verify their conjectures for the integral moments of many different L-functions.

The L-functions of interest in this thesis are intimately connected to quadratic number fields and their associated characters in the following respect. Let K be the quadratic number field $\mathbb{Q}\left(\sqrt{D}\right)$, with $D \neq 0, 1$ a square-free integer, and let d be the discriminant of K:

$$d := \begin{cases} D & \text{if } D \equiv 1 \pmod 4, \\ 4D & \text{if } D \equiv 2, 3 \pmod 4). \end{cases}$$

Each such discriminant induces a corresponding character, namely, the quadratic Dirichlet character $\chi_d(n)$ given by Kronecker's extension of the Legendre symbol. To be more precise, let n be a positive integer with prime decomposition $n = p_1^{\alpha_1} \cdots p_r^{\alpha_r}$. Then

$$\left(\frac{d}{n}\right) = \left(\frac{d}{p_1}\right)^{\alpha_1} \cdots \left(\frac{d}{p_r}\right)^{\alpha_r}$$

defines the Kronecker symbol of d modulo n, with each factor characterized by the Legendre symbol

$$\left(\frac{d}{p}\right)_{p>2 \text{ prime}} = \begin{cases} 0, & \text{if } p|d \\ 1, & \text{if } p \nmid d \text{ and } x^2 \equiv d \pmod p \text{ has solutions } x \in \mathbb{Z}, \\ -1, & \text{otherwise,} \end{cases}$$

and the following extensions:

$$\left(\frac{d}{1}\right) = 1, \qquad \text{and} \qquad \left(\frac{d}{2}\right) = \begin{cases} 1, & \text{if } d \equiv 1, 7 \pmod 8, \\ -1, & \text{if } d \equiv 3, 5 \pmod 8, \\ 0, & \text{otherwise.} \end{cases}$$

Now, the Dirichlet L-series which these quadratic Dirichlet characters induce, namely

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

is an analytic function of $s \in \mathbb{C}$ for $\Re(s) > 1$. In fact, as a result of Dirichlet's class number formula, $L(s, \chi_d)$ analytically continues to an entire function of $\mathbb{C}$, and in this case, we call this function a *quadratic Dirichlet L-function.*

The primary focus of this thesis is to study the asymptotic behavior of the expression

$$\sum_{d \in D(X)} L\left(\frac{1}{2}, \chi_d\right)^k. \tag{1.1}$$

Here, k is a positive integer and

$$D(X) := \{d : d \text{ is a discriminant of } K \text{ with } |\,d\,| \leq X\}.$$

Such an expression defines the *integral moments of* $L\left(\frac{1}{2}, \chi_d\right)$.

Remark. An estimate for the cardinality of $D(X)$ is

$$|\,D(X)\,| = \frac{6}{\pi^2} X + O\left(X^{\frac{1}{2}}\right).$$

In fact, if $D(X)^+$ and $D(X)^-$ denote the set of positive and negative discriminants of K with $|\,d\,| \leq X$, respectively, then

$$\left|\,D(X)^+\,\right| = \left|\,D(X)^-\,\right| = \frac{1}{2}\,|\,D(X)\,| = \frac{3}{\pi^2} X + O\left(X^{\frac{1}{2}}\right).$$

Several conjectures exist for the asymptotics of such moments. For instance, Keating and Snaith [**19**] – motivated by the fundamental work of Katz and Sarnak [**18**] and based on an analogous result in Random Matrix Theory – conjectured a formula for the leading asymptotics of (1.1). Specifically, they conjectured that as $X \to \infty$,

$$\frac{1}{|\,D(X)\,|} \sum_{d \in D(X)} L\left(\frac{1}{2}, \chi_d\right)^k \sim a_k \prod_{j=1}^{k} \frac{j!}{(2j)!} \log(X)^{\frac{k(k+1)}{2}}, \tag{1.2}$$

where a_k is an arithmetic factor which, due to the efforts of Conrey and Farmer [**10**], takes the form

$$a_k = \prod_p \frac{\left(1 - \frac{1}{p}\right)^{\frac{k(k+1)}{2}}}{1 + \frac{1}{p}} \left(\frac{\left(1 - \frac{1}{\sqrt{p}}\right)^{-k} + \left(1 + \frac{1}{\sqrt{p}}\right)^{-k}}{2} + \frac{1}{p} \right).$$

This conjecture, including Conrey and Farmer's arithmetic factor a_k, agrees with theorems of Jutila [**17**] for $k = 1, 2$ and Soundararajan [**25**] for $k = 3$.

With respect to the full asymptotics of (1.1), the services of Random Matrix Theory were once again enlisted when Conrey *et al.*, in their paper [**11**], conjectured the following asymptotic expansion:

$$\sum_{d\in D(\infty)} L\left(\frac{1}{2},\chi_d\right)^k g(|\,d\,|) = \sum_{d\in D(\infty)} Q_k(\log|\,d\,|)\left(1+O\left(|\,d\,|^{-\frac{1}{2}+\epsilon}\right)\right)g(|\,d\,|)\,. \tag{1.3}$$

Here, g is some suitable weight function and Q_k is a polynomial of degree $k(k+1)/2$ whose leading coefficient agrees with the Keating-Snaith conjecture (1.2) (under the correct selection of $g(|\,d\,|)$). [1]

Although Random Matrix Theory served as a fundamental tool in the above conjectures, it is important to make note of an alternative approach. In particular, one can obtain a *similar* result for the cubic moments of $L\left(\frac{1}{2},\chi_d\right)$ by appealing to the philosophy of multiple Dirichlet series, as is described by Diaconu *et al.* in [**13**]. In this instance, the structure of the asymptotics are (heuristically) derived from the polar behavior of the double Dirichlet series

$$Z_3(s,w) = \sum_{d\in D(\infty)} \frac{L(s,\chi_d)^3}{|\,d\,|^w}, \qquad s,w\in\mathbb{C}.$$

Notice the use of the word similar in the above paragraph; we motivate its use as follows. When applying the philosophy of multiple Dirichlet series to the cubic moments of $L\left(\frac{1}{2},\chi_d\right)$, Diaconu *et al.* uncovered some particularly interesting structure in the associated remainder term. Specifically, due to the functional behavior of $Z(s,w)$, an additional lower order term (coined an "exception main term") of the form $bX^{\frac{3}{4}}$, for some computable constant b, comes to fruition. In fact, by building on the work of Diaconu *et al.* and performing some rather complicated residue calculations, Zhang [**28**] further discovered that $b\approx -.2154$, provided some technical conditions involving the analytic continuation and growth of $Z_3(s,w)$ are assumed.

[1] The general definition of the polynomial Q_k is described in §4.1.

Unfortunately, the existence of additional lower order terms in the asymptotics of higher moments ($k \geq 4$) remains a mystery, due to the complicated functional behavior of the associated multiple Dirichlet series. Nonetheless, Diaconu *et al.* remain confident that such terms do exist in the general moments of $L\left(\frac{1}{2}, \chi_d\right)$, contrasting the structure of the remainder term conjectured by Conrey *et al.*

To address the viability of such conjectures, a numerical perspective is beneficial. The computations for the moments of $L\left(\frac{1}{2}, \chi_d\right)$ which we present in this thesis hinge on the efficient computation of $L\left(\frac{1}{2}, \chi_d\right)$ itself for many d values. And this computation is split into two cases according to whether d is positive or negative. In the former case, we exploit a useful algebraic relationship between $L(s, \chi_d)$ and the Dedekind zeta function associated to quadratic fields. Once derived, we then show that the Dedekind zeta function (evaluated at the critical point $s = \frac{1}{2}$) yields a computationally friendly expansion in terms of K-bessel functions.[2] The latter case focuses on more traditional methods, whereby the functional behavior of $L(s, \chi_d)$ is exploited. Specifically, we calculate $L\left(\frac{1}{2}, \chi_d\right)$ using the corresponding smooth approximate functional equation for $L(s, \chi_d)$, which is representable as a combination of certain gamma functions.

The structure of this thesis is as follows. In Chapters 2 and 3, we investigate the computation of $L\left(\frac{1}{2}, \chi_d\right)$ for negative and positive discriminants d, respectively. Firstly, we derive their respective application formulas mentioned above. Secondly, for X the upper bound appearing in (1.2), we then show that the implementation of each formula has complexity $O\left(X^{\frac{3}{2}+\epsilon}\right)$, with the ϵ representing several powers of $\log(X)$. [3] In Chapter 4, an closer examination of the conjectures by Conrey *et al.* and Diaconu *et al* is undertaken. The former involves an heuristic derivation via the recipe set forth by Conrey *et al.* in [**11**]. The latter conjecture is an application of the philosophy of multiple Dirichlet series.

[2]The K used here should not be confused with the K representing the quadratic field $\mathbb{Q}\left(\sqrt{D}\right)$. Rather than K-bessel function, some authors prefer to say modified Bessel function of a second kind.

[3]The powers of $\log(X)$ yielding the ϵ differ slightly in each case.

In this instance, the functional behavior of $Z_3(s,w)$ yields an exceptional main term in the cubic moments of $L\left(\frac{1}{2},\chi_d\right)$, namely $bX^{\frac{3}{4}}$ for some effectively computed constant b. In Chapter 6, we compare the various conjectures for the moments of $L\left(\frac{1}{2},\chi_d\right)$ numerically. And finally, in Chapter 7, we outline three possible directions of further study.

Chapter 2

Computing $L\left(\frac{1}{2}, \chi_d\right)$ for $d < 0$

In this chapter, we introduce the Dedekind zeta function $\zeta_K(s)$ associated to quadratic fields $K = \mathbb{Q}\left(\sqrt{D}\right)$ and produce a formula for computing many values of $L\left(\frac{1}{2}, \chi_d\right)$, $d < 0$, via the algebraic identity[1]

$$\zeta_K(s) = \zeta(s) L(s, \chi_d)\,. \tag{2.1}$$

2.1 The Dedekind Zeta Function and Binary Quadratic Forms

Let $\mathcal{O}_K$ denote the ring of integers of K and for any nonzero integral ideal $\mathfrak{a} \subseteq \mathcal{O}_K$, let $\mathcal{N}(\mathfrak{a})$ be the *absolute norm of* $\mathfrak{a}$ defined as the positive integer[2] for which

$$\mathfrak{a}\bar{\mathfrak{a}} = (\mathcal{N}(\mathfrak{a}))\, \mathcal{O}_K.$$

[1] $\zeta(s)$ denotes the Riemann zeta function.

[2] The fact that $k\mathcal{O}_K = (-k)\mathcal{O}_K$ for any $k \in \mathbb{Z}$ validates the restriction to only positive integers without incurring any loss in generality.

For a continuous variable $s \in \mathbb{C}$, the *Dedekind zeta series* (associated to K) is defined by the series[3]

$$\zeta_K(s) = \sum_{\mathfrak{a} \subseteq \mathcal{O}_K} \frac{1}{\mathcal{N}(\mathfrak{a})^s}, \tag{2.2}$$

where the sum ranges over all nonzero integral ideals in $\mathcal{O}_K$.

The region of absolute convergence and the analytic continuation of $\zeta_K(s)$ are most easily exhibited by first expressing $\zeta_K(s)$ as an infinite product over all prime ideals in $\mathcal{O}_K$ (*Euler product*) and then examining the factoring behavior of rational primes in $\mathcal{O}_K$. To this end, we begin by (formally) writing

$$\zeta_K(s) = \prod_{\mathfrak{p} \subseteq \mathcal{O}_K} \left(1 - \frac{1}{\mathcal{N}(\mathfrak{p})^s}\right)^{-1}. \tag{2.3}$$

The (formal) existence of such an Euler product representation follows from the unique prime factorization of ideals in $\mathcal{O}_K$ and the completely multiplicative nature of $\mathcal{N}$ (which clearly follows by definition).[4]

Let us now classify the factorization of rational primes in $\mathcal{O}_K$. First note that any rational integer a yields $\mathcal{N}(a\mathcal{O}_K) = a^2$. Thus, if we consider a rational prime, say p, with decomposition in $\mathcal{O}_K$ given by

$$p\mathcal{O}_K = \mathfrak{p}_1^{e_1}\mathfrak{p}_2^{e_2}\ldots, \qquad e_1, e_2, \ldots \in \mathbb{Z},$$

then taking norms of both sides yields three possibilities:

$$\begin{cases} \mathcal{N}(\mathfrak{p}_1) = \mathcal{N}(\mathfrak{p}_2) = p, & \text{if } e_1 = e_2 = 1, \\ \mathcal{N}(\mathfrak{p}_1) = p^2, & \text{if } e_1 = 1, \\ \mathcal{N}(\mathfrak{p}_1) = p, & \text{if } e_1 = 2. \end{cases} \tag{2.4}$$

[3]Notice that if $K = \mathbb{Q}$, the $\zeta_K(s) = \zeta(s)$.

[4]The ring of integers $\mathcal{O}_K$ of any algebraic number field K is a Dedekind domain. Hence, any ideal $\mathfrak{a} \subseteq \mathcal{O}_K$ factors as a product of prime ideals (in $\mathcal{O}_K$) in a unique way.

Consequently, we see that

$$p\mathcal{O}_K = \begin{cases} \mathfrak{p}\mathfrak{q}, & \text{if } \mathcal{N}(\mathfrak{p}) = \mathcal{N}(\mathfrak{q}) = p \ (p \textbf{ splits}), \\ \mathfrak{p}, & \text{if } \mathcal{N}(\mathfrak{p}) = p^2 \ (p \textbf{ is inert}), \\ \mathfrak{p}^2, & \text{if } \mathcal{N}(\mathfrak{p}) = p \ (p \textbf{ is ramified}), \end{cases}$$

which in terms of the Kronecker symbol $\left(\frac{d}{p}\right)$, reads

$$p\mathcal{O}_K = \begin{cases} \mathfrak{p}\mathfrak{q}, & \text{if and only if } \left(\frac{d}{p}\right) = 1; \\ \mathfrak{p}, & \text{if and only if } \left(\frac{d}{p}\right) = -1; \\ \mathfrak{p}^2, & \text{if and only if } \left(\frac{d}{p}\right) = 0. \end{cases} \tag{2.5}$$

Now, observe that (2.4) implies that if $\mathfrak{p}$ is a factor in the prime factorization of $p\mathcal{O}_K$, then $\mathcal{N}(\mathfrak{p}) = p$ or p^2. Using this fact, one can (formally) extend the Euler product of $\zeta_K(s)$ to an infinite product over all rational primes in the following way. Let $\delta_{\mathfrak{p}} = 1$ or 2 according as $\mathcal{N}(\mathfrak{p}) = p$ or p^2. Then

$$\zeta_K(s) = \prod_{\mathfrak{p}} \left(1 - \frac{1}{\mathcal{N}(\mathfrak{p})^s}\right)^{-1} = \prod_p \prod_{\mathfrak{p} | p\mathcal{O}_K} \left(1 - \frac{1}{p^{s\delta_{\mathfrak{p}}}}\right)^{-1}. \tag{2.6}$$

The absolute convergence and analytic continuation of $\zeta_K(s)$ can now be readily extracted from (2.6). For the former, observe that (2.6) and the factorization of rational primes in $\mathcal{O}_K$ immediately yields $\zeta_K(s) \leq \zeta^2(s)$, giving the absolute convergence of $\zeta_K(s)$ for $\Re(s) > 1$. For the latter, we further decompose (2.6) in terms of the Kronecker symbol. Namely, we write

$$\begin{aligned} \zeta_K(s) &= \prod_p \prod_{\mathfrak{p} | p\mathcal{O}_K} \left(1 - \frac{1}{p^{s\delta_{\mathfrak{p}}}}\right)^{-1} \\ &= \prod_{\left(\frac{d}{p}\right) = -1} \left(1 - \frac{1}{p^{2s}}\right)^{-1} \prod_{\left(\frac{d}{p}\right) = 1} \left(1 - \frac{1}{p^s}\right)^{-2} \prod_{\left(\frac{d}{p}\right) = 0} \left(1 - \frac{1}{p^s}\right)^{-1} \end{aligned}$$

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

$$= \zeta(s) L(s, \chi_d),$$

where the squared factor is indicative of $\mathfrak{p}$ splitting for $\left(\frac{d}{p}\right) = 1$. As a result, the analytic continuation of $\zeta_K(s)$ mimics that of $\zeta(s)$; that is, it admits a meromorphic continuation to all of $\mathbb{C}$, with a simple pole at $s = 1$. [5]

In conclusion, we see that $\zeta_K(s)$ is in fact a Dirichlet series, absolutely convergent in $\Re(s) > 1$, which analytically continues to the entire complex plane, except for a simple pole at $s = 1$. Moreover, on establishing (2.1), we see that the Dirichlet coefficients of $\zeta_K(s)$ are given by the divisor sum

$$\sum_{m|n} \chi_d(m). \tag{2.7}$$

Conveniently, this divisor sum (and hence $\zeta_K(s)$) can be further identified by appealing to the theory of binary quadratic forms. Before exhibiting this identification, however, let us digress for a moment and take time to introduce binary quadratic forms and discuss some of their properties.

2.1.1 Binary Quadratic Forms

Let $a, b, c \in \mathbb{Z}$ and suppose that k, l are integral indeterminants. We say that a function

$$Q(k,l) = ak^2 + bkl + cl^2 = \begin{pmatrix} k & l \end{pmatrix} \begin{pmatrix} a & b/2 \\ b/2 & c \end{pmatrix} \begin{pmatrix} k \\ l \end{pmatrix}$$

is an *(integral) binary quadratic form* (or simply, a *form*) of discriminant

$$D := b^2 - 4ac.$$

[5]The residue of the simple pole at $s = 1$ yielding the analytic continuation of $\zeta_K(s)$ is significantly more complicated than that of $\zeta(s)$.

For brevity, one often writes $Q = (a, b, c)$.

First observe that $D \equiv 0, 1 \pmod 4$ since the square of any integer is congruent to 0 or 1 modulo 4. Conversely, any integer $D \equiv 0, 1 \pmod 4$ can be realized as the discriminant of a form; simply take the so-called *principal form*

$$\left(1, D \,(\mathrm{mod}\ 4), \frac{D\,(\mathrm{mod}\ 4) - D}{4}\right). \tag{2.8}$$

Ergo, we always know there exists at least one binary quadratic form of discriminant D.

The set of all binary quadratic forms can be partitioned into equivalence classes by saying two forms are equivalent if there exists a unimodular substitution between. More precisely, if two forms $Q_1 = (a_1, b_1, c_1)$ and $Q_2 = (a_2, b_2, c_2)$ are equivalent, written $Q_1 \sim Q_2$, then

$$Q_2(k, l) = Q_1(rk + sl, tk + ul), \qquad \begin{pmatrix} r & s \\ t & u \end{pmatrix} \in \mathrm{SL}_2(\mathbb{Z}).$$

This indeed defines an equivalence relation on the set of all binary quadratic forms and hence partitions the set of such forms into equivalence classes of equivalent forms. In fact, $\sim$ partitions the set of all binary quadratic forms of discriminant D, as equivalent forms share discriminant values (as one may easily check).

By further exploiting the nature of $\sim$, several additional refinements to the aforementioned partition may be attained. Before witnessing such refinements, however, let us first restrict our discussion to only forms for which $D < 0$. (The reason for such a restriction is clarified below, when the notion of *automorphs* of forms is introduced.) Such forms occur in two types according as the leading coefficient is positive or negative. To see this, assume that D is not a perfect square, so that both a and c are nonzero. Then for $a > 0$ (resp. $a < 0$), Q is *positive definite* (resp. *negative definite*); that is, $Q(k, l) \geq 0$ (resp. $Q(k, l) \leq 0$) for all $(k, l) \in \mathbb{Z}^2$. Indeed, on completing the square of Q to get

$$Q(k, l) = \frac{1}{4a}\left[(2ak + bl)^2 - Dl^2\right],$$

it is obvious that a determines the stated types.

Importantly, $\sim$ preserves integer representation. That is, if $Q_1 \sim Q_2$, then there exists $k_1, l_1 \in \mathbb{Z}$ such that $Q_1(k_1, l_1) = n \in \mathbb{Z}$ if and only if there exists $k_2, l_2 \in \mathbb{Z}$ such that $Q_2(k_2, l_2) = n$. Therefore, the forms lying within a particular equivalence class will either be all positive definite or all negative definite. Further, notice that positive and negative definite forms are in 1-1 correspondence with the negative definite forms, the latter being obtained from the former by the mapping $(a, b, c) \mapsto (-a, -b, -c)$. Thus, it suffices to only consider positive definite forms of discriminant $D < 0$, with $\sim$ partitioning the set of such forms accordingly.

Our final refinement is the link which connects the discriminants of binary quadratic forms to the discriminants of quadratic fields. Suppose Q is a binary quadratic form with relatively prime coefficients. Then we say that Q is *primitive* and call its discriminant *fundamental*. In addition to being preserved under $\sim$ (as one may easily check), the introduction of primitivity finds substance in the fact that fundamental discriminants correspond identically to discriminants of quadratic fields. Therefore, since the Dirichlet coefficients of the Dedekind zeta function involves the quadratic Dirichlet character $\chi_d(n)$ indexed by discriminants of quadratic fields, the primitivity refinement is justified.

In conclusion, the binary quadratic forms of relevance in this thesis are the primitive, positive definite forms of negative fundamental discriminant d.

2.1.2 Connecting $\zeta_K(s)$ and Binary Quadratic Forms

Let us now establish the aforementioned connection between the Dedekind zeta function and binary quadratic forms. To begin with, we define the *class number* associated to d as the number of equivalence classes of primitive, positive definite forms of negative fundamental discriminant d. Importantly, $h(d)$ is a finite positive number. Certainly,

$h(d)$ is positive since the principal forms (2.8) always exist and hence define the so-called *principal class*. For finiteness, we use the following theorem of Lagrange.

Theorem 2.1 (Lagrange)**.** *Each equivalence class of primitive, positive definite forms of negative fundamental discriminant d contains at least one form, say $Q = (a, b, c)$, for which $|b| \leq a \leq c$.*

With this theorem in hand, observe that if $Q = (a, b, c)$ is a primitive, positive definite form of discriminant $d < 0$, then

$$|d| = 4ac - b^2 \geq 3a^2 \qquad \Longrightarrow \qquad a \leq \sqrt{\frac{|d|}{3}}.$$

Hence, by Theorem 2.1, there are only finitely many values for a and b. Moreover, as c is determined by the equation

$$c = \frac{b^2 + |d|}{4a},$$

we see that c is also finite.

Now, suppose $Q_1, \ldots, Q_{h(d)}$ are representatives for the $h(d)$ equivalence classes of primitive, positive definite forms of negative fundamental discriminants d. Let $r_Q(n)$ denote the number of representations of $n \in \mathbb{Z}$ by a form Q, i.e., the number of pairs $(k, l) \in \mathbb{Z}^2$ with $Q(k, l) = n$. Put

$$r(n) = \sum_{j=1}^{h(d)} r_{Q_j}(n).$$

As part of Dirichlet's original proof of his class number formula, it was revealed that

$$r(n) = \omega \sum_{m|n} \chi_d(m), \tag{2.9}$$

where

$$\omega = \begin{cases} 2, & \text{if } d < -4, \\ 4, & \text{if } d = -4, \\ 6, & \text{if } d = -3. \end{cases} \tag{2.10}$$

Two equivalent interpretations of ω exist. In algebraic number theory, ω represents the number of roots of unity in the quadratic field of discriminant d. Alternatively, ω represents the number of automorphs of a binary quadratic form of discriminant d; that is, the number of forms which, under $\sim$, are self-equivalent.[6]

Notice that the divisor sum appearing in (2.9) is precisely the Dirichlet coefficient of $\zeta_K(s)$. As a result, the following alternative representation of $\zeta_K(s)$ exists:

$$\zeta_K(s) = \frac{1}{\omega}\sum_{n\geq 1}\frac{r(n)}{n^s} = \frac{1}{\omega}\sum_{j=1}^{h(d)}\sum_{n\geq 1}\frac{r_{Q_j}(n)}{n^s}. \tag{2.11}$$

As a final observation, we further identify the right hand side of (2.11) by introducing another Dirichlet series. Specifically, let Q be a binary quadratic form. Then the *Epstein zeta series* associated to Q is given by

$$\zeta_Q(s) = \sum{}' \frac{1}{Q(k,l)^s}, \qquad \Re(s) > 1,$$

where $\sum'$ denotes the sum over all pairs $(k,l) \in \mathbb{Z}^2$, $(k,l) \neq (0,0)$. Importantly, one can easily observe that

$$\zeta_{Q_j}(s) = \sum_{n\geq 1}\frac{r_{Q_j}(n)}{n^s}$$

for each Q_j in our representative set of forms listed above. Therefore, on appeal to (2.11), we obtain

$$\zeta_K(s) = \frac{1}{\omega}\sum_{j=1}^{h(d)}\zeta_{Q_j}(s). \tag{2.12}$$

[6]For details, see [**12, Chapter 6**].

