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On uncertainty principles, Fourier optimization and the Riemann zeta-function

by

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Dedicado a todxs lxs que han luchado por nuestro derecho de ser nosotrxs mismxs: a lxs que estuvieron y ya no están; lxs que siguen; y lxs que vendrán.

In loving memory of Prof. William Alvarado (University of Costa Rica), teacher and friend to generations of students.

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Abstract

This Ph.D thesis is rooted in the first five research articles of the author, throughout which we study topics at the interface of analytic number theory and harmonic analysis.

From a harmonic analysis perspective, we consider a generalized version of the sign uncertainty principle for the Fourier transform, first proposed by Bourgain, Clozel and Kahane and revisited by Cohn and Gonçalves. In our rough, general framework, we are able to identify sharp constants in some cases.

From a number theory perspective, we study Fourier optimization tools related to bounds in the theory of the Riemann zeta-function and other L-functions, and also to new estimates regarding the distribution of integers and primes represented by quadratic forms. Moreover, we study the number variance of zeta zeros. In particular, conditionally on the Riemann hypothesis and a conjecture for the pair correlation of zeta zeros in longer ranges (which examines how often gaps between zeros can be close to a fixed nonzero value), we prove a conjecture of Berry (1988) for this number variance, in the non-universal regime where random matrix models do not correctly describe the distribution of zeta zeros.

Resumo

Esta tese de doutorado está baseada nos primeiros cinco artigos de pesquisa da autora, onde estudamos tópicos na interseção entre teoria analítica dos números e análise harmônica.

Desde a perspetiva de análise harmônica, consideramos uma versão geral do princípio da incerteza de sinais para a transformada de Fourier, proposto originalmente por Bourgain, Clozel e Kahane e revisitado por Cohn e Gonçalves. Na nossa formulação geral, conseguimos identificar constantes ótimas em alguns casos.

Desde a perspetiva de teoria dos números, estudamos ferramentas de otimização de Fourier relacionadas com cotas na teoria da função zeta de Riemann e outras L-funções, e também com novas estimativas sobre a distribuição de inteiros e primos representados por formas quadráticas. Adicionalmente, estudamos a variância do número de zeros da função zeta. Em particular, condicionalmente à hipótese de Riemann e a uma conjetura sobre a correlação de pares de zeros em intervalos maiores (que examina a frequência com a qual os espaços entre zeros podem ser aproximadamente uma quantidade não nula dada), provamos uma conjetura de Berry (1988) para esta variância, no regime não universal onde os modelos de matrizes aleatórias não descrevem corretamente a distribuição dos zeros da função zeta.

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Chapter 1

Introduction

This thesis lies at the interface of analytic number theory and harmonic analysis. We investigate the following topics: (i) the uncertainty principle in Fourier analysis and its connection to the sphere packings problem; (ii) the distribution of integers and primes represented by quadratic forms; (iii) the theory of the Riemann zeta-function and other L-functions. The exploration of these topics generated the following research articles, on which this thesis is based:

[A1] *Generalized sign Fourier uncertainty* (with E. Carneiro), Ann. Sc. Norm. Super. Pisa, Cl. Sci. DOI: 10.2422/2036-2145.202105_026.

[A2] *Fourier optimization and quadratic forms* (with A. Chirre), Q. J. Math. 73, no. 2 (2022), 539–577. DOI: 10.1093/qmath/haab041.

[A3] *The second moment of $S_n(t)$ on the Riemann hypothesis* (with A. Chirre), Int. J. Number Theory 18, no. 6 (2022), 1203-1226. DOI: 10.1142/S1793042122500610.

[A4] *On the number variance of zeta zeros and a conjecture of Berry* (with M. M. Lugar and M. B. Milinovich), preprint arXiv:2211.14918.

[A5] *On the q-analogue of the pair correlation conjecture via Fourier optimization*, Math. Comp. 91 (2022), 2347-2365. DOI: 10.1090/mcom/3747.

To tackle many of the questions in the above articles, we combine theoretical tools from harmonic analysis, approximation theory, and analytic and algebraic number theory, sometimes with additional computational tools such as numerical optimization methods (including semidefinite programming in particular - see Section 6.3). In the next sections, we will present a brief overview of the topics studied in these articles, their background, and the tools involved in some of our main results. First, we must say some words on notation.

1.1 Notation

Throughout this thesis, we use the following classical notation and conventions.