2.2 $\zeta_K(s)$ as a Series of K-Bessel Functions

In this section, we derive a rapidly convergent expansion for $\zeta_K(s)$ in terms of K-Bessel functions via the Epstein zeta function $\zeta_Q(s)$. Specifically, define

$$B(s) = \frac{8\pi^s 2^{s-\frac{1}{2}}}{a^{\frac{1}{2}}\left|d\right|^{\frac{(2s-1)}{4}}\Gamma(s)} \sum_{n\geq 1} n^{s-\frac{1}{2}}\sigma_{1-2s}(n)\cos\left(\frac{\pi nb}{a}\right) K_{s-\frac{1}{2}}\left(\frac{\pi n\left|d\right|^{\frac{1}{2}}}{a}\right), \tag{2.13}$$

where σ is the divisor sum function

$$\sigma_\nu(n) = \sum_{r|n} r^\nu, \tag{2.14}$$

Γ is the gamma function

$$\Gamma(z) = \int_0^\infty t^{z-1}e^{-t}dt, \qquad \Re(z) > 0, \tag{2.15}$$

and K_ν is the K-Bessel function

$$K_\nu(z) = \frac{1}{2}\int_0^\infty \exp\left(-\frac{z}{2}\left(y+\frac{1}{y}\right)\right) y^{\nu-1}dy, \qquad \Re(z) > 0. \tag{2.16}$$

Then we aim to prove the following result.

Theorem 2.2 (Chowla-Selberg). *Let $Q = (a, b, c)$ be a primitive, positive definite binary quadratic form of negative fundamental discriminant d. Then $\zeta_Q(s)$ analytically continues to all $s \in \mathbb{C}$, except for a simple pole at $s = 1$, and satisfies*

$$\zeta_Q(s) = \frac{2\zeta(2s)}{a^s} + \frac{2a^{s-1}\pi^{\frac{1}{2}}\Gamma\left(s-\frac{1}{2}\right)}{\left(\left|d\right|^{\frac{1}{2}}/2\right)^{2s-1}\Gamma(s)}\zeta(2s-1) + B(s)\,. \tag{2.17}$$

Remark 1. The simple pole at $s = 1$ being claimed in Theorem 2.2 emanates from the $\zeta(2s-1)$ factor. The only other possible pole can occur at the simple pole $s = \frac{1}{2}$ of $\zeta(2s)$. As our goal is to eventually specialize to the critical point $s = \frac{1}{2}$, we must somehow ensure that $\zeta_Q(s)$ does not diverge at this point. Fortunately, this pole is not problematic in this respect and is effectively handled in the proof of Theorem 2.4 below.

Remark 2. The proof we present here follows the one given by Chowla and Selberg in [**5**], whereby the derivation mimics Riemann's classical proof of the functional equation for $\zeta(s)$.

For $\zeta_K(s)$, we appeal to (2.12) and immediately deduce that:

Theorem 2.3. *Let $Q_1, \ldots, Q_{h(d)}$ be representatives for the $h(d)$ equivalence classes of primitive, positive definite binary quadratic forms of negative fundamental discriminant d, with $Q_j = (a_j, b_j, c_j)$ for $1 \leq j \leq h(d)$. Then $\zeta_K(s)$ admits the following expansion:*

$$\zeta_K(s) = \frac{1}{\omega} \sum_{j=1}^{h(d)} \left(\frac{2\zeta(2s)}{a_j^s} + \frac{2a_j^{s-1}\pi^{\frac{1}{2}}\Gamma\left(s-\frac{1}{2}\right)}{\left(|d|^{\frac{1}{2}}/2\right)^{2s-1}\Gamma(s)}\zeta(2s-1) + B(s) \right). \tag{2.18}$$

Remark. Although the analytic continuation of $\zeta_K(s)$ to all $s \in \mathbb{C}$ was previously established in §2.1, notice that the combination of Theorem 2.2 and equation (2.12) provides further justification.

Proof of Theorem 2.2. Assume that $\Re(s) > 1$. By distinguishing the term corresponding to $l = 0$, observe that

$$\zeta_Q(s) = {\sum}' \frac{1}{Q(k,l)^s} = \frac{2\zeta(2s)}{a^s} + \sum_{k\in\mathbb{Z}} {\sum_{l\in\mathbb{Z}}}' \frac{1}{(ak^2 + bkl + cl^2)^s},$$

where ${\sum}'$ indicates that $l = 0$ has been removed. Further, on factoring out a^{-s} and completing the square, the double sum becomes

$$\frac{1}{a^s} \sum_{k\in\mathbb{Z}} {\sum_{l\in\mathbb{Z}}}' \left[\left(k + \frac{lb}{2a}\right)^2 + \frac{l^2\,|d|}{4a^2} \right]^{-s}. \tag{2.19}$$

Label the double sum in (2.19) by $F(s)$. Then we have

$$\zeta_Q(s) = \frac{2\zeta(2s)}{a^s} + \frac{1}{a^s}F(s). \tag{2.20}$$

The key at this step is to follow Riemann's proof of the functional equation of $\zeta(s)$. To this end, we introduce the gamma factor $\pi^{-s}\Gamma(s)$ and consider the expression

$$\pi^{-s}\Gamma(s)F(s) = \frac{1}{\pi^s}\int_0^\infty t^{s-1}e^{-t}\left(\sum_{k\in\mathbb{Z}}\sum_{l\in\mathbb{Z}}{}' \left[\left(k+\frac{lb}{2a}\right)^2 + \frac{l^2\,|\,d\,|}{4a^2}\right]^{-s}\right) dt. \tag{2.21}$$

If we now substitute

$$t = \left[\pi\left(k+\frac{lb}{2a}\right)^2 + \pi\frac{l^2\,|\,d\,|}{4a^2}\right] x,$$

we get

$$\begin{aligned}\pi^{-s}\Gamma(s)F(s) &= \int_0^\infty x^{s-1}\sum_{k\in\mathbb{Z}}\sum_{l\in\mathbb{Z}}{}' \exp\left(-\left[\pi\left(k+\frac{lb}{2a}\right)^2 + \pi\frac{l^2\,|\,d\,|}{4a^2}\right] x\right) dx \\ &= \int_0^\infty x^{s-1}\sum_{l\in\mathbb{Z}}{}' \exp\left(-\frac{\pi l^2\,|\,d\,|}{4a^2}x\right)\sum_{k\in\mathbb{Z}}\exp\left(-\pi\left(k+\frac{lb}{2a}\right)^2 x\right) dx.\end{aligned}$$

Using the identity

$$\sum_{n\in\mathbb{Z}}\exp\bigl(-(n+\alpha)^2\pi x\bigr) = \frac{1}{\sqrt{x}}\sum_{n\in\mathbb{Z}}\exp\left(-\frac{n^2\pi}{x}\right)\cos(2\pi n\alpha)$$

on the second sum gives

$$\int_0^\infty x^{s-1}\sum_{l\in\mathbb{Z}}{}' \exp\left(-\frac{\pi l^2\,|\,d\,|}{4a^2}x\right)\left(\frac{1}{\sqrt{x}}\sum_{k\in\mathbb{Z}}\exp\left(-\frac{\pi k^2}{x}\right)\cos\left(\frac{\pi klb}{a}\right) dx\right)$$

Further, by distinguishing the term corresponding to $k = 0$ and using symmetry, we have

$$\begin{aligned}\pi^{-s}\Gamma(s)F(s) = 2\int_0^\infty & x^{s-\frac{3}{2}}\sum_{l\geq 1}\exp\left(-\frac{\pi l^2\,|\,d\,|}{4a^2}x\right) dx \\ &+ 4\int_0^\infty x^{s-\frac{3}{2}}\sum_{k,l\geq 1}\exp\left(-\frac{\pi l^2\,|\,d\,|}{4a^2}x - \frac{\pi k^2}{x}\right)\cos\left(\frac{\pi klb}{a}\right) dx.\end{aligned} \tag{2.22}$$

Now, let I_1 and I_2 denote the former and latter integrals in (2.22), respectively. For I_1, observe that

$$\begin{aligned}\left(\frac{4a^2}{\pi\,|\,d\,|}\right)^{s-\frac{1}{2}}\Gamma\left(s-\frac{1}{2}\right)\frac{1}{l^{2s-1}} &= \left(\frac{4a^2}{\pi\,|\,d\,|}\right)^{s-\frac{1}{2}}\int_0^\infty t^{s-1}e^{-t}\frac{1}{l^{2s-1}}dt \\ &= \int_0^\infty x^{s-\frac{3}{2}}\exp\left(-\frac{\pi l^2\,|\,d\,|}{4a^2}x\right) dx,\end{aligned}$$

on substitution of

$$t = \frac{\pi l^2 \,|\, d \,|}{4a^2} x.$$

Thus, on summing over $l \geq 1$, we obtain

$$I_1 = \left(\frac{4a^2}{\pi \,|\, d \,|} \right)^{s-\frac{1}{2}} \Gamma\left(s - \frac{1}{2} \right) \zeta(2s-1)\,.$$

For I_2, we substitute

$$x = \frac{2ak}{l \,|\, d \,|^{\frac{1}{2}}} y,$$

and get

$$\begin{aligned} I_2 &= \left(\frac{2a}{|\, d \,|^{\frac{1}{2}}} \right)^{s-\frac{1}{2}} \int_0^\infty y^{s-\frac{3}{2}} \sum_{k,l \geq 1} \left(\frac{k}{l} \right)^{s-\frac{1}{2}} \cos\left(\frac{\pi klb}{a} \right) \exp\left(-\frac{\pi kl \sqrt{|\, d \,|}}{2a} \left[y + \frac{1}{y} \right] \right) dy \\ &= \frac{2 \cdot (2a)^{s-\frac{1}{2}}}{|\, d \,|^{\frac{(2s-1)}{4}}} \sum_{k,l \geq 1} \left(\frac{k}{l} \right)^{s-\frac{1}{2}} \cos\left(\frac{\pi klb}{a} \right) K_{s-\frac{1}{2}} \left(\frac{\pi kl \,|\, d \,|^{\frac{1}{2}}}{a} \right). \end{aligned}$$

Further, if we let $kl = n \geq 1$, then

$$\sum_{kl=n} \left(\frac{k}{l} \right)^{s-\frac{1}{2}} = \sum_{kl=n} \frac{(kl)^{s-\frac{1}{2}}}{l^{2s-1}} = n^{s-\frac{1}{2}} \sigma_{1-2s}(n)\,. \tag{2.23}$$

Hence, I_2 becomes

$$I_2 = \frac{2 \cdot (2a)^{s-\frac{1}{2}}}{|\, d \,|^{\frac{(2s-1)}{4}}} \sum_{n \geq 1} n^{s-\frac{1}{2}} \sigma_{1-2s}(n) \cos\left(\frac{\pi nb}{a} \right) K_{s-\frac{1}{2}} \left(\frac{\pi n \,|\, d \,|^{\frac{1}{2}}}{a} \right).$$

Therefore, on combining the formulas for I_1 and I_2, dividing through by the gamma factor $\pi^{-s}\Gamma(s)$, and plugging the resulting expression for $F(s)$ back into (2.20), we obtain (2.17) as desired. $\square$

2.3 Application Formula for $L\big(\frac{1}{2}, \chi_d\big)$

As we intend to study the integral moments of $L\big(\frac{1}{2}, \chi_d\big)$ in this thesis, let us now specialize to $s = \frac{1}{2}$ and formulate the desired result. To this end, let γ denote Euler's constant:

$$\gamma = \lim_{m\to\infty}\left(\sum_{n=1}^{m}\frac{1}{n} - \log m\right) = -\int_0^\infty e^{-t}\log t dt; \tag{2.24}$$

let $\sigma_0(n)$ be the number of positive divisors of an integer $n \geq 1$:

$$\sigma_0(n) = \sum_{r|n} 1;$$

and let $K_0(z)$ be the K-bessel function

$$K_0(z) = \int_1^\infty \exp\left(-\frac{z}{2}\left(y + \frac{1}{y}\right)\right) y^{-1} dy, \qquad \Re(z) > 0.$$

Then, we have:

Theorem 2.4. *For $Q = (a, b, c)$ a primitive, positive definite binary quadratic form of negative fundamental discriminant d, we have*

$$\zeta_Q\left(\frac{1}{2}\right) = \frac{2}{a^{\frac{1}{2}}}\left(\gamma + \log\left(\frac{|d|^{\frac{1}{2}}}{8\pi a}\right)\right) + \frac{8}{a^{\frac{1}{2}}}\sum_{n\geq 1}\sigma_0(n)\cos\left(\frac{\pi n b}{a}\right) K_0\left(\frac{\pi n |d|^{\frac{1}{2}}}{a}\right). \tag{2.25}$$

Consequently, we may appeal to (2.12) yet again and immediately deduce the following theorem.

Theorem 2.5. *Suppose $Q_1, \ldots, Q_{h(d)}$ are representative forms adhering to the description given in Theorem 2.3. Then we have*

$$\zeta_K\left(\frac{1}{2}\right) = \frac{1}{\omega}\sum_{j=1}^{h(d)}\left[\frac{2}{a_j^{\frac{1}{2}}}\left(\gamma + \log\left(\frac{|d|^{\frac{1}{2}}}{8\pi a_j}\right)\right) + \frac{8}{a_j^{\frac{1}{2}}}\sum_{n\geq 1}\sigma_0(n)\cos\left(\frac{\pi n b_j}{a_j}\right) K_0\left(\frac{\pi n |d|^{\frac{1}{2}}}{a_j}\right)\right]. \tag{2.26}$$

Remark 1. Notice that the limits of integration in the definition of K_0 differ from the general definition (2.16). Indeed, if we write

$$K_0(z) = \frac{1}{2}\left(\int_0^1 + \int_1^\infty\right) \exp\left(-\frac{z}{2}\left(y + \frac{1}{y}\right)\right) \frac{1}{y} dy,$$

and observe that under the substitution $u = y^{-1}$,

$$\int_0^1 \exp\left(-\frac{z}{2}\left(y + \frac{1}{y}\right)\right) \frac{1}{y} dy = \int_1^\infty \exp\left(-\frac{z}{2}\left(u + \frac{1}{u}\right)\right) \frac{1}{u} du,$$

then K_0 is precisely as presented in Theorem 2.4.

Remark 2. Notice that on appeal to (2.1), Theorem 2.5 now yields

$$L\left(\frac{1}{2}, \chi_d\right) = \frac{1}{\zeta\left(\frac{1}{2}\right)} \zeta_K\left(\frac{1}{2}\right) = (-0.68476523608994)\, \zeta_K(s), \tag{2.27}$$

giving a nice application formula for calculating values of $L\left(\frac{1}{2}, \chi_d\right)$.

Proof of Theorem 2.4. Observe that the last term appearing in (2.25) is simply $B\left(\frac{1}{2}\right)$, since $B(s)$ is free of poles at $s = \frac{1}{2}$.

The realization of the leading term in (2.25) is far less obvious and ultimately requires the cancellation of the simple pole at $s = \frac{1}{2}$ emanating from $\zeta(2s)$ factor. To accomplish this cancellation, we express the leading terms of (2.17) in terms of their Laurent expansions about $s = \frac{1}{2}$. In effect, the Laurent expansion for the second term in (2.17) reveals an additional simple pole at $s = \frac{1}{2}$, one which negates the existence of a simple pole at $s = \frac{1}{2}$ in the expression

$$\frac{2\zeta(2s)}{a^s} + \frac{2a^{s-1}\pi^{\frac{1}{2}}\Gamma\left(s - \frac{1}{2}\right)}{\left(|d|^{\frac{1}{2}}/2\right)^{2s-1}\Gamma(s)} \zeta(2s-1)\,.$$

To observe these circumstances more explicitly, we let $s = \frac{1}{2} + \epsilon$ with $\epsilon \to 0$ and establish the following list of expansions:

(1) $\displaystyle \frac{2}{a^s} = \frac{2}{a^{\frac{1}{2}+\epsilon}} = \frac{2}{a^{\frac{1}{2}}}(1 - \epsilon \log a + \cdots).$

(2) $\zeta(2s) = \zeta(1+2\epsilon) = \dfrac{1}{2\epsilon} + \gamma + \cdots.$

(3) $2\pi^{\frac{1}{2}} a^{s-1} = 2\pi^{\frac{1}{2}} a^{-\frac{1}{2}+\epsilon} = \dfrac{2\pi^{\frac{1}{2}}}{a^{\frac{1}{2}}}(1+\epsilon\log a + \cdots).$

(4) $\left(\dfrac{|d|^{\frac{1}{2}}}{2}\right)^{1-2s} = \left(\dfrac{|d|}{4}\right)^{-2\epsilon} = 1 - \epsilon \log\left(\dfrac{|d|}{4}\right) + \cdots.$

(5) $\Gamma\left(s-\dfrac{1}{2}\right) = \Gamma(\epsilon) = \dfrac{1}{\epsilon}(1-\gamma\epsilon+\cdots).$

(6) $\dfrac{1}{\Gamma(s)} = \dfrac{1}{\Gamma\left(\frac{1}{2}+\epsilon\right)} = \dfrac{1}{\pi^{\frac{1}{2}}}(1+(2\log 2+\gamma)\,\epsilon+\cdots).$

(7) $\zeta(2s-1) = \zeta(2\epsilon) = -\dfrac{1}{2} - \epsilon\log(2\pi) + O\left(\epsilon^2\right).$

Suppose, for the moment, that we expansions (1)-(7) at our disposal. Observe that

$$\begin{aligned}\lim_{s\to\frac{1}{2}} \frac{2\zeta(2s)}{a^s} &= \lim_{\epsilon\to 0}\left[\frac{2}{a^{\frac{1}{2}}}(1-\epsilon\log a+\cdots)\left(\frac{1}{2\epsilon}+\gamma+\cdots\right)\right] \\ &= \lim_{\epsilon\to 0}\left[\frac{1}{a^{\frac{1}{2}}\epsilon} + \frac{2\gamma}{a^{\frac{1}{2}}} - \frac{\log a}{a^{\frac{1}{2}}}\right],\end{aligned}$$

on combining (1) and (2). Further, on combining (3)-(7) and expanding the resulting product, the second term in (2.17) has an ϵ^{-1} term of the form

$$\lim_{\epsilon\to 0}\left[\frac{2\pi^{\frac{1}{2}}}{a^{\frac{1}{2}}}\cdot\frac{1}{\epsilon}\cdot\frac{1}{\pi^{\frac{1}{2}}}\cdot -\frac{1}{2}\right] = \lim_{\epsilon\to 0} -\frac{1}{a^{\frac{1}{2}}\epsilon},$$

and a constant term of the form

$$\lim_{\epsilon\to 0}\left[-\frac{1}{a^{\frac{1}{2}}}\left(\log a - \gamma - \log\left(\frac{|d|}{4}\right) + 2\log 2 + \gamma + 2\log 2\pi\right)\right] = \frac{1}{a^{\frac{1}{2}}}\log\left(\frac{|d|}{64\pi^2 a}\right).$$

Consequently, the poles of the two leading terms in (2.17) (i.e. the ϵ^{-1} terms) cancel and we obtain

$$\lim_{s\to\frac{1}{2}}\left[\frac{2\zeta(2s)}{a^s}+\frac{2a^{s-1}\pi^{\frac{1}{2}}\Gamma\left(s-\frac{1}{2}\right)}{\left(|\,d\,|^{\frac{1}{2}}/2\right)^{2s-1}\Gamma(s)}\zeta(2s-1)\right]=\frac{2\gamma}{a^{\frac{1}{2}}}-\frac{\log a}{a^{\frac{1}{2}}}+\frac{1}{a^{\frac{1}{2}}}\log\left(\frac{|\,d\,|}{64\pi^2 a}\right)$$

$$=\frac{2}{a^{\frac{1}{2}}}\left(\gamma+\log\left(\frac{|\,d\,|}{8\pi^2a^2}\right)\right).$$

Therefore, on plugging this expression and $B\left(\frac{1}{2}\right)$ into (2.17), we obtain (2.25).

So, it remains to prove expansions (1)-(7). Expansions (1), (3), and (4) follow from writing $t^z=e^{z\log t}$ ($z\in\mathbb{C}$) and expanding using the power series expansion for e^z.

For expansion (2), recall that $\zeta(z)$ admits a meromorphic continuation to all of $\mathbb{C}$ with a simple pole of residue 1 at $z=1$. Such information is encoded in its Laurent series expansion about $z=1$:

$$\zeta(z)=\frac{1}{z-1}+\sum_{n\geq 0}\frac{(-1)^n}{n!}\gamma_n(z-1)^n, \tag{2.28}$$

where

$$\gamma_n=\lim_{m\to\infty}\left(\sum_{k=1}^{m}\frac{\log^n(k)}{k}-\frac{\log^{n+1}(m)}{n+1}\right)$$

are called the *Stieltjes constants*. So, on replacing z with $1+2\epsilon$, where $1+2\epsilon\to 1$ as $\epsilon\to 0$, we see that the Laurent expansion for $\zeta(2z)$ about $z=\frac{1}{2}+\epsilon$ is precisely expansion (2) (at least the first two terms are clear from this analysis).

Next, recall that

$$\Gamma(z)=\int_0^\infty t^{z-1}e^{-t}dt, \qquad \Re(z)>0,$$

which on appeal to the well-known functional $\Gamma(z)=\frac{1}{z}\Gamma(z+1)$ reads

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

To obtain (5), we begin by expanding t^z as follows:

$$t^z = e^{z \log t} = \sum_{k=0}^{\infty} \frac{(z \log t)^k}{k!}.$$

Recall that the exponential function e^z has an infinite radius of convergence (when viewed as a power series) and converges uniformly for any bounded subset of $\mathbb{C}$. As a result, we may pass the integral through the summation and obtain

$$\Gamma(z) = \frac{1}{z} \sum_{k=0}^{\infty} \frac{z^k}{k!} \int_0^{\infty} e^{-t} \log^k(t) dt = \frac{1}{z}(1 - \gamma z + \cdots), \tag{2.29}$$

from which expansion (5) follows on taking $z = \epsilon$.

To obtain expansion (6), we consider the following Maclaurin series expansion:

$$\frac{1}{\Gamma\left(\frac{1}{2} + \epsilon\right)} = \frac{1}{\Gamma\left(\frac{1}{2}\right)} + \left[\left(\frac{1}{\Gamma\left(\frac{1}{2} + \epsilon\right)}\right)'(0)\right] \epsilon + \cdots = \frac{1}{\Gamma\left(\frac{1}{2}\right)} \left(1 - \frac{\Gamma'\left(\frac{1}{2}\right)}{\Gamma\left(\frac{1}{2}\right)} \epsilon + \cdots\right).$$

First note that $\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}$, as is immediately obvious on appeal to the well-known formula

$$\Gamma(z)\Gamma(1-z) = \frac{\pi}{\sin(\pi z)}.$$

Further, by using the Weierstrass product formula

$$\frac{1}{\Gamma(z)} = z e^{\gamma z} \prod_{n=1}^{\infty} \left(1 + \frac{z}{n}\right) e^{-z/n},$$

one can write

$$-\log \Gamma(z) = \log z + \gamma z + \sum_{n=1}^{\infty} \left(\log\left(1 + \frac{z}{n}\right) - \frac{z}{n}\right).$$

Thus, on differentiating both sides with respect to z, we get

$$-\frac{\Gamma'(z)}{\Gamma(z)} = \frac{1}{z} + \gamma + \sum_{n=1}^{\infty} \left(\frac{1}{1 + \frac{z}{n}} \cdot \frac{1}{n} - \frac{1}{n}\right) = \frac{1}{z} + \gamma + \sum_{n=1}^{\infty} \left(\frac{1}{n+z} - \frac{1}{n}\right),$$

which at $z = \frac{1}{2}$ yields

$$-\frac{\Gamma'\left(\frac{1}{2}\right)}{\Gamma\left(\frac{1}{2}\right)} = 2 + \gamma + 2\left(\sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n} - 1\right) = 2 + \gamma + 2(\log 2 - 1) = 2 \log 2 + \gamma,$$

as desired.

Finally, let us establish expansion (7). Consider the following version of the functional equation for $\zeta(z)$:

$$\zeta(1-z) = 2(2\pi)^{-z}\cos\left(\frac{\pi}{2}z\right)\Gamma(z)\zeta(z).$$

Solving for $\zeta(z)$ and plugging in 2ϵ then gives

$$\begin{aligned}\zeta(2\epsilon) &= \frac{1}{2}\cdot(2\pi)^{2\epsilon}\cdot\sec(\pi\epsilon)\cdot\frac{1}{\Gamma(2\epsilon)}\cdot\zeta(1-2\epsilon)\\ &= \frac{1}{2}(1+2\epsilon\log(2\pi)+\cdots)\cdot\left(1+\frac{1}{2}(\pi\epsilon)^2+\cdots\right)\frac{1}{\Gamma(2\epsilon)}\cdot\zeta(1-2\epsilon)\\ &= \frac{1}{2}(1+2\epsilon\log(2\pi))\cdot\big(1+O\big(\epsilon^2\big)\big)\frac{1}{\Gamma(2\epsilon)}\zeta(1-2\epsilon)\end{aligned}$$

where we have invoked the power series expansions

$$(2\pi)^{2\epsilon} = \sum_{n=0}^{\infty}\frac{(2\epsilon\log(2\pi))^n}{n!} \qquad \text{and} \qquad \sec x = 1+\frac{1}{2}x^2+\frac{5}{24}x^4+\cdots.$$

Now, by the Laurent series expansion (2.28) for $\zeta(z)$, we have

$$\zeta(1-2\epsilon) = -\frac{1}{2\epsilon}+\gamma+O(\epsilon) = -\frac{1}{2\epsilon}\big(1-2\gamma\epsilon+O\big(\epsilon^2\big)\big).$$

Further, on appeal to (2.29) we have

$$\frac{1}{\Gamma(2\epsilon)} = \frac{2\epsilon}{1-2\gamma\epsilon+O(\epsilon^2)}.$$

Therefore, the quotient $\zeta(1-2\epsilon)/\Gamma(2\epsilon)$ yields a contribution of -1 and we are left with

$$\zeta(2\epsilon) = -\frac{1}{2}(1+2\epsilon\log(2\pi))\cdot\big(1+O\big(\epsilon^2\big)\big) = -\frac{1}{2}-\epsilon\log(2\pi)+O\big(\epsilon^2\big),$$

as required. □

2.4 Analysis of Implementation

Given a negative fundamental discriminant d, the computation of $L\big(\frac{1}{2},\chi_d\big)$ is now a relatively easy application of formula (2.27). However, as we intend to compute $L\big(\frac{1}{2},\chi_d\big)$

for large sets of negative discriminants, the need for efficiency (in addition to accuracy) is paramount. To avoid possible inefficiencies, we analyze the implementation more rigorously. Such an analysis is based on several factors, including the incorporation of various mathematical tools, the implementation of numerous hacks (both trivial and clever), and a thorough understanding of how the CPU interprets, and inevitably executes, the code.

For the moment, however, let us ignore such intricacies and focus on providing a broader description of the program. We begin by considering many negative fundamental discriminants simultaneously. Specifically, we let $0 < |d| \le X$ for some X and partition the interval into blocks, say $X_1 \le |d| \le X_2$, of length $\Delta X = X_2 - X_1$. We then search for all integers a, b, c satisfying the following properties:

$$|d| = 4ac - b^2, \qquad 0 < a \le \sqrt{\frac{X_2}{3}}, \qquad 0 \le |b| \le a \le c, \qquad \frac{b^2 + X_1}{4a} \le c \le \frac{b^2 + X_2}{4a}.$$

The motivation for employing such criteria is as follows. Suppose we have found a triple (a, b, c) satisfying each of the above constraints. Then the binary quadratic form furnished by these coefficients (in addition to being primitive, positive definite and having negative fundamental discriminant d) is said to be *reduced*. Importantly, each equivalence class of primitive, positive definite binary quadratic forms of negative fundamental discriminant d contains *one and only one* reduced form. Therefore, since the implementation of our application formula (2.27) inevitably requires the selection of a representative set of forms, we see that considering only reduced forms suffices here.

Now, suppose $Q_j = (a_j, b_j, c_j)$, $1 \le j \le h(d)$, are the reduced forms which constitute a representative set for the $h(d)$ equivalence classes of primitive, positive definite binary quadratic forms of negative fundamental discriminant d. Provided we make the ratio $|d|^{\frac{1}{2}}/a_j$ large for each $1 \le j \le h(d)$, $\zeta_K\left(\frac{1}{2}\right)$ can be accurately approximated using (2.26). This follows from the exponential decay of $K_0(x)$ as $x \to \infty$. Indeed, if one writes

$$y + \frac{1}{y} = \left(y^{\frac{1}{2}} - y^{-\frac{1}{2}}\right)^2 + 2,$$

then on making the substitution $u = x^{\frac{1}{2}}\left(y^{\frac{1}{2}} - y^{-\frac{1}{2}}\right)$, one can observe that

$$|\,K_0(x)\,| \leq \frac{2e^{-x}}{\sqrt{x}} \int_0^\infty e^{-\frac{u^2}{2}} \cdot \frac{1}{y}\left(y^{-\frac{1}{2}} + y^{-\frac{3}{2}}\right)^{-1} du \leq \frac{e^{-x}}{\sqrt{x}} \int_0^\infty e^{-\frac{u^2}{2}} du,$$

since $\frac{1}{y}\left(y^{-\frac{1}{2}} + y^{-\frac{3}{2}}\right)^{-1} \leq \frac{1}{2}$. Moreover, we have

$$\int_0^\infty e^{-\frac{u^2}{2}} du = \sqrt{\frac{\pi}{2}}.$$

For observe that

$$\int_0^\infty e^{-\frac{u^2}{2}} du = \frac{1}{2} \int_{-\infty}^\infty e^{-\frac{u^2}{2}} du = \sqrt{\frac{\pi}{2}},$$

as

$$\left(\int_{-\infty}^\infty e^{-\frac{u^2}{2}} du\right)^2 = \int_{-\infty}^\infty \int_{-\infty}^\infty e^{-\frac{(u^2+v^2)}{2}} dudv = \int_0^{2\pi} \int_0^\infty e^{-\frac{r^2}{2}} r dr d\theta = 2\pi.$$

Therefore, we obtain

$$|\,K_0(x)\,| \leq \sqrt{\frac{\pi}{2x}} e^{-x}, \qquad \text{as } x \to \infty, \tag{2.30}$$

giving us exponential decay as claimed.

With this exponential decay comes many computational conveniences. For example, only 7 terms of the K-Bessel sum in (2.26) are needed to obtain 16 digits precision. To see this, simply consider the extreme case $|\,d\,| = 3$ (so $a = 1$) and use (2.30) to (crudely) observe that

$$n \geq \left\lceil \frac{16 \log(10)}{\sqrt{3}\pi} \right\rceil = 7 \qquad \Longrightarrow \qquad \left|\,K_0\left(\pi n \sqrt{3}\right)\right| \leq 10^{-16}. \tag{2.31}$$

Furthermore, we can avoid the integration associated with the K-Bessel function itself by using a precomputed table of Taylor series expansions. As the size of $|\,d\,|^{\frac{1}{2}}/a_j$ is in direct correlation with the rate of decay, the number of terms needed in the Taylor expansion is governed by this quantity. More precisely, if we want Digits precision, then the number of terms in the Taylor expansion is roughly

$$\frac{a_j (\text{Digits}) \log(10)}{\pi\,|\,d\,|^{\frac{1}{2}}}, \tag{2.32}$$

for a given $1 \leq j \leq h(d)$.

2.4.1 Hacks

By the preceding comments, it is evident that the exponential decay of the K-Bessel function removes accuracy as an obstacle. Efficiency, however, requires more ingenuity and tricks of implementation, as well as some familiarity with the interaction between the processes of fetching data from RAM and accessing the CPU cache. We begin by taking note of the following useful hacks.

Trivial Hacks.

- Since $\cos(x)$ is an even function and b_j gets squared in the discriminant equation $|d| = 4a_jc_j - b_j^2$, we can group $\pm b_j$ together and restrict to only non-negative b_j values.

- Terms such as
$$\frac{2}{a_j^{\frac{1}{2}}}(\gamma - \log(8\pi a_j))$$
appearing in the leading term of (2.26), depend solely on a_j. As such, it is to our advantage to compute this, and all other terms depending solely on a_j, outside the b_j and c_j loops. Similarly, we compute expressions like $\gcd(a_j, b_j)$ outside the c_j loop, and so on.

- For a given a_j, b_j, only one cosine needs to be computed. Indeed, given $\cos\left(\frac{\pi b_j}{a_j}\right)$, we can compute $\cos\left(\frac{\pi n b_j}{a_j}\right)$, for $n = 1, 2, \ldots, 7$, using standard trigonometric identities. For instance, the double angle identity computes the expression for $n = 2$.

- It is a well-known fact that performing divisions in computer programming require (on average) twice as many arithmetic operations than multiplication. Consequently, it is favorable to avoid divisions where possible.

- Experiment with the compiler. A compiler will not optimize your code; the structure of the program and the types of tools being employed ultimately determines the amount of time the compiled program needs to perform arithmetic operations and access RAM and/or CPU cache. For instance, sometimes it is more effective to use pointers to arrays rather than fetching data from RAM in accordance with array indices.

Clever Hacks.

- To test for primitivity, we must compute $\gcd(a_j, b_j, c_j)$ for each $1 \leq j \leq h(d)$. Such gcd computations can cause a bottleneck if handled incorrectly (as witnessed by profiling the code). However, if one computes $g_{a_j,b_j} := \gcd(a_j, b_j)$ outside the c_j loop as previously mentioned, then for a given g_{a_j,b_j}, we can compute one gcd per $c_j \pmod{g_{a_j,b_j}}$ and obtain[7]

$$\gcd(a_j, b_j, c_j) = \gcd\big(g_{a_j,b_j}, c_j \pmod{g_{a_j,b_j}}\big)\,.$$

- An expensive procedure in programming is non-sequential array accessing. When reading an array, the computer loads blocks of consecutive bytes of an array from RAM into the CPU's cache. For this reason, it is much faster to simply access the CPU's cache rather than fetching data from RAM. For instance, in the c_j loop, the values of d are decremented by $4a_j$ in accordance with $d = b_j^2 - 4a_jc_j$, leading to a potentially large decrease in d. Thus, given an array containing the values of $L\big(\frac{1}{2}, \chi_d\big)$, one should 'prefetch' the next value of $L\big(\frac{1}{2}, \chi_d\big)$, corresponding to the decremented d, in anticipation of d being decreased in such a way. C++ contains the necessary tools to perform such a prefetch and should thus be employed accordingly.

[7] An extra improvement could be achieved here by sieving through a table of factors. However, this simple hack removes the gcd computation as a bottleneck, so it suffices.

- It is advantageous to precompute a table of logarithms for the $\log(|\,d\,|)$ factor appearing in (2.26). In this instance, however, both fetching and prefetching from the resulting log table are expensive. Fortunately, we can alleviate some of the cost here by storing $L\left(\frac{1}{2}, \chi_d\right)$ and $\log|\,d\,|$ together as a pair (in a 'struct'). In doing so, a single prefetch is needed to obtain both values at once.[8]

- Since we partitioned the interval $0 < |\,d\,| \leq X$ into blocks $X_1 \leq |\,d\,| \leq X_2$, it is efficient to distribute the blocks across several processors. This will be justified later when we show that the speed at which the program runs is inversely proportional to the size of $\Delta X = X_2 - X_1$.

2.4.2 Complexity

Given that we partition the domain $0 < |\,d\,| \leq X$ into uniform blocks of length ΔX and the fact that for each such $d < 0$ we search for every triple (a, b, c) yielding a reduced form of discriminant d, it is quite clear that the computation of $L\left(\frac{1}{2}, \chi_d\right)$ for many values of $d < 0$ involves four main loops; namely, the loops corresponding to d, a, b, and c, in that order. Here we investigate the amount of work needed to execute this computation, ultimately leading us to establish the previously claimed complexity $O\left(X^{\frac{3}{2}+\epsilon}\right)$.

To begin with, there is a natural contribution to the complexity which arises from the aggregate of all constant-time calculations (i.e., $O(1)$ computations). To quantify this contribution, and for the convenience of arguments to follow, it is conducive to (more explicitly) partition the domain $0 < |\,d\,| \leq X$ as follows:

$$\underbrace{0, \ldots, \Delta X}_{\text{Block 1}}, \underbrace{\Delta X + 1, \ldots, 2\Delta X}_{\text{Block 2}}, \ldots, \underbrace{(m-1)\Delta X + 1, \ldots, m\Delta X}_{\text{Block m}}, \ldots,$$

[8] On combining the last two hacks, the overall running time of the program sped up by a factor of 2 and the array access portion sped up by a factor of 4.

where ΔX is some predetermined block length and the number of blocks (up to X) is given by $\frac{X}{\Delta X}$. [9] So, if L_{neg} denotes the overall length of all loops, then we have

$$L_{\text{neg}} = \sum_{m \le \frac{X}{\Delta X}} \sum_{a \le \sqrt{\frac{m\Delta X}{3}}} \sum_{b \le a} \sum_{c_{m-1} < c \le c_m} 1,$$

where $m, a \ge 1$, $b \ge 0$, and

$$c_{m-1} = \frac{b^2 + (m-1)\Delta X}{4a}, \qquad c_m = \frac{b^2 + m\Delta X}{4a}.$$

We now observe that

$$L_{\text{neg}} \le \sum_{m \le \frac{X}{\Delta X}} \sum_{a \le \sqrt{\frac{m\Delta X}{3}}} \sum_{b \le a} \frac{\Delta X}{4a} \le \frac{\Delta X}{4} \sum_{m \le \frac{X}{\Delta X}} \sum_{a \le \sqrt{\frac{m\Delta X}{3}}} 2 = \frac{\Delta X}{2} \sum_{m \le \frac{X}{\Delta X}} \left\lfloor \sqrt{\frac{m\Delta X}{3}} \right\rfloor,$$

where by using the notation $\lfloor x \rfloor = x - \{x\}$, with $0 \le \{x\} < 1$ the fractional part of x, further evaluation yields

$$L_{\text{neg}} \le \frac{\Delta X^{\frac{3}{2}}}{2\sqrt{3}} \sum_{m \le \frac{X}{\Delta X}} \sqrt{m}.$$

Finally, we appeal to the simple integral bound

$$\sum_{m=1}^{M} \sqrt{m} \le \int_1^M \sqrt{x} dx = \frac{2}{3}\left(M^{\frac{3}{2}} - 1\right) \tag{2.33}$$

to get

$$L_{\text{neg}} \le \frac{\Delta X^{\frac{3}{2}}}{3\sqrt{3}} \left[\left(\frac{X}{\Delta X}\right)^{\frac{3}{2}} - 1\right] \le \frac{X^{\frac{3}{2}}}{3\sqrt{3}}, \tag{2.34}$$

from whence it follows that $L_{\text{neg}} = O\left(X^{\frac{3}{2}}\right)$.

[9] Note that $\left\lceil \frac{X}{\Delta X} \right\rceil$ yields a more precise quantity for the number of blocks. However, in our computations we shall institute that the choice of ΔX be made privy to the condition $\frac{X}{\Delta X} \in \mathbb{Z}$, in which case $\left\lceil \frac{X}{\Delta X} \right\rceil = \frac{X}{\Delta X}$. Moreover, to achieve the desired complexity $O\left(X^{\frac{3}{2}+\epsilon}\right)$, we will eventually take $\Delta X = O\left(\sqrt{X}\right)$, so it is good to keep this in mind.

Further $O(1)$ computations include the K-Bessel expansion associated to $\zeta_K\left(\frac{1}{2}\right)$ and the arithmetic involved in checking for fundamental discriminants. The former follows from the fact that the Taylor series expansion invoked only requires

$$\frac{a\text{Digits}\log(10)}{\pi\,|\,d\,|^{\frac{1}{2}}}$$

terms to achieve Digits precision, with each such term only needing simple arithmetic operations. For the latter check, we simply note that given any integer in our block, say d, it is only a constant-time computation to check if d is a fundamental discriminant, i.e. to check if d or $d/4$ is square-free and then perform the necessary modular arithmetic checks. Thus, since each individual check requires $O(1)$ work, the entire checking process (for each block) requires $O(\Delta X)$ work. Indeed, to keep track of the fundamental discriminants, we must initialize an array of length ΔX for each block. Therefore, across all blocks the work is given by

$$O\left(\Delta X \cdot \frac{X}{\Delta X}\right) = O(X)\,,$$

which gets swallowed by $O\left(X^{\frac{3}{2}}\right)$ contribution previously established.

Besides these constant-time computations, the only other significant contribution to the overall complexity emanates from the gcd computations. As explained in the hacks listed above, for each triple (a, b, c) we compute $\gcd(a, b, c)$ by first computing $g_{a,b} := \gcd(a, b)$ outside the c-loop and then computing $\gcd(g_{a,b}, c \pmod{g_{a,b}})$ inside the c-loop, with the latter calculation being performed at most once per residue class modulo $g_{a,b}$. Following these instructions, we begin by computing $g_{a,b}$ using the Euclidean algorithm, whose run-time is well-known to be $O\left(\log^2 X\right)$ (since a crude approximation for the binary length of both a and b is $\log\sqrt{X}$). Therefore, the contribution for computing $g_{a,b}$ is

$$O\left(\log^2 X \sum_{m\leq\frac{X}{\Delta X}} \sum_{a\leq\sqrt{\frac{m\Delta X}{3}}} a\right) = O\left(\log^2 X \sum_{m\leq\frac{X}{\Delta X}} m\Delta X\right) = O\left(\frac{X^2\log^2 X}{\Delta X}\right),$$

where we have twice applied the asymptotic formula

$$\sum_{a\le x} a = \frac{\lfloor x\rfloor(\lfloor x\rfloor+1)}{2} = \frac{x^2}{2} + O(x)\,. \tag{2.35}$$

Next, to compute $\gcd(g_{a,b}, c \pmod{g_{a,b}})$ we initialize an array of residues modulo $g_{a,b}$ to 0. Since there are precisely $g_{a,b}$ such residues, this initialization requires

$$O\left(\sum_{m\le\frac{X}{\Delta X}}\ \sum_{a\le\sqrt{\frac{m\Delta X}{3}}}\ \sum_{b\le a} g_{a,b}\right)$$

work. We now claim that

$$\sum_{a\le x}\sum_{b\le a} g_{a,b} = \frac{x^2\log x}{2\zeta(2)} + O\big(x^2\big) = \frac{3}{\pi^2}x^2\log x + O\big(x^2\big)\,. \tag{2.36}$$

To see this, we first distinguish the $b=0$ term to give

$$\sum_{a\le x}\sum_{b\le a} g_{a,b} = \sum_{a\le x} a + \sum_{a\le x}{\sum_{b\le a}}' g_{a,b} = \frac{x^2}{2} + \sum_{a\le x}{\sum_{b\le a}}' g_{a,b} + O(x)\,,$$

where $\sum'$ indicates the removal of the $b=0$ term. The inner sum ${\sum_{b\le a}}' g_{a,b}$, which we shall denote $P(a)$, is called *Pillai's arithmetic function*, named after S. S. Pillai, who first introduced these sums in [**23**]. It was in this paper that Pillai discovered an intimate connection between $P(a)$ and Euler's totient function ϕ. Specifically, he proved the following identity:

$$P(a) = \sum_{k|n} \frac{a}{k}\phi(k).$$

Indeed, every term which appears in $P(a)$ is a factor of a. Moreover, each such factor, say g, appears precisely $\phi\Big(\frac{a}{g}\Big)$ times. This clearly follows from the well-known property that $g_{a,b} = g$ if and only if $g|a$, $g|b$, and $\gcd\Big(\frac{a}{g}, \frac{b}{g}\Big) = 1$. Therefore, by extending this argument over all divisors of a, we obtain

$$P(a) = \sum_{g|a} g\phi\left(\frac{a}{g}\right) = \sum_{k|a}\frac{a}{k}\phi(k).$$

Now, write

$$\sum_{a\le x} P(a) = \sum_{a\le x}\sum_{k|a} \frac{a}{k}\phi(k) = \sum_{a\le x} (f*h)(a),$$

where for $f(n) = n$ and $h(n) = \phi(n)$, $f*h$ denotes the Dirichlet convolution

$$(f*h)(a) = \sum_{k|a} f\left(\frac{a}{k}\right) h(k).$$

Further, let $e = f*h$ and define

$$E(x) = \sum_{n\le x} e(n), \qquad F(x) = \sum_{n\le x} f(n), \qquad \text{and} \qquad H(x) = \sum_{n\le x} h(n).$$

Then, by the generalized Dirichlet convolution [**1**]

$$E(x) = \sum_{n\ge x} f(n) H\left(\frac{x}{n}\right) = \sum_{n\le x} h(n) F\left(\frac{x}{n}\right),$$

we have

$$\sum_{a\le x}\sum_{k|a} \frac{a}{k}\phi(k) = \sum_{a\le x} P(a) = E(x) = \sum_{a\le x} \phi(a) F\left(\frac{x}{a}\right),$$

where

$$F(x) = \sum_{n\ge x} n = \frac{x^2}{2} + O(x).$$

Consequently, we have

$$\sum_{a\le x} P(a) = \sum_{a\le x} \phi(a)\left[\frac{1}{2}\left(\frac{x}{a}\right)^2 + O\left(\frac{x}{a}\right)\right] = \frac{x^2}{2}\sum_{a\le x}\frac{\phi(a)}{a^2} + O\left(x\sum_{a\le x}\frac{\phi(a)}{a}\right),$$

where by employing the asymptotic formulae [**1**]

(1) $\displaystyle\sum_{a\le x}\frac{\phi(a)}{a} = \frac{x}{\zeta(2)} + O(\log x)$, and

(2) $\displaystyle\sum_{a\le x}\frac{\phi(a)}{a^2} = \frac{\log x}{\zeta(2)} + C + O\left(\frac{\log x}{x}\right)$, where C is a constant, we obtain (2.36).

Appealing to (2.36), we see that the work associated with initializing the array of residues modulo $g_{a,b}$ is given by

$$\begin{aligned}
O\left(\sum_{m\leq\frac{X}{\Delta X}}\sum_{a\leq\sqrt{\frac{m\Delta X}{3}}}\sum_{b\leq a}g_{a,b}\right) &= O\left(\sum_{m\leq\frac{X}{\Delta X}} m\Delta X\log(m\Delta X)\right)\\
&= O\left(\Delta X\sum_{m\leq\frac{X}{\Delta X}} m\log m + \Delta X\log(\Delta X)\sum_{m\leq\frac{X}{\Delta X}} m\right)\\
&= O\left(\Delta X\left[\left(\frac{X}{\Delta X}\right)^2\log\left(\frac{X}{\Delta X}\right)\right] + \Delta X\log(\Delta X)\left(\frac{X}{\Delta X}\right)^2\right)\\
&= O\left(\frac{X^2\log X}{\Delta X}\right),
\end{aligned}$$

where we have used summation by parts to write

$$\sum_{m\leq N} m\log m = O\big(N^2\log N\big)\,, \qquad \text{for some } N\in\mathbb{N}.$$

Finally, we calculate $\gcd(a,b,c)$ via the computation of $\gcd(g_{a,b}, c \pmod{g_{a,b}})$. Since there are precisely $g_{a,b}$ residue classes modulo $g_{a,b}$ and the Euclidean algorithm requires $O\big(\log^2 X\big)$ work, the above arguments yield

$$O\left(\sum_{m\leq\frac{X}{\Delta X}}\sum_{a\leq\sqrt{\frac{m\Delta X}{3}}}\sum_{b\leq a}g_{a,b}\log^2 X\right) = O\left(\frac{X^2\log^3 X}{\Delta X}\right).$$

Therefore, the complexity of our algorithm is $O\left(X^{\frac{3}{2}+\epsilon}\right)$, provided we choose ΔX of size $\sqrt{X}$.