1. Define the Fourier transform of a function $f \in L^1(\mathbb{R}^d)$ by

$$\mathcal{F}_d[f](\xi) = \widehat{f}(\xi) = \int_{\mathbb{R}^d} e^{-2\pi i x\cdot\xi} f(x)\, \mathrm{d}x.$$

2. For $s \in \mathbb{C}$ we write $s = \sigma + it$, where σ and t are real numbers.

3. We say that $\alpha = O(\beta)$, $\alpha \ll \beta$, and $\alpha \lesssim \beta$ when $|\alpha| \leqslant C\beta$ for some constant $C > 0$, and they may be used interchangeably. In the subscript, we indicate the parameters on which such constant C may depend. We say that $\alpha \simeq \beta$ when $\alpha \lesssim \beta$ and $\beta \lesssim \alpha$. Additionally, the notation $\alpha = O^*(\beta)$ means that $|\alpha| \leqslant \beta$.

4. We denote $f = o(g)$ when $\lim_{x\to\infty} f(x)/g(x) = 0$. We also denote $f \sim g$ when $\lim_{x\to\infty} f(x)/g(x) = 1$.

5. $B_\varepsilon(x)$ denotes the open ball of center x and radius ε in $\mathbb{R}^d$. If $x = 0$ we may simply write B_ε. The Lebesgue measure of a measurable set X is denoted by $|X|$, and $\mathbb{I}_X$ denotes its characteristic function. The dimension d will be clear from context.

6. The function $\mathrm{sgn} : \mathbb{R} \to \mathbb{R}$ is defined by $\mathrm{sgn}(t) = 1$, if $t > 0$; $\mathrm{sgn}(0) = 0$; and $\mathrm{sgn}(t) = -1$, if $t < 0$.

7. We denote by $\lfloor x \rfloor$ the integer part of x, i.e. the largest integer smaller than or equal to x; and $\{x\} := x - \lfloor x \rfloor$ denotes its fractional part.

8. We say that a measurable function $f : \mathbb{R}^d \to \mathbb{R}$ is *eventually non-negative*[1] if $f(x) \geqslant 0$ for all sufficiently large $|x|$.

9. For $x \in \mathbb{R}$, we denote $x_+ := \max\{x, 0\}$.

10. For a radial function $G : \mathbb{R}^d \to \mathbb{C}$, we use the notation $G(x) = G(|x|)$.

11. Sums and products over the variable p run through all prime numbers 2, 3, 5...

12. $\Gamma(s)$ denotes the Gamma function.

13. The function which is identically equal to 0 (resp. 1) is denoted by $\mathbf{0}$ (resp. $\mathbf{1}$).

1.2 Uncertainty principles in Fourier analysis

The Fourier transform is certainly one of the most fundamental objects in mathematics and applied mathematics, as it is used to model a variety of oscillatory phenomena. The expression *Fourier uncertainty* appears recurrently in the literature (see [10, 43] for surveys),

[1] It will be convenient here not to consider only continuous functions in the definition of *eventual non-negativity*, as other works in the literature do. Note, however, that we require that f has a non-negative sign *for all* $|x| > r(f)$, and not only almost everywhere with respect to the Lebesgue measure. Similarly, we may define the concepts of *eventually non-positive* and *eventually zero*.

describing many qualitative and quantitative variants of the same underlying principle: that one cannot have an unrestricted control of a function and its Fourier transform simultaneously. In [12], Bourgain, Clozel and Kahane introduced a novel uncertainty principle, in connection to a problem in algebraic number theory. It essentially says that a function f and its Fourier transform $\widehat{f}$ cannot have their negative mass arbitrarily concentrated near the origin, when facing a competing condition that $f(0) \leqslant 0$ and $\widehat{f}(0) \leqslant 0$. The authors realized that the essence of the problem was captured by eigenfunctions of the Fourier transform with eigenvalue $s = +1$. Later, Cohn and Gonçalves [35] proposed a suitable variant of the sign uncertainty principle associated to the eigenvalue $s = -1$. To formulate this precisely, for an eventually non-negative function $f : \mathbb{R}^d \to \mathbb{R}$, we define

$$r(f) := \inf\{r > 0 \ : \ f(x) \geqslant 0 \text{ for all } |x| \geqslant r\}.$$