Chapter 3

Computing $L\left(\frac{1}{2}, \chi_d\right)$ for $d > 0$

In this chapter, we derive the smooth approximate functional equation for $L(s, \chi_d)$ via the modified L-function

$$\Lambda(s, \chi_d) := \left(\frac{d}{\pi}\right)^{\frac{s}{2}} \Gamma\left(\frac{s}{2}\right) L(s, \chi_d),$$

and use it to compute many values of $L\left(\frac{1}{2}, \chi_d\right)$ for $d > 0$. More specifically, we show that $\Lambda(s, \chi_d)$ satisfies the (symmetric) functional equation

$$\Lambda(s, \chi_d) = \Lambda(1 - s, \chi_d)\,, \tag{3.1}$$

from which the desired smooth approximate functional equation is an easy deduction.

3.1 The Smooth Approximate Functional Equation for $L\left(\frac{1}{2}, \chi_d\right)$

Although it is possible to derive the desired functional equation using local properties, it is more informative, and no more tedious, to consider any primitive Dirichlet character χ

modulo q and first derive the functional equation for $\Lambda(s,\chi)$. To this end, we let

$$\Lambda(s,\chi)=\left(\frac{q}{\pi}\right)^{\frac{s}{2}}\Gamma\left(\frac{s}{2}\right)L(s,\chi)$$

and first show that

$$\Lambda(s,\chi)=\frac{1}{2}\int_1^\infty\left[x^{\frac{s}{2}-1}\psi(x,\chi)+\frac{\sqrt{q}}{G(1,\bar{\chi})}x^{-\frac{1}{2}(s+1)}\psi(x,\bar{\chi})\right]dx, \tag{3.2}$$

where ψ and G are functions to be defined below and $\bar{\chi}$ represents the complex conjugate of χ. More symmetrically stated, this reads

$$\Lambda(s,\chi)=\frac{G(1,\chi)}{\sqrt{q}}\Lambda(1-s,\bar{\chi}). \tag{3.3}$$

3.1.1 Functional Equation of $\Lambda(s,\chi)$

Recall that the quadratic characters χ_d are precisely the real primitive Dirichlet characters associated to the quadratic field $K:=\mathbb{Q}\left(\sqrt{D}\right)$. Further, as we are assuming that $d>0$ in this instance, $\chi_d(-1)=1$ (i.e. χ_d is *even*). Accordingly, it is acceptable to restrict our discussion here to only even primitive Dirichlet characters modulo q.

The derivation we present here follows the presentation given in [**12**], which is in turn based on a proof by de la Vallée Poussin (1896), who established the result by mimicking Riemann's proof of the functional equation of $\zeta(s)$. We begin by considering the gamma function $\Gamma\left(\frac{s}{2}\right)$. Substituting $t=\frac{n^2\pi x}{q}$, we get

$$\Gamma\left(\frac{s}{2}\right)=\left(\frac{\pi}{q}\right)^{\frac{s}{2}}n^s\int_0^\infty x^{\frac{s}{2}-1}\exp\left(-\frac{n^2\pi x}{q}\right)dx, \qquad \Re(s)>0.$$

Thus, on dividing through by $\left(\frac{\pi}{q}\right)^{\frac{s}{2}}n^s$, multiplying through by $\chi(n)$ and summing both sides over all $n\geq 1$, we obtain

$$\Lambda(s,\chi):=\left(\frac{q}{\pi}\right)^{\frac{s}{2}}\Gamma\left(\frac{s}{2}\right)L(s,\chi)=\int_0^\infty x^{\frac{s}{2}-1}\left[\sum_{n\geq 1}\chi(n)\exp\left(-\frac{n^2\pi x}{q}\right)\right]dx, \tag{3.4}$$

for $\Re(s) > 1$. Further, since $\chi(0) = 0$ by definition and $\chi(-1) = 1$ by assumption, the summation on the right hand side of (3.4) can be extended to a sum over all integers n. Specifically, we can write

$$\Lambda(s,\chi) = \frac{1}{2}\int_0^\infty x^{\frac{s}{2}-1}\psi(x,\chi)\,dx, \qquad \psi(x,\chi) := \sum_{n\in\mathbb{Z}}\chi(n)\exp\left(-\frac{n^2\pi x}{q}\right). \tag{3.5}$$

Remark. The interchange of summation and integration in (3.4) is justified by the uniform convergence of

$$\sum_{n\geq 1}\chi(n)\int_0^\infty x^{\frac{s}{2}-1}\exp\left(-\frac{n^2\pi x}{q}\right)dx, \qquad x \geq 0.$$

Indeed, for $x \geq 1$, the Weierstrass M-test implies the uniform convergence of

$$\sum_{n\geq 1}\chi(n)\exp\left(-\frac{n^2\pi x}{q}\right);$$

simply observe that

$$\left|\chi(n)\exp\left(-\frac{n^2\pi x}{q}\right)\right| \leq \exp\left(-\frac{n^2\pi x}{q}\right) < \frac{q}{n^2\pi x} \leq \frac{q}{n^2\pi}, \qquad x \geq 1.$$

Similar upper bounds can be obtained for $0 \leq x < 1$ on appeal to the functional equation (3.8) given below.

Now, in Riemann's proof of the functional equation of $\zeta(s)$, the introduction of an auxiliary function is a crucial step. Specifically, one must introduce the so-called θ-function

$$\theta(x) := \sum_{n\in\mathbb{Z}}\exp\left(-n^2\pi x\right), \qquad x > 0, \tag{3.6}$$

and apply its corresponding functional equation

$$\theta\left(\frac{1}{x}\right) = \sqrt{x}\,\theta(x) \tag{3.7}$$

in order to obtain the desired functional equation for $\zeta(s)$. In a similar fashion, we introduce the function $\psi(x,\chi)$ and derive its corresponding functional equation

$$G(1,\overline{\chi})\psi(x,\chi) = \sqrt{\frac{q}{x}}\,\psi\left(\frac{1}{x},\overline{\chi}\right) \tag{3.8}$$

where $G(n,\chi)$ denotes the Gaussian sum

$$G(n,\chi) := \sum_{k=1}^{q} \chi(k) \exp\left(\frac{2\pi i n k}{q}\right).$$

In fact, as we shall see, a more general form of the functional equation (3.6) is precisely the key ingredient needed to formulate (3.8).

On the way to proving (3.8), and for the benefit of what follows, there are several standard results which need be incorporated. For convenience, we collect those results here and refer interested readers to [**12**] for details and proofs.

Proposition 3.1. *Any even primitive Dirichlet character modulo q can be written as*

$$\chi(n) = \frac{1}{G(1,\overline{\chi})} \sum_{m=1}^{q} \overline{\chi}(m) \exp\left(\frac{2\pi i n m}{q}\right) = \frac{G(n,\overline{\chi})}{G(1,\overline{\chi})}, \qquad \textit{for all } n \in \mathbb{N}. \tag{3.9}$$

Proposition 3.2. *For any even primitive Dirichlet character for the modulus q, we have*[1]

$$q = |\,G(1,\chi)\,|^2 = G(1,\chi)\overline{G(1,\chi)} = G(1,\chi)G(1,\overline{\chi}). \tag{3.10}$$

Proposition 3.3. *For all $x > 0$ and $\alpha \in \mathbb{R}$, we have*

$$\sum_{n\in\mathbb{Z}} \exp\left(-\frac{(n+\alpha)^2\pi}{x}\right) = \sqrt{x} \sum_{n\in\mathbb{Z}} \exp\left(-n^2\pi x + 2\pi i n \alpha\right). \tag{3.11}$$

With each of these preliminaries in hand, the functional equation (3.8) is now a simple deduction. First observe that Proposition 3.1 gives

$$G(1,\overline{\chi})\psi(x,\chi) = \sum_{n\in\mathbb{Z}} \left(\sum_{m=1}^{q} \overline{\chi}(m) \exp\left(\frac{2\pi i m n}{q}\right) \right) \exp\left(-\frac{n^2\pi x}{q}\right).$$

So, by combining the exponentials and applying Proposition 3.3, we get

$$\begin{aligned} G(1,\overline{\chi})\psi(x,\chi) &= \sum_{m=1}^{q} \overline{\chi}(m) \sqrt{\frac{q}{x}} \sum_{n\in\mathbb{Z}} \exp\left(-\frac{(n+m/q)^2\pi q}{x}\right) \\ &= \sqrt{\frac{q}{x}} \sum_{m=1}^{q} \overline{\chi}(m) \sum_{n\in\mathbb{Z}} \exp\left(-\frac{(nq+m)^2\pi}{xq}\right). \end{aligned}$$

[1] The last equality follows from the fact that $\chi(-1) = 1$.

Finally, put $k = nq + m$. Then $\overline{\chi}(m) = \overline{\chi}(k)$ and so

$$G(1,\overline{\chi})\psi(x,\chi) = \sqrt{\frac{q}{x}} \sum_{k\in\mathbb{Z}} \overline{\chi}(k) \exp\left(-\frac{k^2\pi}{xq}\right) = \sqrt{\frac{q}{x}}\, \psi\left(\frac{1}{x},\overline{\chi}\right).$$

We now return to (3.5), splitting the integral into two parts as follows:

$$\begin{aligned}\Lambda(s,\chi) &= \frac{1}{2}\left[\int_0^1 x^{\frac{s}{2}-1}\psi(x,\chi)\,dx + \int_1^\infty x^{\frac{s}{2}-1}\psi(x,\chi)\,dx\right] \\ &= \frac{1}{2}\int_1^\infty \left[x^{\frac{s}{2}-1}\psi(x,\chi) + x^{-\frac{s}{2}-1}\psi\left(\frac{1}{x},\chi\right)\right] dx, \end{aligned} \tag{3.12}$$

with the last line produced by substituting $x = t^{-1}$. Further, on replacing χ by $\overline{\chi}$ in the functional equation (3.8) and noting that

$$G(1,\chi)G(1,\overline{\chi}) = G(1,\chi)\overline{G(1,\chi)} = q$$

by Proposition 3.2, observe that

$$\psi\left(\frac{1}{x},\chi\right) = \sqrt{x}\,\frac{G(1,\chi)G(1,\overline{\chi})}{\sqrt{q}\,G(1,\overline{\chi})}\psi(x,\overline{\chi}) = \frac{\sqrt{q}}{G(1,\overline{\chi})}\sqrt{x}\psi(x,\overline{\chi})\,.$$

Hence, on plugging this into (3.12), we obtain the functional equation (3.2).

Importantly, the right hand side of (3.2) defines a holomorphic function of s, thus giving the analytic continuation of $L(s,\chi)$ to the entire complex plane. Further, notice that (3.2) is invariant, up to a factor depending on q and χ, under the mappings $s \mapsto 1-s$ and $\chi \mapsto \overline{\chi}$. Specifically, observe that the effect of multiplying through by $\sqrt{q}/G(1,\chi)$ is exactly identical to replacing s by $1-s$ and χ by $\overline{\chi}$. Therefore, for any even primitive Dirichlet character, (3.2) has the more symmetric form given in (3.3).

3.1.2 Functional Equation of $L(s,\chi_d)$

The functional equation of $L(s,\chi_d)$ is now a simple consequence of (3.2). Given a fundamental discriminant $d > 0$, χ_d is an real even primitive Dirichlet character modulo d, so

$\overline{\chi}_d = \chi_d$ and $\chi_d(-1) = 1$. Thus, (3.2) becomes

$$\Lambda(s,\chi_d) = \frac{1}{2}\int_1^\infty \left[x^{\frac{s}{2}-1}\psi(x,\chi_d) + \frac{\sqrt{d}}{G(1,\chi_d)}x^{-\frac{1}{2}(s+1)}\psi(x,\chi_d)\right]dx, \tag{3.13}$$

and (3.3) becomes

$$\Lambda(1-s,\chi_d) = \left(\frac{\sqrt{d}}{G(1,\chi_d)}\right)\Lambda(s,\chi_d). \tag{3.14}$$

Further, we claim that $G(1,\chi_d) = \sqrt{d}$. Indeed, by Proposition 3.2 we have

$$\sqrt{d} = |\,G(1,\chi_d)\,| = (G(1,\chi_d)G(1,\overline{\chi}_d))^{\frac{1}{2}} = \left(G(1,\chi_d)^2\right)^{\frac{1}{2}} = G(1,\chi_d).$$

Therefore, the factor $\sqrt{d}/G(1,\chi_d)$ equals 1 in both (3.13) and (3.14), displaying total invariance under the mapping $s \mapsto 1-s$ and thus yielding the required functional equation (3.1).

Remark. For the benefit of later discussions, we record a unified functional equation of $\Lambda(s,\chi_d)$ for both positive and negative discriminants d. In particular, if we let

$$a = \begin{cases} 0 & \text{if } d \geq 0, \\ 1 & \text{if } d < 0, \end{cases}$$

then we may write

$$\left(\frac{|\,d\,|}{\pi}\right)^{\frac{s+a}{2}}\Gamma\left(\frac{s+a}{2}\right)L(s,\chi_d) = \left(\frac{|\,d\,|}{\pi}\right)^{\frac{1-s+a}{2}}\Gamma\left(\frac{1-s+a}{2}\right)L(1-s,\chi_d), \tag{3.15}$$

where $|\,d\,|$ is the modulus of χ_d. More symmetrically stated, this reads

$$L(s,\chi_d) = |\,d\,|^{\frac{1}{2}-s}X(s,a)L(1-s,\chi_d), \tag{3.16}$$

where $X(s,a)$ represents the gamma factor

$$X(s,a) = \pi^{s-\frac{1}{2}}\frac{\Gamma\left(\frac{1-s+a}{2}\right)}{\Gamma\left(\frac{s+a}{2}\right)}. \tag{3.17}$$

3.1.3 Smooth Approximate Functional Equation for $L\left(\frac{1}{2}, \chi_d\right)$

The smooth approximate functional equation for $L\left(\frac{1}{2}, \chi_d\right)$ can now be easily deduced from the functional equation (3.1). Let $G(z, w)$ denote the *normalized incomplete gamma function*

$$G(z,w) := \int_1^\infty t^{z-1} e^{-wt} dt = w^{-z} \int_w^\infty x^{z-1} e^{-x} = w^{-z} \Gamma(z,w),$$

with $\Gamma(z, w)$ the *incomplete gamma function*.[2] Noting that

$$\psi(x, \chi_d) = 2 \sum_{n \geq 1} \chi_d(n) \exp\left(-\frac{n^2 \pi x}{d}\right)$$

in this instance, the functional equation (3.13) can be rewritten as

$$\Lambda(s, \chi_d) = \sum_{n \geq 1} \chi_d(n) G\left(\frac{s}{2}, \frac{n^2 \pi}{d}\right) + \sum_{n \geq 1} \chi_d(n) G\left(\frac{1-s}{2}, \frac{n^2 \pi}{d}\right). \tag{3.18}$$

So, on specializing to $s = \frac{1}{2}$, (3.18) yields

$$\left(\frac{d}{\pi}\right)^{\frac{1}{4}} \Gamma\left(\frac{1}{4}\right) L\left(\frac{1}{2}, \chi_d\right) := \Lambda\left(\frac{1}{2}, \chi_d\right) = 2 \sum_{n \geq 1} \chi_d(n) G\left(\frac{1}{4}, \frac{n^2 \pi}{d}\right).$$

Therefore, we have

$$L\left(\frac{1}{2}, \chi_d\right) = 2 \left(\frac{\pi}{d}\right)^{\frac{1}{4}} \sum_{n \geq 1} \chi_d(n) \frac{G\left(\frac{1}{4}, \frac{n^2 \pi}{d}\right)}{\Gamma\left(\frac{1}{4}\right)} = 2 \sum_{n \geq 1} \frac{\chi_d(n)}{\sqrt{n}} \frac{\Gamma\left(\frac{1}{4}, \frac{n^2 \pi}{d}\right)}{\Gamma\left(\frac{1}{4}\right)}, \tag{3.19}$$

giving the smooth approximate functional equation for $L\left(\frac{1}{2}, \chi_d\right)$.

3.2 Analysis of Implementation

Similar to the investigation conducted in §2.4, we analyze the process of implementing the smooth approximate functional equation (3.19) and quantify the associated numerical

[2] The notation $G(z, w)$ should not be confused with the Gaussian sum notation $G(n, \chi)$ used above.

complexity here. As it turns out, the complexity in this instance is also $O\left(X^{\frac{3}{2}+\epsilon}\right)$, matching the complexity for $d < 0$. Unlike the implementation for $d < 0$, however, there are several numerical issues which crop up here. For instance, due to the sporadic value distribution of $\chi_d(n)$, calculating the amount of cancellation involved and the correct truncation point become important factors to be handled carefully. The remainder of this section is devoted to treating these numerical issues and establishing the aforementioned complexity.

3.2.1 Numerical Issues

To motivate why cancellation is such a numerical issue, it is instructive to consider the following example. Consider the problem of naively computing the series expansion

$$e^{-x} = \sum_{n \geq 0} \frac{(-x)^n}{n!}$$

at, say, $x = 100$. Then

$$e^{-100} = 1 - 100 + \frac{100^2}{2!} - \frac{100^3}{3!} + \cdots,$$

so initially the terms, and the intermediate partial sums, tend to be rather large relative to the final answer. This suggests the occurrence of a considerable amount of cancellation and indeed this is the case. As a result, it becomes essential to maintain a certain degree of extra precision in order to capture the cancellation involved.

Such a phenomena is quite common when performing floating point computations. Typically, one is forced to keep track of how large the terms get relative to the final answer, so as to determine the loss in precision incurred. Fortunately for us, however, the smooth approximate functional equation (3.19) is not problematic in this respect. Nonetheless, determining the cancellation involved and the correct truncation point can be easily achieved, so we continue to pursue these endeavors here.

Put

$$f(t) = \frac{2}{\sqrt{t}} \frac{\Gamma\left(\frac{1}{4}, \frac{t^2\pi}{d}\right)}{\Gamma\left(\frac{1}{4}\right)},$$

and note that $f(t) = O\left(t^{-\frac{1}{2}}\right)$ since the latter ratio is close to 1 if t^2/d is large. In fact, $f(t) \to 0$ as $t \to \infty$ since $\Gamma(z, w) \sim e^{-w} w^{z-1}$. Now, observe that summation by parts yields

$$\sum_{n \leq N} \chi_d(n) f(n) = f(N) \sum_{n \leq N} \chi_d(n) - \int_1^N \left(\sum_{n \leq t} \chi_d(n) \right) f'(t) dt. \tag{3.20}$$

Thus, on letting $N \to \infty$, we obtain

$$L\left(\frac{1}{2}, \chi_d\right) = \sum_{n \geq 1} \chi_d(n) f(n) = -\int_1^\infty \left(\sum_{n \leq t} \chi_d(n) \right) f'(t) dt. \tag{3.21}$$

Moreover, by subtracting (3.20) from (3.21), we get an estimate for the tail:

$$\sum_{n=N+1}^{\infty} \chi_d(n) f(n) = -f(N) \sum_{m \leq N} \chi_d(m) - \int_N^\infty \left(\sum_{m \leq t} \chi_d(m) \right) f'(t) dt. \tag{3.22}$$

One could use the trivial bound $|\chi_d(n)| \leq 1$ here and get reasonable estimates for the size of the partial sums and the associated tail. However, something closer to the truth is obtained by using the conjectured (more realistic) bound

$$\sum_{n \leq x} \chi_d(n) = O\left(x^{\frac{1}{2}+\epsilon} d^\epsilon\right). \tag{3.23}$$

The purpose of using this more realistic bound is to provide a more accurate measure for the amount of cancellation actually taking place. Of course, to perform more rigorous computations, one is encouraged to use a more explicit bound. Nonetheless, by employing the more realistic bound (3.23), we get

$$f(N) \sum_{n \leq N} \chi_d(n) = O((Nd)^\epsilon), \tag{3.24}$$

and

$$\int_1^N \left(\sum_{n \leq t} \chi_d(n) \right) f'(t) dt = O\left(d^\epsilon \int_1^N t^{\frac{1}{2}+\epsilon} f'(t) dt \right) = O((Nd)^\epsilon), \tag{3.25}$$

where we have applied integration by parts to get the last equality in (3.25). Therefore, by plugging (3.24) and (3.25) back into (3.20), we obtain

$$\sum_{n\le N} \chi_d(n) f(n) = O\big((Nd)^{\epsilon}\big)\,. \tag{3.26}$$

Formula (3.26) gives us an estimate for the degree of extra precision required to capture the cancellation involved. A similar analysis shows that the tail of the series satisfies

$$\sum_{n=N+1}^{\infty} \chi_d(n) f(n) = O\left((Nd)^{\epsilon} \cdot \exp\left(-\frac{N^2\pi}{d}\right)\right). \tag{3.27}$$

So, focusing on the exponential factor in (3.27), we get an estimate for the truncation point:

$$N = \sqrt{\frac{d}{\pi}\log(10)\cdot \text{Digits}.} \tag{3.28}$$

Here, Digits denotes the working precision invoked plus a small amount, say $O(\epsilon \log d)$, to overcome the d^{ϵ} factors in the cancellation bound and the tail.

3.2.2 Hacks

The implementation of various hacks, both trivial and nontrivial, played an instrumental role in the computation of critical values $L\left(\frac{1}{2}, \chi_d\right)$ for negative fundamental discriminants $d < 0$. The role of hacks is slightly diminished here. Nonetheless, they remain an important aspect of computation, so we list a few which were helpful in the implementation of the smooth approximate functional equation (3.19).

- $\chi_d(n)$ can be efficiently computed by repeatedly extracting powers of 2 and applying quadratic reciprocity when useful.
- As in the case for $d < 0$, it is to our advantage to partition the domain $0 < d \le X$ into blocks $X_1 \le d \le X_2$ and farm the work out to many processors.

- Due to the presence of $\chi_d(n)$ in the (3.19), it is more efficient to place the d-loop on the inside and the n-loop on the outside. This swap alleviates the need of applying quadratic reciprocity each time we want to calculate $\chi_d(n)$ for a new pair d, n.

- Because n is typically much smaller than d (going up to $|d|^{\frac{1}{2}+\epsilon}$), it pays to store a precomputed table of $\chi_d(n)$ (regarded as a character modulo n or $8n_0$, for n_0 the odd part of n) so long as each residue class gets hit, on average, more than once (perhaps slightly more because of the overhead involved in storing the values and looking up the array.) In our implementation, with blocks of length 10^6, $0 < d < 10^{10}$, or so, and 16 digits working precision, it conducive to do so.[3]

- Compute the normalized incomplete gamma function $G(z, w)$, evaluated at $z = \frac{1}{4}$ and $w = \frac{n^2\pi}{d}$, as follows. For $w > 37$, return 0 (since $\exp(-37) < 10^{-16}$). For $1 < w < 37$, use a precomputed table of Taylor series, centering each Taylor series at multiples of .01 (so nearly 4000 Taylor series) and taking terms up to degree 7 (less for larger w because of the exponential decay.) Otherwise, for $w < 1$, employ the complimentary incomplete gamma function

$$\gamma(z, w) := \Gamma(z) - \Gamma(z, w) = \int_0^w e^{-x} x^{z-1} dx, \qquad \Re(z) > 0, \, |\arg w| < \pi.$$

  Specifically, set

$$g(z, w) = w^{-z}\gamma(z, w) = \int_0^1 e^{-wt} t^{z-1} dt,$$

  so $G(z, w) = w^{-z}\Gamma(z) - g(z, w)$, and integrate by parts to yield

$$g(z, w) = e^{-w} \sum_{j=0}^{\infty} \frac{w^j}{(z)_{j+1}},$$

[3] One could also create a larger precomputed table of $\chi_d(n)$ values for all the jobs (i.e. for each block of 10^6). Further, one could also save a bit by factoring n and only constructing tables for prime n. In the end, however, doing so would have made things a bit too complicated, and would not have reduced the main bottleneck, which is executing a sum of length $\sqrt{d}$.

where

$$(z)_j = \begin{cases} z(z+1)\cdots(z+j-1) & \text{if } j > 0; \\ 1 & \text{if } j = 0. \end{cases}$$

Then, by calculating $\Gamma(z)$ and $g(z, w)$ efficiently (truncating the sum once the tail is less than 10^{-16}), one can obtain a value for $G(z, w)$.