Let $s \in \{+1, -1\}$ denote a sign, and consider the following family of functions:

$$\mathcal{A}_s^*(d) = \left\{ \begin{array}{l} f \in L^1(\mathbb{R}^d)\backslash\{\mathbf{0}\} \text{ continuous, even, real-valued and such that } \widehat{f} = sf; \\ sf(0) \leqslant 0, f \ \text{ is eventually non-negative.} \end{array} \right\}.$$

We then define

$$\mathbb{A}_s^*(d) := \inf_{f \in \mathcal{A}_s^*(d)} r(f).$$

Bourgain, Clozel and Kahane [12] (for $s = 1$) and Cohn and Gonçalves [35] (for $s = -1$) showed that

$$\mathbb{A}_s^*(d) \simeq \sqrt{d}.$$

Historically, quests to find the sharp forms of functional inequalities have been non-trivial and beautiful problems, whose solution often reveals new information about the underlying structures. In this particular case, the sharp forms and extremizers have only been identified in four special cases. Cohn and Gonçalves observed that the solutions in the cases $(s, d) = (-1, 1)$, $(-1, 8)$ and $(-1, 24)$ follow from the recent breakthroughs in the sphere packing problem by Cohn and Elkies [34], Viazovska [103] and Cohn, Kumar, Miller, Radchenko and Viazovska [37]. Cohn and Gonçalves then go further by adapting their techniques, and developing new ones, to settle the case $(s, d) = (+1, 12)$.

In Chapter 2, based on the manuscript [A1], we propose a generalized weighted version of the sign uncertainty principle in Euclidean space. In our setup, the signs of a function and its Fourier transform resonate with a generic given function P outside of a ball. One essentially wants to know if and how soon this resonation can happen, when facing a suitable competing weighted integral condition. All the four eigenvalues of the Fourier transform appear in this formulation, but the new possibilities go far beyond. Formally, Let $P \in L^1_{\text{loc}}(\mathbb{R}^d)$ be a real-valued function that is either even or odd. That is, $P(-x) = (-1)^{\mathfrak{r}} P(x)$ for some $\mathfrak{r} \in \{0, 1\}$.

Then, we consider the following class of functions:

$$\mathcal{A}_s^*(P;d) = \left\{ \begin{array}{l} f \in L^1(\mathbb{R}^d)\backslash\{\mathbf{0}\} \text{ continuous, real-valued and such that } \widehat{f} = si^{\mathrm{r}} f; \\ Pf \in L^1(\mathbb{R}^d); \\ \int_{\mathbb{R}^d} Pf \leqslant 0\,; \\ Pf \text{ is eventually non-negative.} \end{array} \right\}.$$

We also define

$$\mathbb{A}_s^*(P;d) = \inf_{f \in \mathcal{A}_s^*(P;d)} r(Pf).$$

The original version of the problem corresponds to the particular case $P \equiv 1$. In the first part of the chapter (Theorems 2.3, 2.5 and 2.6), we attempt to push the existing techniques to their limit, to discuss general situations where the class $\mathcal{A}_s^*(P;d)$ is non-trivial and the presence of suitable admissible conditions that give a generic formulation of the principle. In the second part of the chapter (Theorem 2.7 and its two corollaries), we introduce the novel mechanism of dimension shifts, which allows us to relate some of the sign uncertainty principles under different weights and dimensions. This is especially useful when dealing with singular weights, and allows us to fully settle the problem (finding sharp constants and extremizers) in 14 new situations with polynomial weights, modulo symmetries given by the orthogonal group (Corollary 2.8). For instance, we obtain the following two sharp constants.

Theorem 1.1 (c.f. Corollary 2.8)**.** *Let*

$$P_1(x_1, \ldots x_d) = x_1\ ;\ P_2(x_1,x_2,x_3,x_4) = \big(x_1^3 + x_1^2(x_2 - x_3) - x_1(x_2^2 + 2x_3^2) - x_2^3 + x_2^2 x_3 + 2x_2 x_3^2\big) x_4.$$

Then,

$$\mathbb{A}_{+1}^*(P_1;22) = 2 \quad \textit{and} \quad \mathbb{A}_{+1}^*(P_2;4) = \sqrt{2}.$$

Another interesting special case is that of the sign uncertainty principle with power weights $P(x) = |x|^\gamma$:

Theorem 1.2 (c.f. Corollary 2.9)**.** *Let $d \in \mathbb{N}$ with $d \geqslant 5$ and let $\gamma > -d$ be a real number. Assume that $\gamma \notin \left(\frac{-d-3}{2}, \frac{-d+3}{2}\right)$. Then,*

$$\sqrt{\min\left\{d, |d+2\gamma|\right\}} \ll \mathbb{A}_{+1}(|x|^\gamma; d) \ll \sqrt{\max\{d+\gamma\,,\, -\gamma\}}.$$

The case $\gamma = 0$ corresponds to the original formulation by Bourgain, Clozel, and Kahane. In the singular case where $-d < \gamma < 0$, there are crucial obstructions to the classical arguments used to establish the sign uncertainty principles in previous works (see the remarks in Section 2.6.3). New tools were therefore needed, and this is where our dimension shifts mechanism, and other new ideas, came into play.

1.3 Theory of the Riemann zeta-function and other L-functions

In this section, we briefly introduce the topics of the articles [A3], [A4], and [A5], which we will present in detail in Chapters 4, 5 and 6.

1.3.1 The Riemann zeta-function and the distribution of its zeros

Understanding the behavior of the Riemann zeta-function and the distribution of its zeros is a crucial problem in number theory, being related to the distribution of primes. The Riemann zeta-function is defined in the half-plane $\mathrm{Re}\, s > 1$ by

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s} = \prod_p \left(1 - \frac{1}{p^s}\right)^{-1}. \tag{1.3.1}$$

The *Euler product* - the product over primes in (1.3.1) - is the starting point of the connection between this function and the distribution of primes. By partial summation, for $\mathrm{Re}\, s > 1$,

$$\zeta(s) = -s \int_1^{\infty} \frac{\{x\}}{x^{s+1}}\, \mathrm{d}x + \frac{s}{s-1}.$$

Since the integral in the right-hand side is convergent and analytic for $\mathrm{Re}\, s > 0$, this shows that $\zeta(s)$ can be analytically continued to a meromorphic function in the half-plane $\mathrm{Re}\, s > 0$. Moreover, it satisfies the functional equation

$$\zeta(s) = 2^s \pi^{s-1} \sin(\pi s/2) \Gamma(1-s) \zeta(1-s),$$

which implies that it can be extended to a meromorphic function in the entire plane, with a simple pole at $s = 1$. From the functional equation, one can see that $\zeta(-2n) = 0$ for all positive integers n, and these are called the *trivial zeros.* Furthermore, from the Euler product and the functional equation, one can see that all non-trivial zeros of $\zeta(s)$ must lie on the *critical strip* $\{s \in \mathbb{C} : 0 < \mathrm{Re}\, s < 1\}$. The Riemann hypothesis (RH), conjectured in 1859 [91], states that all non-trivial zeros actually lie on the *critical line*, $\mathrm{Re}\, s = \frac{1}{2}$. For further background on the theory of $\zeta(s)$, and its connection to the distribution of primes, see [41, 69, 84, 102].

Throughout this thesis, we will also sometimes consider other families of L-functions, which are generalizations of the Riemann zeta-function in different contexts. See [69, Chapter 5] for a general framework regarding the theory of L-functions. In particular, in Chapter 6 we work primarily with Dirichlet L-functions, which were originally introduced to study primes in arithmetic progressions. For a positive integer q, a Dirichlet character $\chi \pmod q$ is a character of the multiplicative group of units $(\mathbb{Z}/q\mathbb{Z})^{\times}$, extended to a completely multiplicative q-periodic function over all integers by taking $\chi(n) = 0$ whenever $\gcd(n, q) \neq 1$ (see e.g. [41, 69] for details). We may consider the Dirichlet L-function defined initially (and then analytically continued), for $\operatorname{Re} s > 1$, by

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

In Chapter 6, we also describe and work with a family of automorphic L-functions, following a framework in [26]. In Chapter 3, we describe and work with Hecke L-functions, which generalize Dirichlet L-functions to algebraic number fields, since, as we shall explain therein, they can codify information about quadratic forms.