3.2.3 Complexity

Both methods, for $d < 0$ and $d > 0$, yield the same estimate for the number of arithmetic operations needed for 16 digits precision: $O\left(X^{\frac{3}{2}+\epsilon}\right)$. The powers of $\log(X)$ appearing in both estimates (hence the presence of an extra power of ϵ in $O\left(X^{\frac{3}{2}+\epsilon}\right)$) can be controlled by taking ΔX slightly larger than $\sqrt{X}$ (e.g., $\sqrt{X}\log^2(X)$ or $\sqrt{X}\log^3(X)$, depending on implementation). In the case that $d < 0$, we have already seen this to be true. In the present case, we jusitfy this claim as follows.

For $d < 0$, the powers of $\log(X)$ came from computing gcds. In this instance, they come from computing the character $\chi_d(n)$ via quadratic reciprocity. The time required to create a precomputed table of characters $\chi_d(n)$ can be quantified by considering the expression

$$\sum_{m \leq \frac{X}{\Delta X}} \sum_{n \leq M} \left(\frac{a}{n}\right),$$

where

$$M = \sqrt{\frac{m\Delta X}{\pi}\log(10)\cdot \text{Digits}.}$$

Each character $\left(\frac{a}{n}\right)$ can be calculated in time $O(\text{size}(a)\text{size}(\text{n}))$ (see [**6**] for details). Thus, since both a and n are of size X in this case, the precomputation time needed here is given by

$$O\left(\log^2(X)\sum_{m \leq \frac{X}{\Delta X}} \sum_{n \leq M} 1\right),$$

which after two applications of the estimate (2.35), reduces to

$$O\left(\frac{X^2\log^2(X)}{\Delta X}\right).$$

So, by choosing ΔX a bit larger than $\sqrt{X}$, the number of arithmetic operations performed (for 16 digits precision) in both cases is indeed $O\left(X^{\frac{3}{2}+\epsilon}\right)$.

Of course, one may inquire about the necessity of precomputing a table of character values. In carrying out computations, issues such as storage become important aspects to be handled carefully. To this point, one must ask whether it is better to precompute and store a table of roughly 10^{10} characters $\chi_d(n)$ (for all residue classes modulo $n = O\left(\sqrt{|d|}\right)$) valid for all blocks of one million, or to read from disk and transfer portions of an enormous table into RAM? Moving huge amounts of memory from disk to RAM and then cache could end up being more of a bottleneck, in practice, performing a precomputation for each block separately. In practice, we did the latter.

Due to the estimate for the number of arithmetic operations in both cases, one can reduce the time spent on the gcd and quadratic reciprocity computations entirely by choosing ΔX slightly larger than $\sqrt{X}$ at the expense of having larger arrays. As ΔX increases, there is a tradeoff between doing less computation and having larger arrays. There is a definite advantage (by a constant factor depending on the particular hardware) to having arrays that fit entirely within the cache memory of the cpu, but at some point the logarithm factors begin to outweigh that advantage.

In the case of binary quadratic forms ($d < 0$), the nice thing is that, on average, the number of triples a, b, c that are required is $O\left(\sqrt{|d|}\right)$, which does not depend on the desired precision. Precision becomes a factor only in regards to computing the particular contribution from each triple (e.g., the number of terms needed for the various K-Bessel Taylor series expansions).

In the case of the smooth approximate functional equation ($d > 0$), both the length of the sum and the amount of work needed to compute the individual terms of the sum depends on the desired precision. So, the main difference in these two approaches is the length of the sum.

For $d < 0$, an estimate for the length of the sum is

$$L_{\text{neg}} \leq \frac{1}{3\sqrt{3}} X^{\frac{3}{2}} = .19...X^{\frac{3}{2}},$$

as was calculated in §2.4.2. In the case of $d > 0$, the length of the main d, n loops, summed over all blocks of length ΔX, is quantified by

$$L_{\text{pos}} = \sum_{m \leq \frac{X}{\Delta X}} \sum_{(m-1)\Delta X < d \leq m\Delta X} \sum_{n \leq N} 1,$$

with N given by (3.28). And this quantity simplifies as follows. Applying the integral bound (2.33) twice gives

$$L_{\text{pos}} \leq \sqrt{\frac{\log(10) \cdot \text{Digits}}{\pi}} \sum_{m \leq \frac{X}{\Delta X}} \frac{2}{3} \left[(m\Delta X)^{\frac{3}{2}} - ((m-1)\,\Delta X)^{\frac{3}{2}} \right],$$

with the summand appearing here yielding a simplification via the Binomial Theorem. Specifically, observe that

$$(m-1)^{\frac{3}{2}} = \sum_{k=0}^{\infty} \binom{3/2}{k} m^{\frac{3}{2}-k} (-1)^k = m^{\frac{3}{2}} - \frac{3}{2} m^{\frac{1}{2}} + \frac{3}{8} m^{-\frac{1}{2}} - \cdots,$$

where the binomial coefficients are calculated using

$$\binom{r}{k} = \frac{r(r-1)\cdots(r-k+1)}{k!}.$$

Thus, the summand is bounded above by $m^{\frac{1}{2}} \Delta X^{\frac{3}{2}}$, yielding

$$L_{\text{pos}} \leq \sqrt{\frac{\log(10) \cdot \text{Digits}}{\pi}} \cdot \Delta X \sum_{m \leq \frac{X}{\Delta X}} m^{\frac{1}{2}}.$$

Finally, we apply the integral bound (2.33) once more and obtain

$$L_{\text{pos}} \leq \frac{2}{3} \sqrt{\frac{\log(10) \cdot \text{Digits}}{\pi}} X^{\frac{3}{2}}.$$

So, if Digits $= 16$, then $L_{\text{pos}} \leq 2.28\ldots X^{\frac{3}{2}}$, which is about ten times larger than L_{neg}. In practice, the run-time for $d < 0$ was an order or so of magnitude faster, consistent with the lengths of the loops.

Chapter 4

Integral Moments of $L\left(\frac{1}{2}, \chi_d\right)$

As previously mentioned in the introduction, Keating and Snaith [**19**] conjectured a formula for the leading asymptotics of

$$\sum_{d \in D(X)} L\left(\frac{1}{2}, \chi_d\right)^k, \qquad k \in \mathbb{Z}^+.$$

When investigating the asymptotic behavior of any function, however, one often desires to go beyond the leading asymptotics and determine the full asymptotics of the associated main term(s), as well as reveal the structure of the remainder term (if possible). Today's knowledge about the moments of L-functions is the aggregate of work, both classical and recent, accredited to a plethora of mathematicians. Due to their efforts, many theorems and conjectures for the moments of various L-functions exist. Here we focus our efforts on the integral moments of $L\left(\frac{1}{2}, \chi_d\right)$.

4.1 A Conjecture for the Integral Moments of $L\left(\frac{1}{2}, \chi_d\right)$

Under a correlation assumption between the value distributions of moments of L-functions and the eigenvalue distributions of random unitary matrices, Conrey *et al.* [**11**] were able to apply number theoretic heuristics to derive an asymptotic expansion for the integral moments of $L\left(\frac{1}{2}, \chi_d\right)$. Specifically, they conjectured the following.

Conjecture 4.1 (Conrey, Farmer, Keating, Rubinstein, Snaith)**.** *Suppose $g(t)$ is a suitable weight function with support in either $(0, \infty)$ or $(-\infty, 0)$, and let*

$$X_d(s) = |\,d\,|^{\frac{1}{2}-s}\, X(s, a),$$

where $X(s, a)$ is the gamma factor given in the functional equation (3.16). Summing over fundamental discriminants d, we have

$$\sum_{d \in D(\infty)} L\left(\frac{1}{2}, \chi_d\right)^k g(|\,d\,|) = \sum_{d \in D(\infty)} Q_k(\log |\,d\,|)\Big(1 + O\Big(|\,d\,|^{-\frac{1}{2}+\epsilon}\Big)\Big)\, g(|\,d\,|)\,, \tag{4.1}$$

where $Q_k(x)$ denotes the polynomial of degree $k(k+1)/2$ given by the k-fold residue

$$Q_k(x) = \frac{(-1)^{\frac{k(k-1)}{2}} 2^k}{k!(2\pi i)^k} \oint \cdots \oint \frac{G(z_1, \ldots, z_k)\Delta(z_1^2, \ldots, z_k^2)^2}{\prod_{j=1}^k z_j^{2k-1}} e^{\frac{x}{2}\sum_{j=1}^k z_j} dz_1 \ldots dz_k. \tag{4.2}$$

Here Δ is the Vandermonde

$$\Delta(z_1, \ldots, z_k) = \prod_{1 \le i < j \le k} (z_i - z_j)\,,$$

and

$$G(z_1, \ldots, z_k) = A_k(z_1, \ldots, z_k) \prod_{j=1}^k X\left(\frac{1}{2} + z_j, a\right)^{-\frac{1}{2}} \prod_{1 \le i \le j \le k} \zeta(1 + z_i + z_j)\,, \tag{4.3}$$

where A_k is the Euler product, absolutely convergent for $|\Re(z_j)| < \frac{1}{2}$, defined by

$$A_k(z_1, \ldots, z_k) = \prod_p \prod_{1 \le i \le j \le k} \left(1 - \frac{1}{p^{1+z_i+z_j}}\right) \times \left(1 + \left(1 + \frac{1}{p}\right)^{-1} \sum_{j=1}^{\infty} \sum_{\substack{e_1, \ldots, e_k \in \mathbb{Z} \\ e_1 + \cdots + e_k = 2j}} \prod_{i=1}^k \frac{1}{p^{e_i(s+z_i)}}\right). \tag{4.4}$$

Remark. If we take $g(|d|) = \chi_{[0,X]}(|d|)$ (the characteristic function on $[0, X]$) and use the estimate

$$|D(X)| = \frac{6}{\pi^2}X + O\Big(X^{\frac{1}{2}}\Big),$$

then Conjecture 4.1 can be stated as

$$\sum_{d\in D(X)} L\left(\frac{1}{2}, \chi_d\right)^k = \frac{6}{\pi^2}X\,\mathcal{Q}_k(\log X) + O\Big(X^{\frac{1}{2}+\epsilon}\Big). \tag{4.5}$$

Here, $\mathcal{Q}_k$ is a polynomial of degree $k(k+1)/2$ whose leading coefficient agrees with the Keating-Snaith conjecture (1.2).

4.2 Heuristic Derivation of Conjecture 4.1

In this section we heuristically derive Conjecture 4.1. To achieve this, we adhere to the general recipe for conjecturing moments of L-functions set forth by Conrey *et al.* in [**11**, §4.1]. The recipe is flawed in the fact that individual steps are performed without rigorous justification (as carefully emphasized by the authors of [**11**]). Nonetheless, when considered as a whole, the recipe serves to generate a conjecture for the moments of $L\big(\frac{1}{2}, \chi_d\big)$ which is consistent with its random matrix analogues.

So, for a fixed k, we would like to produce an asymptotic expression for the moment

$$\sum_{d\in D(\infty)} L\left(\frac{1}{2}, \chi_d\right)^k g(|d|), \tag{4.6}$$

with g a suitable weight function supported on $(-\infty, 0)$ or $(0, \infty)$. Although many traditional surveys of this problem (and of the moments of other L-functions) focus on the moments of central values $L\big(\frac{1}{2}, \chi_d\big)$, it is more informative to perturb the critical values by small shifts, say $\alpha_1, \dots, \alpha_k$, and instead consider the moment

$$\sum_{d\in D(\infty)} L\left(\frac{1}{2}+\alpha_1, \chi_d\right)\cdots L\left(\frac{1}{2}+\alpha_k, \chi_d\right) g(|d|). \tag{4.7}$$

By introducing such shifts, hidden structure in the moments is revealed in the form of symmetries. Further, these shifts tend to keep calculations relatively simple by removing higher order poles. At the appropriate time, of course, we can simply let each of $\alpha_1, \ldots, \alpha_k$ tend to 0 and obtain results for the desired moment (4.6).

To ease notation and make our arguments more aesthetically pleasing, we develop an asymptotic expansion for the moments of a slightly different L-function. Namely, we consider the Z-function

$$Z(s, \chi_d) = X_d(s)^{-\frac{1}{2}} L(s, \chi_d),$$

where $X_d(s)$ is given in the statement of Conjecture 4.1 above. Notice that $Z(s, \chi_d)$ satisfies the more symmetric functional equation $Z(s, \chi_d) = Z(1 - s, \chi_d)$ since $X_d(s)X_d(1-s) = 1$.

So, we would like to, in turn, produce an asymptotic expansion for the k shifted moment

$$L_d(s) := \sum_{d \in D(\infty)} Z(s; \alpha_1, \ldots, \alpha_k)\,, \qquad Z(s; \alpha_1, \ldots, \alpha_k) = \prod_{j=1}^{k} Z(s + \alpha_j, \chi_d)\,.$$

To do so, we adhere to the following recipe.

1. Start with the product of k shifted L-functions $Z(s; \alpha_1, \ldots, \alpha_k)$.

2. Take note of the approximate functional equation for $L(s, \chi_d)$ and replace each Z-function by its corresponding approximate functional equation, ignoring the remainder term. Multiply out to get an expression of the form

$$(\text{product of } X_d(s) \text{ factors}) \sum_{n_1, \ldots, n_k} (\text{summand})\,.$$

3. Average the resulting expression over all fundamental discriminants. Simplify the summand by appealing to the orthogonality relation for quadratic Dirichlet characters.

4. Extend each of $n_1, \ldots, n_k$ to all positive integers and call the total $M(s; \alpha_1, \ldots, \alpha_k)$.

5. The conjecture is

$$\sum_{d\in D(\infty)} Z\left(\frac{1}{2};\alpha_1,\ldots,\alpha_k\right) g(|d|) = \sum_{d\in D(\infty)} M\left(\frac{1}{2};\alpha_1,\ldots,\alpha_k\right)\left(1+O\left(|d|^{-\frac{1}{2}+\epsilon}\right)\right) g(|d|)\,.$$

Let us now exhibit the technical details involved in each of these steps. We begin by taking note of the approximate functional equation[1]

$$L(s,\chi_d) = \sum_{n<x}\frac{\chi_d(n)}{n^s} + X_d(s)\sum_{n<y}\frac{\chi_d(n)}{n^{1-s}} + \text{error}. \tag{4.8}$$

When applied to $Z(s,\chi_d)$, this yields

$$Z(s,\chi_d) = X_d(s)^{-\frac{1}{2}}\sum\frac{\chi_d(n)}{n^s} + X_d(1-s)^{-\frac{1}{2}}\sum\frac{\chi_d(n)}{n^{1-s}} + \text{error}.$$

So, since $s=\frac{1}{2}+\alpha_j$ implies that $1-s=\frac{1}{2}-\alpha_j$, we have

$$\begin{aligned} L_d(s) &= \sum_{d\in D(\infty)}\prod_{j=1}^{k}\left(X_d\left(\frac{1}{2}+\alpha_j\right)^{-\frac{1}{2}}\sum\frac{\chi_d(n)}{n^{\frac{1}{2}+\alpha_j}} + X_d\left(\frac{1}{2}-\alpha_j\right)^{-\frac{1}{2}}\sum\frac{\chi_d(n)}{n^{\frac{1}{2}-\alpha_j}} + \text{error}\right) \\ &= \sum_{d\in D(\infty)}\sum_{\varepsilon_j\in\{-1,1\}}\prod_{j=1}^{k}\left(X_d\left(\frac{1}{2}+\varepsilon_j\alpha_j\right)^{-\frac{1}{2}}\sum\frac{\chi_d(n)}{n^{\frac{1}{2}+\varepsilon_j\alpha_j}} + \text{error}\right). \end{aligned}$$

We then ignore the error term and multiply out to get[2]

$$L_d(s) = \sum_{d\in D(\infty)}\sum_{\varepsilon_j\in\{-1,1\}}\left(\prod_{j=1}^{k}X_d\left(\frac{1}{2}+\varepsilon_j\alpha_j\right)^{-\frac{1}{2}}\right)\sum_{n_1,\ldots,n_k}\frac{\chi_d(n_1\cdots n_k)}{\prod_{j=1}^{k} n_j^{\frac{1}{2}+\varepsilon_j\alpha_j}}. \tag{4.9}$$

The next step is to average over all fundamental discriminants d. As a preliminary task, we prove the following orthogonality relation for quadratic Dirichlet characters.

[1] The values of x and y are irrelevant here, since the ranges of summation will eventually be extended to infinity, as explained in step 4. We only include them here for esthetic reasons.

[2] Here we have rearranged the terms in the expansion even though absolute convergence is absent, as well as used the fact that χ_d is completely multiplicative.

Lemma 4.2. *Let* $a_m = \prod_{p|m}\left(1+\frac{1}{p}\right)^{-1}$. *Then*

$$\frac{1}{|\,D(\infty)\,|}\sum_{d\in D(\infty)}\chi_d(m) = \begin{cases} a_m & \text{if } m=\square \text{ (i.e., a perfect square)},\\ 0 & \text{otherwise.}\end{cases} \tag{4.10}$$

Proof. We prove the main contribution here and refer the interested reader to either [**11**] or [**17**, Lemma 1] for the proof when m is squarefree.

Fix a perfect square number m. In this instance, we know that $\chi_d(m) = 1$ unless $\gcd(d,m) > 1$ (in which case $\chi_d(m) = 0$). So, for $\gcd(d,m) = 1$ we are simply pulling out the subset of fundamental discriminants with no common divisor with m. To quantify the size of this subset, we must first count fundamental discriminants.

The set of fundamental discriminants consists of all square-free integers congruent to 1 modulo 4 (i.e. odd fundamental discriminants) and all such numbers multiplied by -4 and ± 8 (i.e. even fundamental discriminants). The odd fundamental discriminants may be counted by considering the series

$$\sum_{d\text{ odd}}{}^{\star}\frac{1}{|\,d\,|^s},$$

where the sum ranges over all odd fundamental discriminants. In fact, this is a Dirichlet series. For observe that

$$\sum_{d\text{ odd}}{}^{\star}\frac{1}{|\,d\,|^s} = 1+\frac{1}{3^s}+\frac{1}{5^s}+\frac{1}{7^s}+\cdots = \prod_{p>2}\left(1+\frac{1}{p^s}\right) = \frac{\zeta(s)}{\zeta(2s)}\left(1+\frac{1}{2^s}\right)^{-1},$$

where

$$\frac{\zeta(s)}{\zeta(2s)} = \sum_{n=1}^{\infty}\frac{|\,\mu(n)\,|}{n^s}$$

is the Dirichlet series which generates the square-free numbers. So, by following the definition of fundamental discriminants given above, we can count fundamental discriminants using the Dirichlet series

$$\left(1+\frac{1}{4^s}+\frac{2}{8^s}\right)\frac{\zeta(s)}{\zeta(2s)}\left(1+\frac{1}{2^s}\right)^{-1}=\left(1+\frac{1}{4^s}+\frac{2}{8^s}\right)\underbrace{\prod_{p>2}\left(1+\frac{1}{p^s}\right)}_{l_p(s)}. \tag{4.11}$$

Now, to omit those discriminants with $\gcd(d,m)>1$, we just omit the corresponding factors in $l_p(s)$. What's missing is

$$\prod_{\substack{p>2\\p\mid m}}\left(1+\frac{1}{p^s}\right),$$

so the relative density (compared to all fundamental discriminants d) can be quantified using

$$\frac{1}{l_p(s)}\cdot\prod_{\substack{p>2\\p\nmid m}}\left(1+\frac{1}{p^s}\right)=\prod_{\substack{p>2\\p\mid m}}\left(1+\frac{1}{p^s}\right)^{-1}.$$

The main contribution here comes from the simple pole at $s=1$, just as is the case in the proof of the prime number theorem. In fact, $p=2$ also fits at $s=1$ since $1+\frac{1}{4}+\frac{2}{8}=1+\frac{1}{2}$. Thus, we obtain

$$\frac{1}{|\,D(\infty)\,|}\sum_{d\in D(\infty)}\chi_d(m)=\prod_{p\mid m}\left(1+\frac{1}{p}\right)^{-1},$$

as desired. □

We now use Lemma 4.2 to simplify the summand in (4.9). This yields the heuristic expression

$$L_d\left(\frac{1}{2}\right)=\sum_{d\in D(\infty)}\underbrace{\sum_{\varepsilon_j\in\{-1,1\}}\prod_{j=1}^{k}X_d\left(\frac{1}{2}+\varepsilon_j\alpha_j\right)^{-\frac{1}{2}}R_k\left(\frac{1}{2};\varepsilon_1\alpha_1,\ldots,\varepsilon_k\alpha_k\right)}_{:=M\left(\frac{1}{2};\varepsilon_1\alpha_1,\ldots,\varepsilon_k\alpha_k\right)}. \tag{4.12}$$

Here, R_k denotes the double sum

$$R_k\left(\frac{1}{2};\alpha_1,\ldots,\alpha_k\right)=\sum_{m=1}^{\infty}\sum_{n_1\cdots n_k=m^2}\frac{a_m}{n_1^{\frac{1}{2}+\alpha_1}\cdots n_k^{\frac{1}{2}+\alpha_k}}, \tag{4.13}$$

indicating the extension of $n_1, \ldots, n_k$ to all positive integers.

The recipe now leads us to the following conjecture:

$$\sum_{d \in D(\infty)} Z\left(\frac{1}{2}; \alpha_1, \ldots, \alpha_k\right) g(|d|) = \sum_{d \in D(\infty)} M\left(\frac{1}{2}; \alpha_1, \ldots, \alpha_k\right)\left(1 + O\left(|d|^{-\frac{1}{2}+\epsilon}\right)\right) g(|d|)\,. \tag{4.14}$$

The stated conjecture is problematic, however, with respect to convergence. Specifically, the sum which defines $R_k(s; \alpha_1, \ldots, \alpha_k)$ actually diverges at $s = \frac{1}{2}$ for most choices of $\alpha_1, \ldots, \alpha_k$. For instance, it converges absolutely when $s = \frac{1}{2}$ and all the $\alpha_j > 0$, but diverges if any of the $\alpha_j < 0$.

To rectify this situation, we eliminate these divergent sums by replacing each with their corresponding analytic continuation. This is, in turn, established by expressing R_k in terms of its Euler product representation. To this end, we write $R_k = \prod_p R_{k,p}$, where

$$R_{k,p}(s; \alpha_1, \ldots, \alpha_k) = 1 + \left(1 + \frac{1}{p}\right)^{-1} \sum_{j=1}^{\infty} \sum_{e_1 + \cdots + e_k = 2j} \prod_{i=1}^{k} \frac{1}{p^{e_i(s+\alpha_i)}}. \tag{4.15}$$

Indeed, for each $p|m$ in (4.13), we want the overall power of p (from the product of n_j's) to be even. Thus, if we suppose that $p^{e_j}||n_j$, then $\sum e_j$ must be even as $\prod n_j = m^2$, which is precisely what the summation in (4.15) indicates.

The leading order poles of R_k can now be readily identified by expressing the main contribution of $R_{k,p}$ in powers of $1/p^2$. To obtain this form, we first recall the expansion

$$\left(1 + \frac{1}{p}\right)^{-1} = 1 - \frac{1}{p} + \frac{1}{p^2} - \frac{1}{p^3} + \cdots\,,$$

and write $R_{k,p}$ as

$$R_{k,p} = 1 + \sum_{l=0}^{\infty} \sum_{j=1}^{\infty} \sum_{e_1 + \cdots + e_k = 2j} \prod_{i=1}^{k} \frac{(-1)^q}{p^{e_i(s+\alpha_i)+l}}.$$

We now remark that only the terms for which $e_1 + \cdots + e_k = 2$ produce poles. For observe that $R_{k,p}$ can be written as

$$R_{k,p} = 1 + \sum_{1 \le i \le j \le k} \frac{1}{p^{2s+\alpha_i+\alpha_j}} + O\left(p^{-1-2s+\epsilon}\right) + O\left(p^{-3s+\epsilon}\right), \tag{4.16}$$

where the main summation emanates from the case $l = 0$ and $j = 1$ (i.e. $e_1 + \cdots + e_k = 2$).

Written in product form, (4.16) reads

$$R_{k,p} = \prod_{1 \le i \le j \le k} \left(1 + \frac{1}{p^{2s+\alpha_i+\alpha_j}}\right) \times \left(1 + O\big(p^{-1-2s+\epsilon}\big) + O\big(p^{-3s+\epsilon}\big)\right). \tag{4.17}$$

Now, since

$$\prod_p \left(1 + \frac{1}{p^{2s}}\right) = \frac{\zeta(2s)}{\zeta(4s)}$$

has a simple pole at $s = \frac{1}{2}$ and

$$\prod_p \left(1 + O\big(p^{-1-2s}\big) + O\big(p^{-3s}\big)\right)$$

is analytic in $\Re(s) > \frac{1}{3}$, we see that $\prod_p R_{k,p}$ has a pole at $s = \frac{1}{2}$ of order $k(k+1)/2$ if $\alpha_1 = \cdots = \alpha_k = 0$. In particular, the Euler product is now convergent at $s = \frac{1}{2}$ for each α_j's in some sufficiently small neighborhood of 0.

With the divergent sums replaced by their analytic continuation and the leading order poles clearly identified, we now put the conjecture (4.14) in a more desirable form. To this end, we first rewrite R_k as

$$\begin{aligned} R_k(s;\alpha_1,\ldots,\alpha_k) &= \prod_{1 \le i \le j \le k} \zeta(2s+\alpha_i+\alpha_j) \prod_p \left(R_{k,p}(s;\alpha_1,\ldots,\alpha_k) \prod_{1 \le i \le j \le k} \left(1 - \frac{1}{p^{2s+\alpha_i+\alpha_j}}\right)\right) \\ &= \left(\prod_{1 \le i \le j \le k} \zeta(2s+\alpha_i+\alpha_j)\right) A_k(s;\alpha_1,\ldots,\alpha_k). \end{aligned} \tag{4.18}$$

Here, A_k defines an absolutely convergent Dirichlet series for $\Re(s) > \frac{1}{2} + \delta$ for some $\delta > 0$ and for all α_j's in some sufficiently small neighborhood of 0. Subsequently, we have

$$M\left(\frac{1}{2};\varepsilon_1\alpha_1,\ldots,\varepsilon_k\alpha_k\right) = \sum_{\varepsilon_j \in \{-1,1\}} \prod_{j=1}^{k} X_d\left(\frac{1}{2} + \varepsilon_j\alpha_j\right)^{-\frac{1}{2}} A_k\left(\prod_{1 \le i \le j \le k} \zeta(1+\alpha_i+\alpha_j)\right),$$

where $A_k = A_k\left(\frac{1}{2}; \varepsilon_1\alpha_1, \ldots, \varepsilon_k\alpha_k\right)$, and the conjectured asymptotic expansion takes the form

$$\sum_{d \in D(\infty)} Z\left(\frac{1}{2}; \alpha_1, \ldots, \alpha_k\right) g(|d|)$$
$$= \sum_{d \in D(\infty)} \sum_{\varepsilon_j \in \{-1,1\}} \prod_{j=1}^{k} X_d\left(\frac{1}{2} + \varepsilon_j\alpha_j\right)^{-\frac{1}{2}} A_k \prod_{1 \le i \le j \le k} \zeta(2s + \alpha_i + \alpha_j) \tag{4.19}$$

Finally, to obtain the polynomial $Q_k(x)$ as stated in Conjecture 4.1, we substitute

$$X_d\left(\frac{1}{2} + \varepsilon_j\alpha_j\right)^{-\frac{1}{2}} = |d|^{\frac{1}{2}(\varepsilon_j\alpha_j)} X\left(\frac{1}{2} + \varepsilon_j\alpha_j, a\right), \qquad j = 1, \ldots, k,$$

and borrow the following lemma from [**11**].

Lemma 4.3. *Suppose F is a symmetric function of k variables, analytic near $(0, \ldots, 0)$, and $f(s)$ has a simple pole of residue 1 at $s = 0$ and is otherwise analytic in a neighborhood of $s = 0$, and let*

$$K(a_1, \ldots, a_k) = F(a_1, \ldots, a_k) \prod_{1 \le i \le j \le k} f(a_i + a_j).$$

If $\alpha_i + \alpha_j$ are contained in the region of analyticity of $f(s)$, then

$$\sum_{\varepsilon_j \in \{-1,1\}} K(\varepsilon_1\alpha_1, \ldots, \varepsilon_k\alpha_k) =$$
$$\frac{(-1)^{k(k-1)/2}}{(2\pi i)^k} \frac{2^k}{k!} \oint \cdots \oint K(z_1, \ldots, z_k) \frac{\Delta(z_1^2, \ldots, z_k^2) \prod_{j=1}^{k} z_j}{\prod_{1 \le i,j \le k} (z_i - \alpha_j)(z_i + \alpha_j)} dz_1 \cdots dz_k,$$

where the paths of integration encloses each of the $\pm\alpha_j$'s.

4.3 Mathematical Violations

Executing the recipe outlined in the previous section requires us to make several heuristic assumptions without providing rigorous justification. Here, we expose these mathematical violations and briefly explain the extent to which each bends reality. Following the recipe step-by-step, we have:

1. Definition.

2. Approximate functional equations often play a significant role in the analytic study of L-functions. Due to the impending structure of the recipe, the ranges of the two summations appearing in (4.8) become irrelevant. When considering the reality of the situation, however, it is worth noting that the bounds x, y ultimately depend on the modulus $|d|$. Specifically, both x and y have size $O\left(|d|^{\frac{1}{2}+\epsilon}\right)$. Neglecting this connection is one of the more subtle heuristics made in this recipe, one which continues to propagate throughout the remaining steps.

3. Off-diagonal terms are completely ignored in this step due to the application of the orthogonality relation for quadratic Dirichlet characters. The derivation of the orthogonality relation we presented in the previous section fixed each of $n_1, \ldots, n_k$ as positive integers (whether perfect square or not) and allowed the modulus $|d|$ to become arbitrarily large. This, in addition to neglecting the aforementioned connection between the n_j's and the modulus $|d|$, is problematic for the following reason. Studying moments rigorously involves the examination of a double sum: one over integers n and one over fundamental discriminants d. By fixing n, the bound which one gets is not strong enough to yield moments. For our heuristic purposes, however, it is enough to know what happens for fixed n (since we only want a sense of which terms contribute) and this has the effect of completely ignoring a (perhaps nontrivial) contribution from off-diagonal terms.

4. By extending each of $n_1, \ldots, n_k$ to all positive integers, we have again ignored the relationship these indices share with the modulus $|d|$.

5. Complete disregard with respect to divergence is undertaken in this step. Indeed, the replacement of each diverging sum $R_k\left(\frac{1}{2}; \alpha_1, \ldots, \alpha_k\right)$ by its corresponding analytic continuation increases our chances of further deviating from reality.

4.4 Multiple Dirichlet Series and the Cubic Moments of $L\left(\frac{1}{2}, \chi_d\right)$

In the field of mathematics, the existence of several solutions to the same problem is a recurrent theme. With respect to the moments of $L\left(\frac{1}{2}, \chi_d\right)$, such a theme continues to persist. In particular, due to the efforts of Diaconu *et al.* [**13**], the moments of $L\left(\frac{1}{2}, \chi_d\right)$ appearing in Conjecture 4.1 can be reformulated (at least conjecturally) by appealing to the philosophy of multiple Dirichlet series. In their paper, it was revealed that the analytic properties of $L\left(\frac{1}{2}, \chi_d\right)$, and more importantly its moments, were somehow encoded in the double Dirichlet series

$$Z_k(s, w) = \sum_{d \in D(\infty)} \frac{L(s, \chi_d)^k}{|d|^w}.$$

In fact, they showed that one may formulate a conjecture for the cubic moments of $L\left(\frac{1}{2}, \chi_d\right)$, which is *similar* to that formulated in Conjecture 4.1, by investigating the polar behavior of $Z_3(s, w)$.

Surprisingly, there is a slight discrepancy in the conclusions which the respective approaches yield in this case (hence the use of the word *similar*). As is evident by (4.5), the application of Random Matrix Theory to the moments of $L\left(\frac{1}{2}, \chi_d\right)$ yields an associated remainder term of size $O\left(X^{\frac{1}{2}+\epsilon}\right)$. A sufficient condition for obtaining this optimal error term is the meromorphic continuation of $Z_k\left(\frac{1}{2}, w\right)$ up to $\Re(w) > \frac{1}{2}$, which although widely believed to be true, remains unproven. In the special case $k = 3$, the best known approximation to this optimal error term is given by Diaconu *et al.* [**13**], where on establishing the meromorphic continuation of $Z_3\big(\frac{1}{2}, w\big)$ up to $\Re(w) > \frac{4}{5}$, they proved that

$$\sum_{d \in D(X)} L\left(\frac{1}{2}, \chi_d\right)^3 = X\mathcal{R}_3(\log X) + O\left(X^{\frac{47-\sqrt{265}}{36}+\epsilon}\right). \tag{4.20}$$

Here, $\mathcal{R}_3$ is a polynomial of degree 6 whose leading coefficient agrees with the Keating-Snaith conjecture (1.2).

During the process of obtaining this optimal statement, evidence indicating the possible existence of lower order terms of the form bX^α, $\frac{1}{2} < \alpha < 1$, came to fruition. Specifically, Diaconu *et al.* conjectured that

$$\sum_{d \in D(X)} L\left(\frac{1}{2}, \chi_d\right)^3 = X\mathcal{R}_3(\log X) + bX^{\frac{3}{4}} + O\left(X^{\frac{1}{2}+\epsilon}\right), \tag{4.21}$$

for some nonzero constant b, which they claimed could be effectively computed. In fact, although higher moments were never investigated explicitly in [**13**], Diaconu *et al.* conveyed to the reader that additional lower order terms were expected to persist in such circumstances.

Building on the foundations of Diaconu *et al.* in the cubic moment case, Zhang [**28**] used a suitable growth condition to conjecture the constant $b \approx -.2154$.[3] The conjectural nature of this constant (and the impending asymptotic expansion) is due to the fact that Zhang's arguments are completely dependent on the assumption that $Z_3\big(\frac{1}{2}, w\big)$ admits a meromorphic continuation up to $\Re(w) > \frac{1}{2}$, which, as indicated above, is only conjectural. For this reason, a skeptic may argue that b should be zero, in which case $bX^{\frac{3}{4}}$ is not a true main term and Zhang's conjecture, as well as that of Diaconu *et al.*, reduces to coincide with Conjecture 4.1 (for $k = 3$).

As the emergence of such a lower order main term in the cubic moment of $L\big(\frac{1}{2}, \chi_d\big)$ was the inspiration from which this thesis emanated, we digress for the moment and take time

[3] In fact, Zhang electronically communicated to my supervisor, Dr. Rubinstein, that the constant b is approximately $-.07$ for $d < 0$ and $-.14$ for $d > 0$.

to investigate the application of multiple Dirichlet series to this case. In particular, we explore the evidence which led Diaconu *et al.* and Zhang [**28**] to conjecture the existence of and coefficient of such an exceptional main term, respectively.

4.4.1 The Functional Equations of $Z_3(s,w)$

Many traditional applications of multiple Dirichlet series to the moment problem typically involve a thorough investigation of the analytic properties of $Z_k(s,w)$, with special emphasis placed on its polar behavior. Continuing in this tradition, we begin by establishing the following functional equations of $Z_3(s,w)$:

$$\alpha:\ (s,w)\mapsto\left(1-s,w+3s-\frac{3}{2}\right),\qquad \beta:\ (s,w)\mapsto\left(s+w-\frac{1}{2},1-w\right). \tag{4.22}$$

Although heuristic circumstances exist (see below) in which these functional equations are easily verified, working directly with $Z_3(s,w)$ to derive them is, in general, an exhaustive approach. To compensate for these difficulties, Diaconu *et al.*[**13**] adapted their arguments by extending $Z_3(s,w)$ to a sum over all integers d. In turn, this requires the introduction of suitable correction factor and hence the introduction of analogous multiple Dirichlet series. More precisely, we must introduce the (related) multiple Dirichlet series

$$Z_M(s,w;a,b)=\sum_{(d,M)=1}\frac{L(s,\chi_a\chi_{d_0})^3\,\chi_b(d_0)\,P_d^a(s)}{d^w}\prod_{p|M}\left(1-\frac{\chi_a(p)\chi_{d_0}(p)}{p^s}\right)^3. \tag{4.23}$$

Then, on applying the correct sieving process needed to isolate fundamental discriminants, it can be shown that $Z_M(s,w;a,b)$ is precisely the utility which yields all analytic properties of $Z_3(s,w)$, including its analytic continuation, functional equations α and β, and polar behavior.[4]

[4]Importantly, these new multiple Dirichlet series are meant to act as the building blocks of $Z(s,w)$, with each block satisfying the functional equations α and β (at least in s and w aspect).

Let us clarify some of the notation used here. In this situation, d is a positive integer with square-free part d_0 (so $d = d_0 d_1^2$), M is a positive square-free even integer, a, b are some relatively prime divisors (both positive and negative) of M, and $P_d^a(s)$ is some suitable Dirichlet polynomial. In fact, the Dirichlet polynomial $P_d^a(s)$ can be uniquely specified by introducing an auxiliary Dirichlet polynomial $Q_n^b(w)$, $n = n_0 n_1^2$ with n_0 square-free, satisfying the following two properties.

(1) (Functional Equations)

$$d_1^{3s} P_d^a(s) = d_1^{3(1-s)} P_d^a(1-s), \qquad n_1^w Q_n^b(w) = n_1^{1-w} Q_n^b(1-w).$$

(2) (Quadratic Reciprocity Law)

$$\begin{aligned} Z_M(s, w; a, b) &= \sum_{(d,M)=1} \frac{L(s, \chi_a \chi_{d_0})^3 \, \chi_b(d_0) \, P_d^a(s)}{d^w} \prod_{p|M} \left(1 - \frac{\chi_a(p)\chi_{d_0}(p)}{p^s}\right)^3 \\ &= \sum_{(n,M)=1} \frac{L(w, \chi_b \bar{\chi}_{n_0}) \, \chi_a(n_0) \, Q_n^b(w)}{n^s} \prod_{p|M} \left(1 - \frac{\chi_b(p)\bar{\chi}_{n_0}(p)}{p^w}\right) \\ &:= Z_M^*(s, w; a, b), \end{aligned}$$

where, in this instance, $\bar{\chi}_{d_0} = \left(\frac{\cdot}{d_0}\right)$ is obtained by applying quadratic reciprocity to χ_{d_0}.[5]

In this way, $P_d^a(s)$ and $Q_n^b(w)$ are precisely the (unique) Dirichlet polynomials required to ensure that $Z_M(s, w; a, b)$ satisfies functional equations of the form α and β, respectively. An explicit formulation of both functional equations is given in [**13**] and [**28**]. Here, we shall motivate this claim by giving a simple heuristic derivation of α and β in the special case that every integer, d and otherwise, is a positive fundamental discriminant.

[5] Notice that the roles of s and w have interchanged and the power on the L-function has been reduced to first order.

Since d is a (positive) fundamental discriminant, χ_d is primitive and $L(s,\chi_d)$ satisfies the functional equation

$$L(s,\chi_d) = d^{\frac{1}{2}-s} X(s,a) L(1-s,\chi_d),$$

with $X(s,a)$ the gamma factor given in (3.17). If we ignore the gamma factor, admitting the simplified functional equation

$$L(s,\chi_d) = d^{\frac{1}{2}-s} L(1-s,\chi_d), \tag{4.24}$$

then

$$Z_3(s,w) = \sum_{d\in D(\infty)} \frac{L(s,\chi_d)^3}{d^w} = \sum_{d\in D(\infty)} \frac{L(1-s,\chi_d)^3}{d^{w+3s-\frac{3}{2}}} = Z_3\left(1-s, w+3s-\frac{3}{2}\right), \tag{4.25}$$

which agrees with the functional equation α. [6]

To obtain β, first observe that

$$L(s,\chi_d)^3 = \sum_{n_1\geq 1} \frac{\chi_d(n_1)}{n_1^s} \sum_{n_2\geq 1} \frac{\chi_d(n_2)}{n_2^s} \sum_{n_3\geq 1} \frac{\chi_d(n_3)}{n_3^s} = \sum_{n\geq 1} \frac{d_3(n)\chi_d(n)}{n^s},$$

where d_3 is the divisor sum

$$d_3(n) = \sum_{n_1 n_2 n_3 = n} 1.$$

It then follows that

$$Z_3(s,w) = \sum_{d\in D(\infty)} \frac{L(s,\chi_d)^3}{d^w} = \sum_{d\in D(\infty)} \frac{1}{d^w} \sum_{n\geq 1} \frac{d_3(n)\chi_d(n)}{n^s}.$$

A weak version of the quadratic reciprocity law, namely

$$\chi_d(n) = \chi_n(d),$$

[6] It is quite evident that there is connection between the functional equation (4.24) and the functional equations of $P_d^a(s)$ and $Q_n^b(w)$. In fact, one can view these as analogues, giving some justification that property (1) is used to ensure that $Z_M(s,w;a,b)$ satisfies the functional equation α.

can now be invoked to give

$$Z_3(s,w) = \sum_{n\geq 1} \frac{d_3(n)}{n^s} \sum_{d\in D(\infty)} \frac{\chi_n(d)}{d^w} = \sum_{n\geq 1} \frac{d_3(n)L(w,\chi_n)}{n^s}. \tag{4.26}$$

Thus, on application of the simplified functional equation (4.24) yet again, we have

$$Z(s,w) = \sum_{n\geq 1} \frac{d_3(n)L(w,\chi_n)}{n^s} = \sum_{n\geq 1} \frac{d_3(n)L(1-w,\chi_n)}{n^{s+w-\frac{1}{2}}} = Z\left(s+w-\frac{1}{2}, 1-w\right), \tag{4.27}$$

yielding the other functional equation β. [7]

Of course, this example is indeed a heuristic as we have clearly over-simplified several properties. Remarkably, however, by using $Z_M(s,w;a,b)$ and the subsequent collection of properties associated to its correction factor, this heuristic can be made precise in the derivation of the (extended) functional equations of α and β. For explicit formulas defining the functional equations of $Z_M(s,w;a,b)$ and depicting the relationship between $Z_M(s,w;a,b)$, as well as in depth discussion about the sieving process (which sieves back to $Z_3(s,w)$), see [**13**] and [**28**].

4.4.2 Poles of $Z_3(s,w)$ and Zhang's Constant

Using Bochner's theorem and successive application of the functional equations α and β, Diaconu *et al.* [**13**, Proposition 4.10] obtained the meromorphic continuation of $Z_M(s,w;a,b)$ to all s and w in $\mathbb{C}$. Using similar treatments, they deduced that $Z_M\left(\frac{1}{2},w;a,b\right)$ was a meromorphic function of w, with the only possible poles appearing at $w=1$ and $w=\frac{3}{4}$.

[7] Just as in property (2), the roles of s and w have interchanged and the power on the L-function has been reduced to first-order (as exhibited in (4.26)). This, in addition to using a weak version of quadratic reciprocity, clearly indicates a connection between (4.27) and property (2). In fact, just as before, one may view these properties as analogues, giving some evidence that property (2) does indeed ensure that $Z_M(s,w;a,b)$ satisfies the functional equation β.

These poles can be observed as follows. Indeed, the pole at $w = 1$ appears in the buliding block $Z_M^*\left(\frac{1}{2}, w; a, 1\right)$ (and subsequently in $Z_M\left(\frac{1}{2}, w; a, 1\right)$), where for $n = 1$ (hence $n_0 = 1$), we have

$$L(w, \bar{\chi}_{n_0}\chi_b) = \zeta(w).$$

Now, any other pole of $Z_M\left(\frac{1}{2}, w; a, 1\right)$ must emanate as the image of the pole at $w = 1$ under transformations involving α and β. To this end, we first observe that

$$\alpha\left(\frac{1}{2}, w\right) = \left(\frac{1}{2}, w\right) \qquad \text{and} \qquad \beta\left(\frac{1}{2}, w\right) = (w, 1 - w)\,.$$

Thus, α fixes w and β sends $w \mapsto 1 - w$, yielding another possible pole of $Z_M\left(\frac{1}{2}, w; a, 1\right)$ at $w = 0$. This pole may be disregarded, however, as it lies outside the region of assumed continuation (i.e $\Re(w) > \frac{1}{2}$).

Next, we consider where the transformation $\alpha\beta$ sends $w = 1$. Observe that

$$\alpha\beta(s, w) = \alpha\left(s + 2 - \frac{1}{2}, 1 - w\right) = \left(\frac{3}{2} - s - w, 3s + 2w - 2\right),$$

so that on specializing to $s = \frac{1}{2}$, we have

$$\alpha\beta\left(\frac{1}{2}, w\right) = \left(1 - w, 2w - \frac{1}{2}\right).$$

Thus, we obtain a possible pole at

$$2w - \frac{1}{2} = 1 \qquad \Longrightarrow \qquad w = \frac{3}{4},$$

which does lie within the region of assumed continuation.

No other transformations need be checked, since α, β and $\alpha\beta$ characterize all possible images of the pole at $w = 1$. This follows from the fact that the set of functional equations generated by α and β form the finite group D_6 (the dihedral group of order 6) under multiplication.[8] Indeed, one may easily check that

$$\alpha^2 = \beta^2 = (\alpha\beta)^6 = (\beta\alpha)^6 = id.$$

Due to the difficulties involved with the sieving process, especially convergence of infinite series, the analyticity of $Z_3\left(\frac{1}{2}, w\right)$ becomes significantly constricted. For example, Diaconu *et al.* [**13**], by subduing some of the difficulties involved, managed to obtain the meromorphic continuation of $Z_3\left(\frac{1}{2}, w\right)$ up to $\Re(w) > \frac{4}{5}$, with the only pole being the one of order 7 at $w = 1$. By then proceeding with complex Tauberian theorems, they were able to establish (4.20), the best known approximation for the error term involved in the cubic moments of $L\left(\frac{1}{2}, \chi_d\right)$.

What of the pole at $w = \frac{3}{4}$? Is it possible to analytically continue $Z_3\left(\frac{1}{2}, w\right)$ to a larger region with the promise of attaining a legitimate pole at $w = \frac{3}{4}$? Such questions lead naturally to the work of Zhang [**28**], who further conjectured that, under suitable technical conditions, $Z_3\left(\frac{1}{2}, w\right)$ admits a simple pole at $w = \frac{3}{4}$ with complex residue

$$\operatorname*{Res}_{w=\frac{3}{4}} Z_3\left(\frac{1}{2}, w\right) \approx -0.1616.$$

Using this and complex Tauberian theorems, Zhang conjectured the existence of an exceptional main term, namely $bX^{\frac{3}{4}}$ with $b \approx -.2154$, in the asymptotic expansion for the cubic moments of $L\left(\frac{1}{2}, \chi_d\right)$.

As indicated above, however, there is a rather significant contingency associated with Zhang's arguments. Throughout his paper [**28**], it is assumed that $Z_3\left(\frac{1}{2}, w\right)$ can be continued to a meromorphic function of w up to $\Re(w) > \frac{1}{2}$, which, as previously mentioned above, is widely believed to be true, but remains unproven. Due to the difficulties involved with the application of the sieving process and complex Tauberian theorems, obtaining the

[8] It is unfortunate to note that the finiteness of the group generated by the functional equations associated to $Z_M(s, w; a, b)$ (and hence, to $Z_3(s, w)$) does not persist for higher moments. Indeed, even when encountering the fourth moments of $L\left(\frac{1}{2}, \chi_d\right)$, for example, the group of functional equations is infinite.

analyticity of $Z_3\big(\frac{1}{2}, w\big)$ up to $\Re(w) > \frac{1}{2}$ seems to be quite the formidable task. However, if one assumes that such analyticity can be obtained, then the following conjecture seems plausible.