Returning to the Riemann zeta-function, let $N(t)$ be the number of zeros $\rho = \beta + i\gamma$ of $\zeta(s)$ such that $0 < \gamma \leqslant t$ and $0 < \beta < 1$ (counted with multiplicity, and where the zeros with $\gamma = t$ are counted with weight $\frac{1}{2}$). The classical Riemann von-Mangoldt formula states that

$$N(t) = \frac{t}{2\pi} \log \frac{t}{2\pi} - \frac{t}{2\pi} + \frac{7}{8} + S(t) + O\left(\frac{1}{t}\right). \tag{1.3.2}$$

Here, for $t \neq \gamma$,

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

where the argument is obtained by a continuous variation along the straight line segments joining the points 2, $2 + it$ and $\frac{1}{2} + it$, and we take $\arg \zeta(2) = 0$. If $t = \gamma$, we define

$$S(t) = \lim_{\varepsilon \to 0} \frac{S(t+\varepsilon) + S(t-\varepsilon)}{2}.$$

Furthermore, we may define the complex logarithm of $\zeta(s)$ on the critical line as

$$\log \zeta(\tfrac{1}{2} + it) := \log |\zeta(\tfrac{1}{2} + it)| + i\pi S(t).$$

By equation (1.3.2) and the facts that $S(t) \ll \log t$ and $\int_0^T S(t)\, \mathrm{d}t \ll \log T$, we can think of $S(t)$ as the difference between the actual and average number of zeros around height t. Therefore, to understand the distribution of the zeros, we wish to understand the statistical and oscillatory behavior of $S(t)$ and $\log |\zeta(\frac{1}{2} + it)|$.

From (1.3.2), we expect that there are about δ zeros of $\zeta(s)$ with ordinates in the interval $[t, t + \frac{2\pi\delta}{\log T}]$ when $0 < t \leqslant T$ and T is large. We define the *number variance* of the zeros of $\zeta(s)$ by

$$\int_0^T \left[N\left(t + \tfrac{2\pi\delta}{\log T}\right) - N(t) - \delta\right]^2 \mathrm{d}t. \tag{1.3.3}$$

This quantity has been studied by a number of authors, for instance [5, 6, 45, 46, 47, 50]. By (1.3.2), up to a small error, the integral in (1.3.3) is equal to

$$\int_0^T \left[S\left(t + \tfrac{2\pi\delta}{\log T}\right) - S(t)\right]^2 \mathrm{d}t.$$

1.3.2 The pair correlation conjecture

Before discussing the known properties of $S(t)$, the number variance of zeta zeros, and our contributions in the theory, we must make a brief interlude on the pair correlation of the zeros of $\zeta(s)$. In 1973, Montgomery [81] studied finer aspects of the vertical distribution of the zeros of $\zeta(s)$, assuming RH. While studying this distribution, he formulated his pair correlation conjecture, which states that

$$\sum_{\substack{0<\gamma,\,\gamma'\leqslant T\\ 0<\gamma-\gamma'\leqslant\frac{2\pi\beta}{\log T}}} 1 \sim N(T)\int_0^\beta \left\{1-\left(\frac{\sin\pi u}{\pi u}\right)^2\right\}\,\mathrm{d}u, \tag{1.3.4}$$

as $T\to\infty$, for any fixed $\beta>0$, where the sum runs over the ordinates of pairs of non-trivial zeros of $\zeta(s)$.

By (1.3.2), the pair correlation conjecture gives an asymptotic formula for the number of pairs of zeros whose distance is at most β times the average gap between zeros, $\frac{2\pi}{\log T}$. Based on (1.3.4), Montgomery further conjectured that the imaginary parts of the zeros of $\zeta(s)$ behave like the eigenvalues of a random matrix from a certain probability distribution called the Gaussian Unitary Ensemble (GUE).

Montgomery wanted to understand sums involving the differences $(\gamma-\gamma')$, such as the left-hand side of (1.3.4). With this goal in mind, for any $R\in L^1(\mathbb{R})$ such that $\widehat{R}\in L^1(\mathbb{R})$, Fourier inversion yields the convolution formula

$$\sum_{0<\gamma,\,\gamma'\leqslant T} R\left(\frac{(\gamma-\gamma')\log T}{2\pi}\right) w(\gamma-\gamma') = \frac{T\log T}{2\pi}\int_{\mathbb{R}} F(\alpha)\,\widehat{R}(\alpha)\,\mathrm{d}\alpha,$$

where we introduce a weight $w(u):=\frac{4}{4+u^2}$, and Montgomery's function $F(\alpha)$ is the (suitably weighted and normalized) Fourier transform of the distribution function of the differences $(\gamma-\gamma')$. It is defined as