Conjecture 4.4 (Zhang)**.** *Let $w = \sigma + it$ and assume that $Z_3\big(\frac{1}{2}, w\big)$ satisfies the growth condition*

$$Z_3\left(\frac{1}{2}, \sigma + it\right) \ll (2 + |\,t\,|)^{r+\epsilon},$$

for any $\epsilon > 0$ and some positive constant $r < 3 - 4\sigma$. Then we have

$$\sum_{d \in D(X)} L\left(\frac{1}{2}, \chi_d\right)^3 = X\mathcal{R}_3(\log X) + bX^{\frac{3}{4}} + O\left(X^{\frac{r+\sigma}{r+1}}\right),$$

where $\mathcal{R}_3$ agrees with the polynomial appearing in (4.21) and $b \approx -.2154$ (with $b \approx -.07$ if $d < 0$ and $b \approx -.14$ if $d > 0$).

Remark. The residue calculations needed to prove this conjecture are far to technically involved to be explicitly included here. We refer the interested reader to [**24**, §4] for details.

Chapter 5

Numerical Data

In this chapter, we compare the various conjectures for the moments of $L\left(\frac{1}{2}, \chi_d\right)$ from a numerical perspective. Due to physical limitations, we restrict our examination here to the first eight moments of $L\left(\frac{1}{2}, \chi_d\right)$. As expected, the collected data further verfifies the main term appearing in the moments of $L\left(\frac{1}{2}, \chi_d\right)$. With respect to the remainder term, however, there are several instances in which the numerics seem to suggest the presence of additional structure. For example, in the case of the cubic moments of $L\left(\frac{1}{2}, \chi_d\right)$, the collected data tends to agree with the conjectures of Diaconu *et al.* and Zhang regarding the existence of an exceptional main term.

To witness these intriguing properties, two quantities are of particular importance. Namely, the ratio

$$R_k(X) := \frac{\displaystyle\sum_{d \in D(X)^{\pm}} L\left(\frac{1}{2}, \chi_d\right)^k}{\displaystyle\sum_{d \in D(X)^{\pm}} Q_k(\log |\, d\,|)}, \tag{5.1}$$

and difference

$$D_k(X) := \sum_{d \in D(X)^{\pm}} L\left(\frac{1}{2}, \chi_d\right)^k g(|\, d\,|) \;-\; \sum_{d \in D(X)^{\pm}} Q_k(\log |\, d\,|)\, g(|\, d\,|)\,, \tag{5.2}$$

for $k = 1, \ldots, 8$ and both positive and negative discriminants d.[1] The former quantity measures the consistency of the main term, while the latter yields information about the associated remainder term. The numerator of (5.1) is calculated by computing many values of $L\big(\frac{1}{2}, \chi_d\big)$ while the denominator uses numerically approximated values of Q_k (computed in the same manner performed in [**11**]). The left- and right-hand terms of (5.2) are computed in a similar way.

Tables 5.1 and 5.2, reproduced from [**11**], list the various coefficients for the polynomials Q_k. Table 5.3 examines, for $k = 1, \ldots, 8$ and $g(|\,d\,|) = 1 - \frac{|d|}{X}$, the ratio $R_k(X)$ and difference $D_k(X)$ restricted to negative fundamental discriminants d. This information, including the mean up to X (indicated by the green line), is depicted in Figures 1 and 3, respectively.

In the former figure, notice that each graph clearly hovers above and below one, with the extent of fluctuation involved becoming progressively amplified as k increases (as indicated by the varying vertical scales). One can attribute this property to the size of $L\big(\frac{1}{2}, \chi_d\big)$ for higher values of k. The mean up to X does, however, remains fairly close to one, validating the main term. The latter figure also depicts fluctuation which amplifies with the order k. In this instance, however, the range of fluctuation tends to be much more dramatic (as indicated by the dramatic variation in the vertical scales). As a result, there are several instances (e.g. $k = 3$) in which the mean up to X clearly deflects away from the zero line. Such deviations raise questions about the structure of the associated remainder terms. In the cubic moment case, for instance, such deviations tend to reinforce the conjectured asymptotics of Zhang, as we show below.

Table 5.4 and Figures 2 and 4 compare and depict the same ratio and difference, respectively, but for $d > 0$. Similar fluctuations and deviations occur here as well.

To obtain the plots for $R_k(X)$ and $D_k(X)$ in both instances (i.e. $d < 0$ and $d > 0$),

[1] We use the notation $D(X)^{\pm}$ to emphasize that these quantities were calculated separately for positive and negative discriminants.

the data was sampled and collected at $X = 100000, 200000, \ldots$. For $d > 0$, we stopped the sampling at 1.2×10^{10}, yielding approximately 10000 data points. In the case of $d < 0$, the sampling was stopped at 5×10^{10}, yielding approximately 50000 data points.

5.1 Analyzing the Cubic Moment Data

Let us now concentrate our efforts on the cubic moments of $L\left(\frac{1}{2}, \chi_d\right)$ and analyze the associated data more thoroughly. Figures 5 and 6 depict the difference $D_3(X)$ for $d > 0$ and $d < 0$, respectively. In both instances, the mean up to X (indicated by a green line) and a line indicating the (running) average of the differences (indicated by a blue line) are plotted. For $d > 0$, a downward shift begins to (visibly) occur around 2×10^9 for both the mean line and average line (as depicted in Figure 5). For $d < 0$, the amplified number of data points tends to hide both the mean and average line (as one can clearly observe in Figure 6). Nevertheless, we can zoom in on the data and observe that a similar downward shift persists in this case. This is the content of Figure 7.

The depicted average line is developed as follows. For the first M differences, we sample the average of $D_3(X)$ at $X = m \cdot 10^6$, for $m = 1, \ldots, M$. That is, for $X = m \cdot 10^6$, we consider the expression

$$\frac{1}{M} \sum_{m=1}^{M} D_3(X) = \frac{1}{M} \sum_{m=1}^{M} \left(\sum_{d \in D(X)^{\pm}} L\left(\frac{1}{2}, \chi_d\right)^3 g(|d|) - \sum_{d \in D(X)^{\pm}} Q_3(\log |d|)\, g(|d|) \right).$$

According to Diaconu *et al.*, this expression takes the conjectured form

$$\frac{1}{M} \sum_{m=1}^{M} \left(b \cdot \left(m \cdot 10^6\right)^{\frac{3}{4}} + O\left(\left(m \cdot 10^6\right)^{\frac{1}{2}+\epsilon}\right)\right),$$

where by Zhang's conjecture, $b \approx -.14$ or $b \approx -.07$ according as $d > 0$ or $d < 0$. The main term which appears here can be simplified using an easy integral bound. Specifically, observe that

$$b \cdot \left(10^6\right)^{\frac{3}{4}} \cdot \frac{1}{M} \sum_{m=1}^{M} m^{\frac{3}{4}} \sim b \cdot \left(10^6\right)^{\frac{3}{4}} \cdot \frac{1}{M} \int_1^M t^{\frac{3}{4}} dt \sim \frac{4}{7} b x^{\frac{3}{4}},$$

for $x = M \cdot 10^6$.

The nature of these downward shifts and the description of the average lines certainly tend to corroborate the conjectures of Diaconu *et al.* and Zhang. It is reasonable to contest that some sort of bias exists here, perhaps due to human error in the calculation of $D_3(X)$. In an effort to alleviate such concerns, both here and with respect to other moments, the computations yielding our numerics were executed again (in a limited way) using higher precision. As anticipated, these higher precision results remained consistent with the initial results, reducing the possibility of such a bias existing.

5.2 Tables and Figures

r	$d_r(1)$	$d_r(2)$	$d_r(3)$	$d_r(4)$
0	.3522211004995828	.1238375103096e-1	.1528376099282e-4	.31582683324433e-9
1	.61755003361406	.18074683511868	.89682763979959e-3	.50622013406082e-7
2		.3658991414081	.17014201759477e-1	.32520704779144e-5
3		-.13989539029	.10932818306819	.10650782552992e-3
4			.13585569409025	.18657913487212e-2
5			-.23295091113684	.16586741288851e-1
6			.47353038377966	.59859999105052e-1
7				.52311798496e-2
8				-.1097356195
9				.55812532
10				.19185945

r	$d_r(5)$	$d_r(6)$	$d_r(7)$	$d_r(8)$
0	.671251761107e-16	.1036004645427e-24	.886492719e-36	.337201e-49
1	.23412332535824e-13	.67968140667178e-22	.98944375081241e-33	.59511917e-46
2	.35711692341033e-11	.20378083365099e-19	.51762930260135e-30	.500204322e-43
3	.31271184907852e-9	.36980514080794e-17	.16867245856115e-27	.2664702284e-40
4	.17346173129392e-7	.45348387982697e-15	.38372675160809e-25	.1010164552e-37
5	.63429411057027e-6	.39728668850800e-13	.64746354773372e-23	.29004988867e-35
6	.15410644373832e-4	.2563279107877e-11	.84021141030379e-21	.65555882460e-33
7	.2441498848698e-3	.12372292296e-9	.85817644593981e-19	.11966099802e-30
8	.2390928284571e-2	.44915158297e-8	.70024645896e-17	.17958286298e-28
9	.127561073626e-1	.1222154548e-6	.4607034349989e-15	.22443685425e-26
10	.24303820161e-1	.2461203700e-5	.2455973970377e-13	.2357312577e-24
11	-.333141763e-1	.3579140509e-4	.106223013225e-11	.20942850060e-22
12	.25775611e-1	.3597968761e-3	.3719625461492e-10	.15805997923e-20
13	.531596583	.230207769e-2	.1048661496741e-8	.10159435845e-18
14	-.325832	.7699469185e-2	.2357398870407e-7	.55665248752e-17
15	-1.34187	.4281359929e-2	.416315210727e-6	.25985097519e-15
16		-.2312387714e-1	.564739434674e-5	.103134457e-13
17		.109503	.56831273239e-4	.346778002e-12
18		.2900464	.40016131254e-3	.982481680e-11
19		-.9016	.1755324808e-2	.232784142e-9
20		-.89361	.340409901e-2	.456549799e-8
21		-.181	-.2741804e-2	.7309216472e-7
22			.353555e-3	.9368893764e-6
23			.117734	.9348804928e-5
24			.20714e-1	.69517414e-4
25			-.9671	.356576507e-3
26			-.284	.1059852e-2
27			1.3	.8242527e-3
28			-1.	-.206921e-2

Table 5.1: Coefficients of$Q_k(x) = d_0(k)x^{k(k+1)/2} + d_1(k)x^{k(k+1)/2} + \cdots$, for $k = 1, \ldots, 8$ and $d < 0$.

r	$e_r(1)$	$e_r(2)$	$e_r(3)$	$e_r(4)$
0	.3522211004995828	.1238375103096e-1	.1528376099282e-4	.31582683324433e-9
1	-.4889851881547	.6403273133043e-1	.60873553227400e-3	.40700020814812e-7
2		-.403098546303	.51895362572218e-2	.19610356347280e-5
3		.878472325297	-.20704166961612e-1	.4187933734219e-4
4			-.4836560144296e-1	.32338329823195e-3
5			.6305676273171	-.7264209058150e-3
6			-1.23114954368	-.97413031149e-2
7				.6254058547e-1
8				.533803934e-1
9				-1.125788
10				2.125417

r	$e_r(5)$	$e_r(6)$	$e_r(7)$	$e_r(8)$
0	.671251761107e-16	.1036004645427e-24	.886492719e-36	.337201e-49
1	.2024913313373e-13	.6113326104277e-22	.91146378e-33	.556982629e-46
2	.261100345555e-11	.16322243213252e-19	.437008961e-30	.43686422e-43
3	.187088892376e-9	.2605311255687e-17	.1297363095e-27	.216465856e-40
4	.8086250862418e-8	.2766415183453e-15	.2670392090e-25	.7604817313e-38
5	.2126496335545e-6	.2056437432502e-13	.404346681e-23	.201532781e-35
6	.319415704903e-5	.10957094998959e-11	.46631481394e-21	.418459324e-33
7	.21201987479e-4	.42061728711797e-10	.41831543311e-19	.698046515e-31
8	-.33900555230e-4	.11491097182922e-8	.29548572643e-17	.951665168e-29
9	-.775061385e-3	.21545094604323e-7	.1652770327e-15	.1073015400e-26
10	.333997849e-2	.25433712247032e-6	.73192383650e-14	.1008662234e-24
11	.22204682e-1	.1448397731463e-5	.25506469557e-12	.7945270901e-23
12	-.1538433	-.2179868777201e-5	.6901276286e-11	.5257922143e-21
13	-.19794e-1	-.54298634893e-4	.141485467e-9	.2924082555e-19
14	2.01541	.1698771341e-3	.210241720e-8	.1363867915e-17
15	-4.451	.22887524e-2	.20651382e-7	.5311448709e-16
16		-.1042e-1	.101650951e-6	.1714154659e-14
17		-.4339429e-1	-.16979129e-6	.453180963e-13
18		.343054	-.37367e-5	.9644403068e-12
19		-.1947171	.97069e-5	.160742335e-10
20		-3.16910	.18351e-3	.200188929e-9
21		7.31266	-.54878e-3	.16931900e-8
22			-.5621e-2	.7257434e-8
23			.284e-1	-.14329111e-7
24			.639e-1	-.25913136e-6
25			-.7	.6473933e-6
26			.86	.138673e-4
27			5.	-.2339e-4
28			-.1e2	-.48124e-3

Table 5.2: Coefficients of $Q_k(x) = e_0(k)x^{k(k+1)/2} + e_1(k)x^{k(k+1)/2} + \cdots$, for $k = 1, \ldots, 8$ and $d > 0$.

k	moment	conjecture	ratio	difference
1	25458527125.3765	25458526443.0851	1.00000002680011	682.291400909424
1	52401254983.3979	52401252573.3514	1.00000004599215	2410.04650115967
1	79904180421.7457	79904180600.9019	0.999999997757862	-179.156204223633
1	107770905413.087	107770904521.066	1.00000000827701	892.021011352539
1	135908144579.9	135908144595.649	0.99999999988412	-15.7490081787109
2	695798091128.962	695797942880.624	1.00000021306234	148248.338012695
2	1505736931971.68	1505736615081.97	1.00000021045494	316889.709960938
2	2362905062077.15	2362905209666.86	0.999999937538878	-147589.709960938
2	3251727763805.56	3251727486319.23	1.00000008533505	277486.330078125
2	4164586513531.53	4164586544704.79	0.999999992514681	-31173.2602539062
3	35923488939395.6	35923434720073.8	1.00000150930228	54219321.8046875
3	82792501873632.1	82792433101707.4	1.00000083065471	68771924.6875
3	134707236936019	134707230960903	1.00000004435631	5975116
3	190139826789407	190139791751013	1.00000018427702	35038394
3	248315000391821	248315015388794	0.99999993960505	-14996973
4	2.62216772015079e15	2.62215426148555e15	1.00000513267485	13458665240
4	6.48460654252297e15	6.48459187992768e15	1.00000226114389	14662595290
4	1.09871964707935e16	1.09871878848222e16	1.00000078145303	8585971300
4	1.59561231814031e16	1.5956125546013e16	0.999999851805509	-2364609900
4	2.12995355148029e16	2.12995409110151e16	0.999999746651244	-5396212200
5	2.35419374721785e17	2.3541622006477e17	1.00001340033841	3154657015008
5	6.27717267114645e17	6.2771414322685e17	1.0000049766089	3123887794944
5	1.11068908536146e18	1.1106862772711e18	1.000002528248	2808090359936
5	1.66286324284991e18	1.66286838497409e18	0.999996907678186	-5142124179968
5	2.27240250776101e18	2.27240484232311e18	0.999998972646926	-2334562099968
6	2.42254871622434e19	2.42247808189372e19	1.00002915788223	706343306199040
6	6.98802246409075e19	6.98795544874549e19	1.000009590122	670153452601344
6	1.29379682106315e20	1.29378875862885e20	1.00000623164659	806243429990400
6	1.99967529784789e20	1.99970133063147e20	0.999986981664121	-2.60327835798733e15
6	2.80059250886771e20	2.8006019455853e20	0.999996630468102	-943671758979072
7	2.74712571777423e21	2.74697762671744e21	1.00005391054348	1.48091056789914e17
7	8.59431066562339e21	8.59415893116067e21	1.00001765553371	1.51734462720246e17
7	1.66743403869214e22	1.66740957094856e22	1.00001467410527	2.44677435799372e17
7	2.66330275023537e22	2.66339641977569e22	0.999964830792884	-9.36695403200381e17
7	3.82588166641253e22	3.8259132201782e22	0.999991752618564	-3.15537656693916e17
8	3.35169775526293e23	3.35140684068409e23	1.00008680371935	2.90914578839655e19
8	1.13946580450882e24	1.13942904804314e24	1.00003225867003	3.67564656800128e19
8	2.31935906884942e24	2.31928230131293e24	1.00003309969487	7.67675364899952e19
8	3.83145462724565e24	3.83173855869501e24	0.999925900098608	-2.83931449359721e20
8	5.64909301637731e24	5.6491832095572e24	0.999984034297252	-9.01931798900947e19

Table 5.3: Moments of $L(\frac{1}{2}, \chi_d)$ up to X versus conjectured asymptotics up to X, for $k = 1, \ldots, 8$ and $d < 0$. Each block is sampled at $X = 10^{10}, 2 \times 10^{10}, \ldots, 5 \times 10^{10}$.

k	moment	conjecture	ratio	difference
1	4074391863.44469	4074392042.93877	0.999999955945801	-179.494079589844
1	8445624718.02429	8445624023.31381	1.00000008225686	694.710479736328
1	12928896894.5904	12928896383.1457	1.00000003955826	511.444700241089
1	17484928279.5793	17484927921.5002	1.0000000204793	358.0791015625
1	22095062063.1137	22095062690.7385	0.999999971594342	-627.624797821045
2	76310075816.4656	76310057832.3198	1.00000023567202	17984.1458129883
2	168051689378.933	168051603484.026	1.00000051112221	85894.9070129395
2	266303938917.289	266303916920.62	1.00000008259987	21996.6690063477
2	368948427173.219	368948308826.37	1.0000003207681	118346.848999023
2	474942139636.155	474942177549.675	0.999999920172346	-37913.5199584961
3	2478393690176.25	2478391641054.51	1.00000082679497	2049121.74023438
3	5878735240405.92	5878729153410.41	1.00000103542711	6086995.50976562
3	9720154390088.39	9720158187579.47	0.999999609317975	-3797491.08007812
3	13873264940981.6	13873252832528.8	1.00000087279119	12108452.7988281
3	18271480140004.1	18271496263135.1	0.99999911758015	-16123131
4	108684254847368	108684097510165	1.00000144765616	157337203
4	279749805201690	279749156684971	1.00000231820795	648516719
4	484732760732189	484733296056915	0.99999889563038	-535324726
4	714931674293147	714929616642460	1.00000287811645	2057650687
4	965640462899128	965643346476594	0.999997013827645	-2883577466
5	5.7022430562904e15	5.70223224068973e15	1.000001896731	108684097510165
5	1.59997376762599e16	1.5999653478756e16	1.00000526245797	84197503900
5	2.91304302919673e16	2.91304950122491e16	0.999997778263577	-64720281800
5	4.44827164173005e16	4.4482376920928e16	1.00000763215448	339496372496
5	6.17072908903673e16	6.17077088697785e16	0.999993226463616	-417979411200
6	3.36582908140978e17	3.3658163201404e17	1.00000379143369	1276126937984
6	1.03269331133762e18	1.03268168488978e18	1.00001125850106	11626447840000
6	1.97924258066123e18	1.97925154912564e18	0.999995468759687	-8968464409856
6	3.13323798444742e18	3.13318904016406e18	1.00001562123534	48944283359744
6	4.46859415120687e18	4.46864874024817e18	0.999987783993669	-54589041299968
7	2.15991539085973e19	2.15989246212753e19	1.00001061568231	229287322001408
7	7.26312167991914e19	7.26295668030914e19	1.00002271796697	1.64999610000179e15
7	1.46733199899907e20	1.46734533114348e20	0.999990914105816	-1.33321444099686e15
7	2.41042340833943e20	2.41036160843122e20	1.0000256392684	6.17999082097869e15
7	3.5369407873606e20	3.53700808054158e20	0.999980974547005	-6.72931809801011e15
8	1.47589977366401e21	1.47585964179895e21	1.00002719219628	4.01318650597868e16
8	5.44909066717911e21	5.44885361218154e21	1.00004350548105	2.37054997569733e17
8	1.16160296153376e22	1.16162279275691e22	0.999982928001005	-1.983122315013e17
8	1.98161815943723e22	1.98155052338218e22	1.00003413289454	6.76360550497649e17
8	2.99340300076072e22	2.99348464881333e22	0.999972724746512	-8.16480526100595e17

Table 5.4: Moments of $L\left(\frac{1}{2}, \chi_d\right)$ up to X versus conjectured leading term up to X, for and $k = 1, \ldots, 8$ and $d > 0$. Each block is sampled at $X = 2 \times 10^9, 4 \times 10^9, \ldots, 10^{10}$.

d	average of moments	average of conjectures	ratio of average
< 0	3.26052668116201e23	3.26058331976247e23	0.99998262930436
> 0	1.68629369822128e21	1.68629519213256e21	0.999999114086739

Table 5.5: Average of moments versus average of conjectured asymptotics.

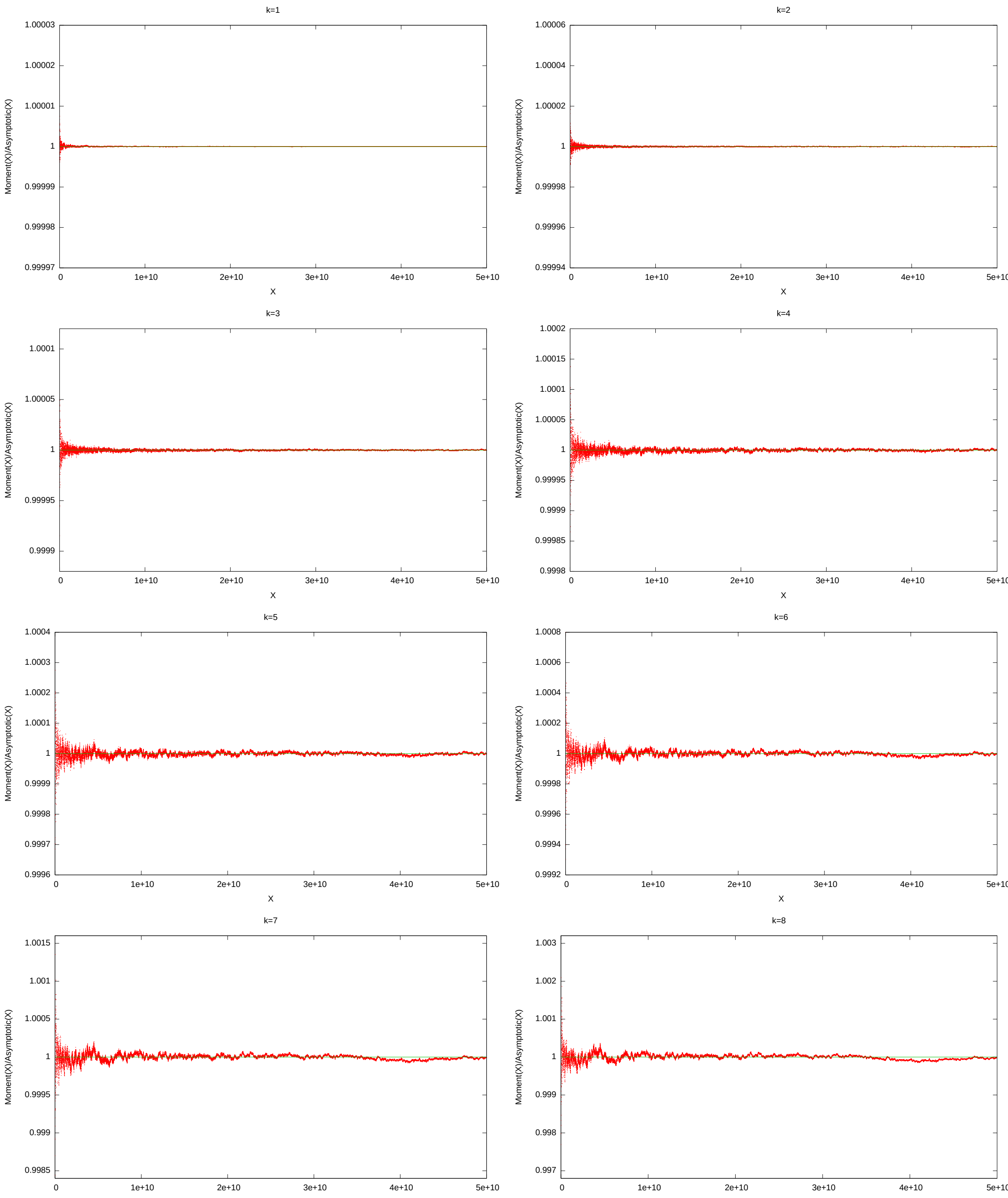

Figure 1: These plots depict the ratio $R_k(X)$ for $k = 1, \ldots, 8$ and $d < 0$, sampled at $X = 100000, 200000, \ldots, 5 \times 10^{10}$. The horizontal axis is X, the vertical axis is the difference $R_k(X)$, and the line through the data is the mean up to X.

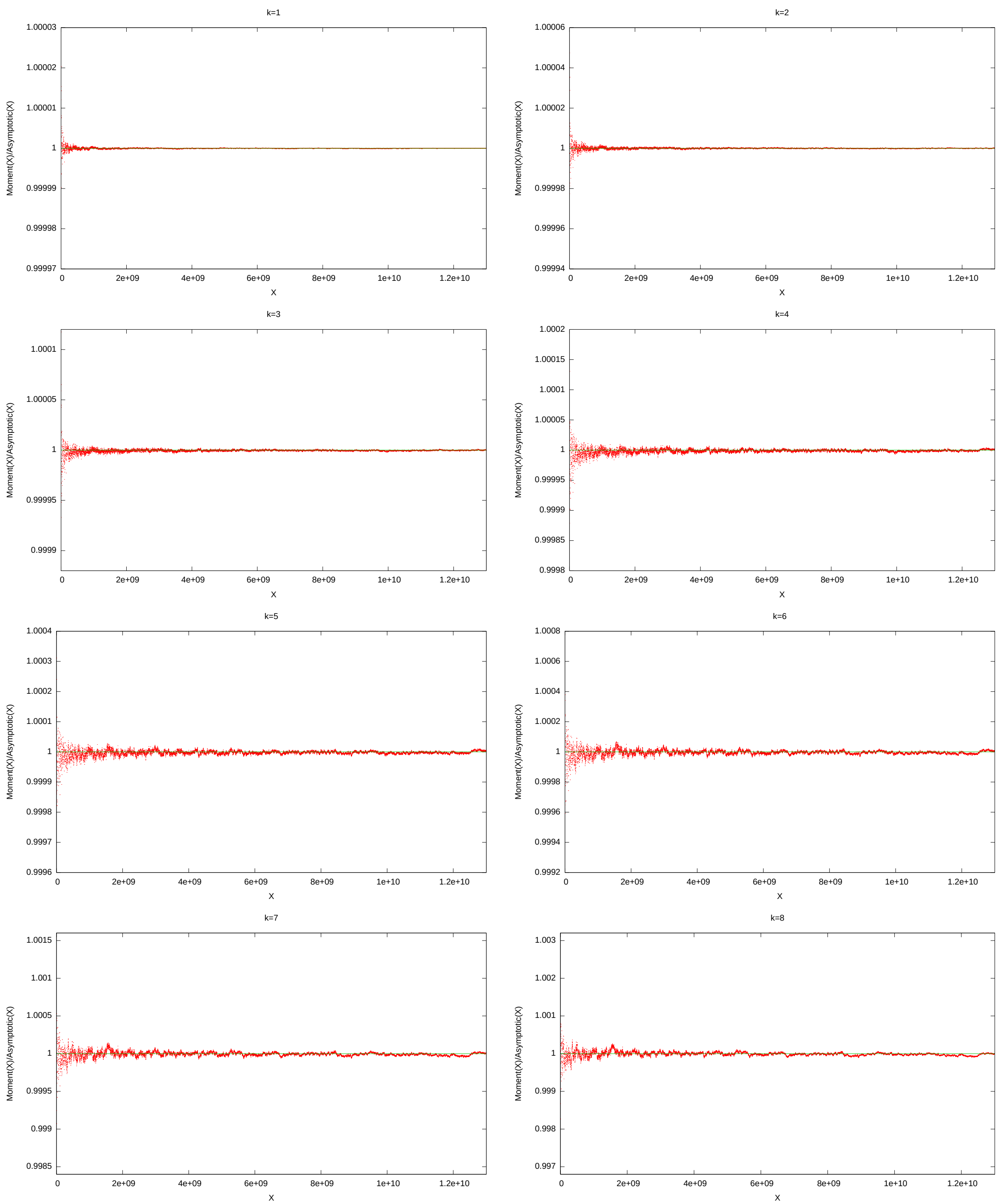

Figure 2: These plots depict the ratio $R_k(X)$ for $k = 1, \ldots, 8$ and $d > 0$, sampled at $X = 100000, 200000, \ldots, 1.2 \times 10^{10}$. The horizontal axis is X, the vertical axis is the difference $R_k(X)$, and the line through the data is the mean up to X.

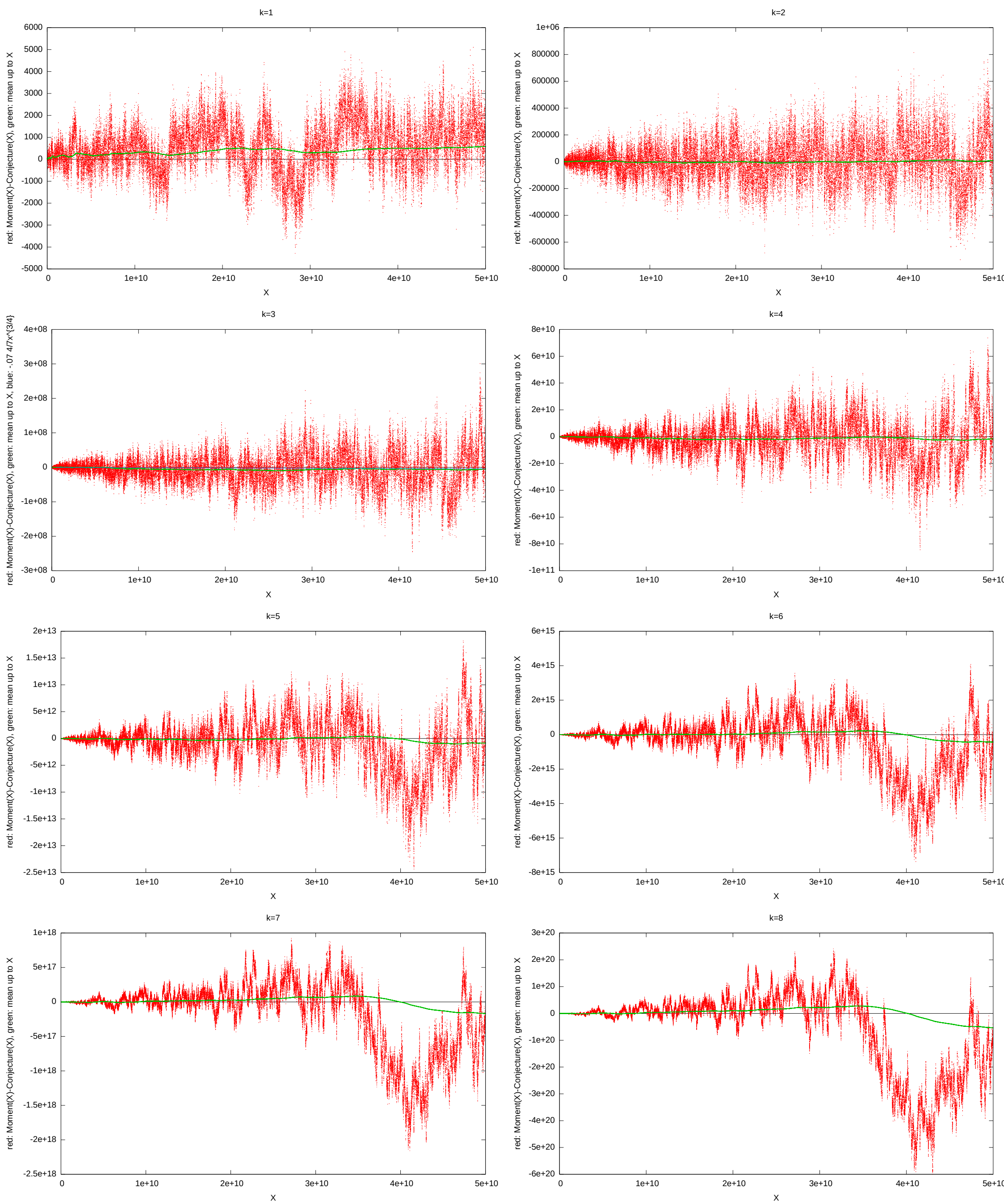

Figure 3: These plots depict the difference $D_k(X)$ for $k = 1, \ldots, 8$ and $d < 0$, sampled at $X = 100000, 200000, \ldots, 5 \times 10^{10}$. The horizontal axis is X, the vertical axis is the difference $D_k(X)$, and the line through the data is the mean up to X.

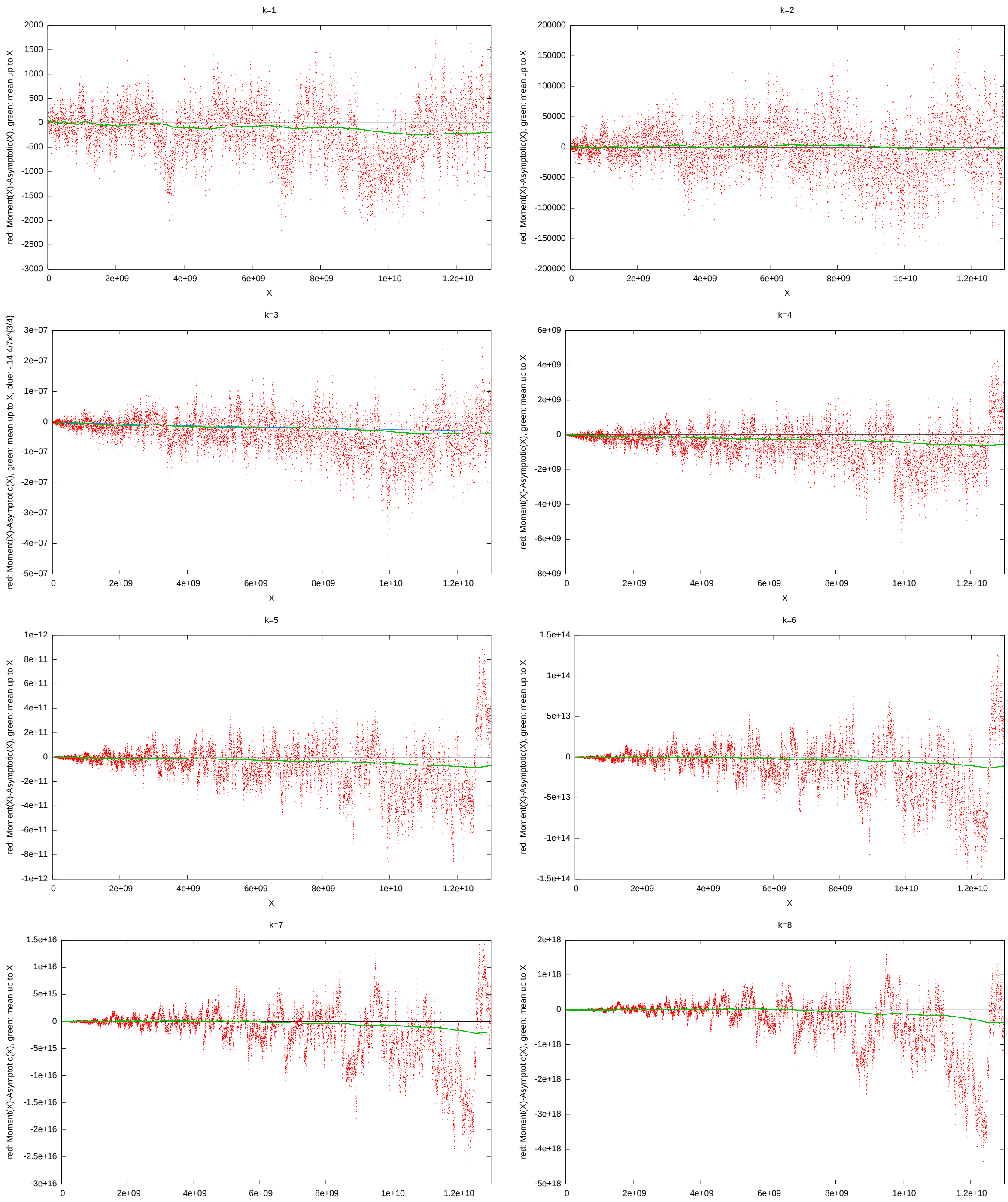

Figure 4: These plots depict the difference $D_k(X)$ for $k = 1, \ldots, 8$ and $d > 0$, sampled at $X = 100000, 200000, \ldots, 1.2 \times 10^{10}$. The horizontal axis is X, the vertical axis is the difference $D_k(X)$, and the line through the data is the mean up to X.

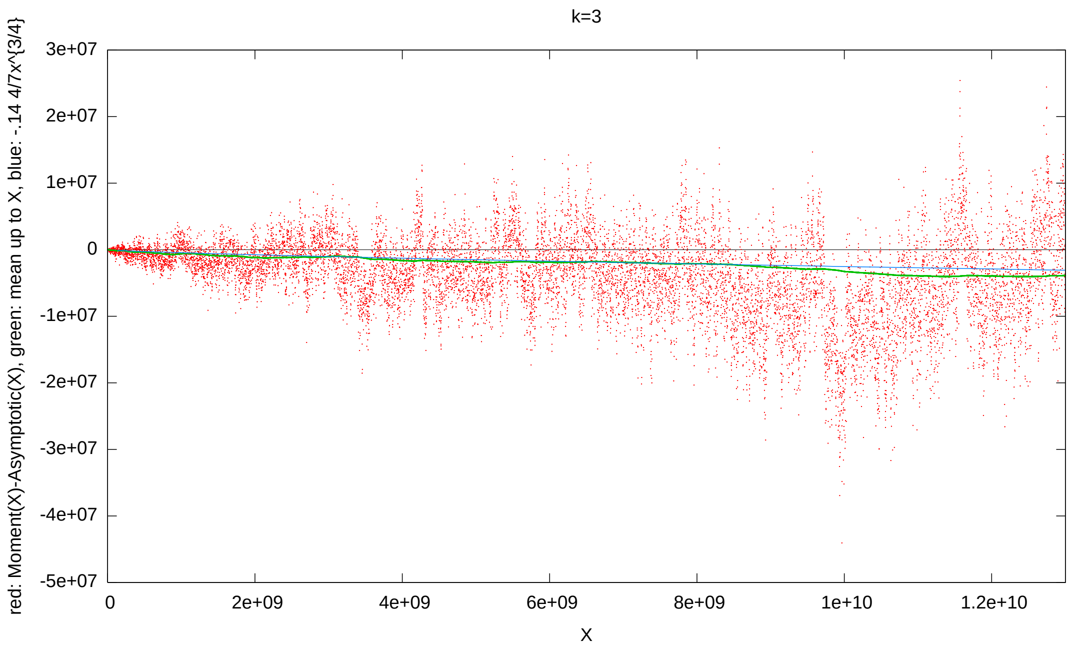

Figure 5: This graph depicts the difference $D_3(X)$ for $d > 0$. The lines through the data are the mean up to X and the running average of $D_3(X)$ up to X. Observe that both the mean line and average line deflect away from 0 in a similar fashion.

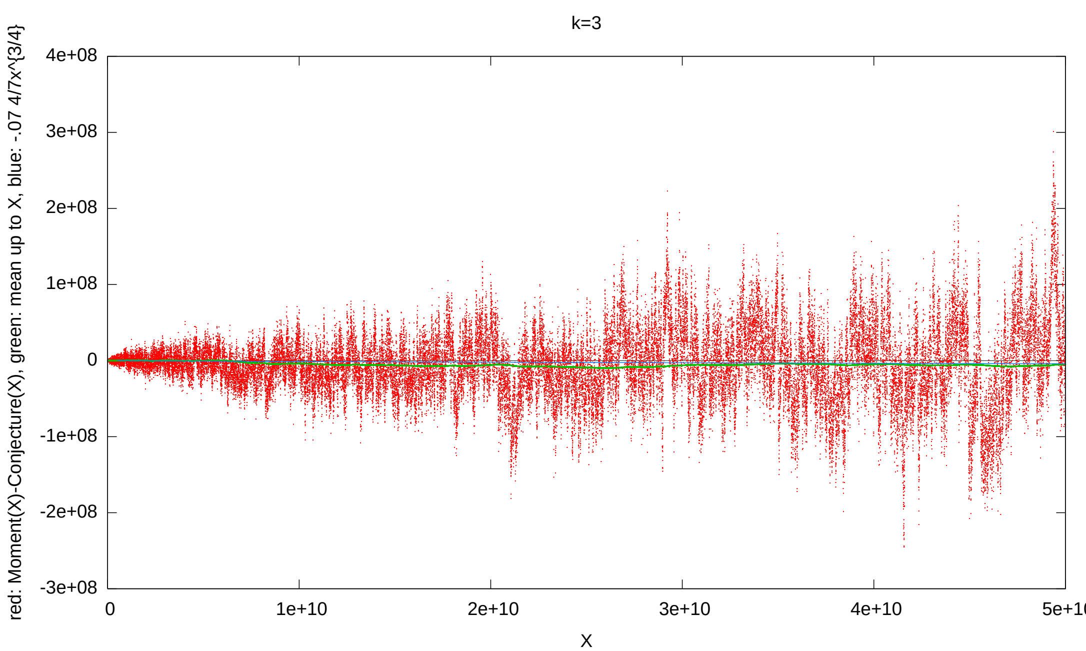

Figure 6: This graph depicts the difference $D_3(X)$ for $d < 0$. The lines through the data are the mean up to X and the running average of $D_3(X)$ up to X.

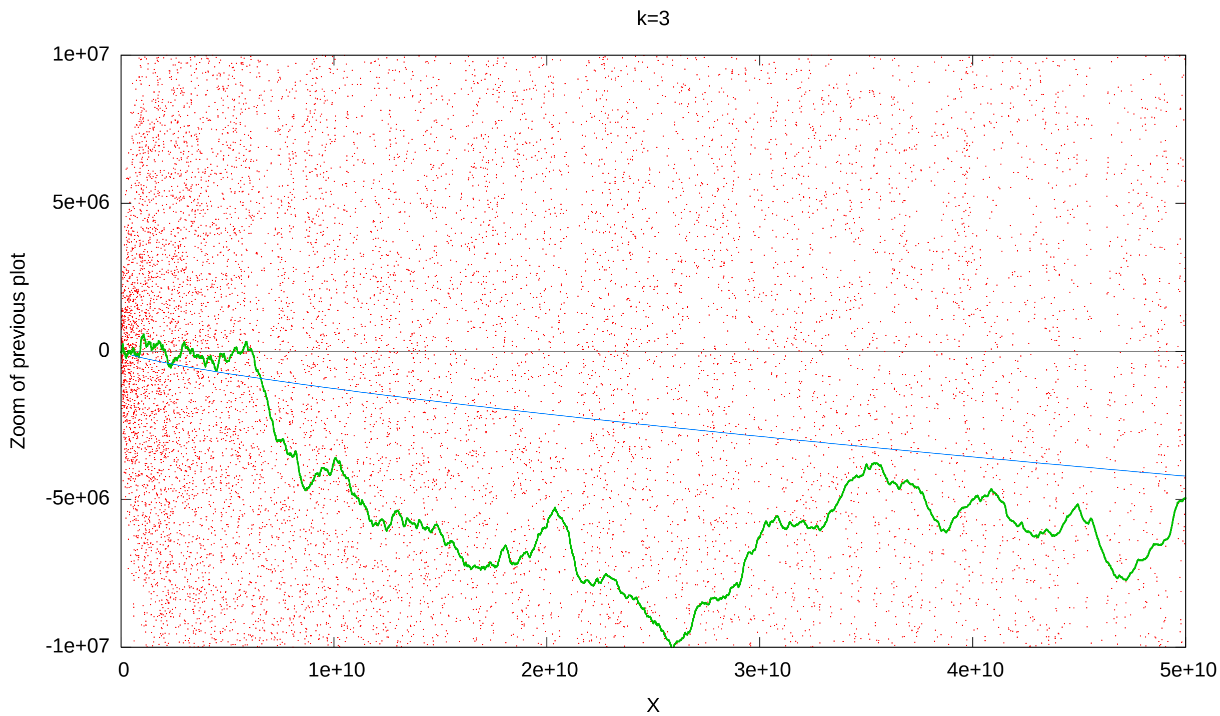

Figure 7: This is a zoomed plot of the difference $D_3(X)$ for $d < 0$. The lines through the data are the mean up to X and the running average of $D_3(X)$ up to X. Observe that both the mean line and average line deflect away from 0.

Chapter 6

Further Advancements

Current stages of investigation seem to indicate three possible avenues to pursue further.

6.1 Complexity Improvements

At a recent number theory conference (Automorphic Forms and L-functions: Computational Aspects) held at the University of Montreal, A. Booker and D. Goldfeld communicated several ideas to my supervisor (Dr. M. Rubinstein) which may prove to significantly enhance the efficiency of our algorithms. Specifically, they indicated the promising fact that the L-values in question appear as the Fourier coefficients of a certain Eisenstein series of half weight. As a result, it would then seem plausible to borrow Hejhal's phase two algorithm – developed for computing Fourier coefficients of Maass forms – to design a version based on the Fast Fourier Transform (FFT) and then apply it to our situation. This promises to reduce the complexity of our algorithm from $O\left(X^{\frac{3}{2}+\epsilon}\right)$ to $O(X^{1+\epsilon})$. For the practical implementation of the FFT portion, we would consult with Bill Hart and Gonzalo Tornaria who recently carried out an FFT on polynomials of degree one trillion.

6.2 Theoretical Investigation

As previously indicated, Diaconu *et al.* recently used the philosophy of multiple Dirichlet series to conjecture the existence of an exceptional main term of the form $bX^{\frac{3}{4}}$ appearing in the cubic moments of $L\left(\frac{1}{2}, \chi_d\right)$. In his thesis, Zhang determined that $b \approx -.2154$. The numerical data collected above appears to support the existence of such a lower order main term, though Zhang's constant seems to be a bit off. Accordingly, questions now arise concerning the possible existence of extra lower order main terms in the asymptotic expansions of other moments. In certain cases, especially the first two moments, the collected data reveals interesting structure in the associated remainder term, and it would be worthwhile to study this further.

6.3 Generalizations

The family of quadratic Dirichlet L-functions is merely one example within the class of all L-functions. As a result, it is natural to wonder if properties such as the existence of lower order main terms in the moment expansions of more general L-functions persist. In particular, we could consider the moments for the family of quadratic twists of elliptic curve L-functions (sometimes referred to as the Hasse-Weil L-function). An elliptic curve L-function can be represented by an L-function whose coefficients are indicative of the underlying properties of the elliptic curve. For example, if we suppose that E is an elliptic curve over the rational field $\mathbb{Q}$ (which is typically the only case of interest in the theory of elliptic curves), then the coefficients of the induced elliptic curve L-function count, roughly, the number of points (in the finite field of p elements) which "miss" the curve E. Importantly, the ideas given above might lead to the existence of a lower order term in the moments of, for example, quadratic twists of a given elliptic curve. Presumably the constant factor in this lower term would depend on the properties of the underlying elliptic curve, giving a whole set of testable predicitons that ought to be convincing one way or the other.

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