$$F(\alpha)=F(\alpha,T):=\frac{2\pi}{T\log T}\sum_{0<\gamma,\,\gamma'\leqslant T} T^{i\alpha(\gamma-\gamma')}w(\gamma-\gamma'), \tag{1.3.5}$$

where $\alpha\in\mathbb{R}$ and $T\geqslant 2$. Thanks to the convolution formula, to understand sums over pairs of zeros, and therefore expressions such as the left-hand side of (1.3.4), it is useful to study the asymptotic behavior of $F(\alpha)$, for large T. Montgomery [81] and Goldston and Montgomery [58] showed, assuming RH, that

$$F(\alpha,T)=(T^{-2|\alpha|}\log T+|\alpha|)\left(1+O\left(\sqrt{\frac{\log\log T}{\log T}}\right)\right), \tag{1.3.6}$$

uniformly for $0\leqslant|\alpha|\leqslant 1$, as $T\to\infty$. Moreover, Montgomery conjectured that $F(\alpha,T)\sim 1$, for $|\alpha|\geqslant 1$ as $T\to\infty$, uniformly for α in compact intervals. This is the *strong pair correlation conjecture*, and it implies (1.3.4) by taking suitable functions R in the convolution formula.

1.3.3 Selberg's central limit theorem

We now return to the theory of $S(t)$, with the goal of understanding the distribution of the zeros of $\zeta(s)$. A celebrated and classical result of Selberg is that the real and imaginary parts of the logarithm of the Riemann zeta-function are normally distributed on the critical line. He proved this by estimating moments of $S(t)$, first assuming RH and then later without any conditions with the same main term and a slightly weaker error term [93, 94]. Assuming RH, Selberg showed that, for $k \in \mathbb{N}$ and $T \geqslant 3$,

$$\int_0^T S(t)^{2k} \, \mathrm{d}t = \frac{(2k)!}{k!(2\pi)^{2k}} T(\log\log T)^k \left[1 + O\left(\frac{1}{\log\log T}\right)\right]. \tag{1.3.7}$$

In other words, the moments of $S(t)$ are Gaussian. In this way, Selberg [95] deduces a *central limit theorem* for $S(t)$:

$$\lim_{T\to\infty} \frac{1}{T} \operatorname{meas}\left\{T \leqslant t \leqslant 2T : \frac{\pi S(t)}{\sqrt{\frac{1}{2}\log\log T}} \in [a,b]\right\} = \frac{1}{\sqrt{\pi}} \int_a^b e^{-x^2/2} \, \mathrm{d}x. \tag{1.3.8}$$

This tells us $\pi S(t)$ is normally distributed for $t \in [T, 2T]$ with mean 0 and variance $\frac{1}{2}\log\log T$, when T is large. Selberg (unpublished) also considered the moments of $\log|\zeta(\frac{1}{2} + it)|$. The details were worked out by Tsang [80], who used Selberg's methods to prove, assuming RH, that

$$\int_0^T \log^{2k}|\zeta(\tfrac{1}{2} + it)| \, \mathrm{d}t = \frac{(2k)!}{k!2^{2k}} T(\log\log T)^k \left[1 + O\left(\frac{1}{\log\log T}\right)\right]. \tag{1.3.9}$$

These moments can be calculated unconditionally with a slightly weaker error term. A corresponding central limit theorem for $\log|\zeta(\frac{1}{2} + it)|$, analogous to (1.3.8), follows from the work Selberg and Tsang. See Radziwiłł and Soundararajan [90] for a recent and simplified proof of Selberg's central limit theorem for $\log|\zeta(\frac{1}{2} + it)|$.

1.3.4 The variance in Selberg's central limit theorem

Selberg modeled $\log\zeta(s)$ near the critical line using information from the primes and the zeros of $\zeta(s)$. He arrives at the main term in (1.3.7) using information from the primes. The information about the zeros is cleverly contained in his error term.

Recall that the *variance* of a distribution is given by its second moment, which corresponds to taking $k = 1$ in (1.3.7). Goldston [53] gave a refined estimate for the variance of $S(t)$ in Selberg's central limit theorem utilizing finer information from both the primes and the zeros of $\zeta(s)$ in his representation of $\log\zeta(s)$. He does so through methods relying, in part, on Montgomery's work [81] on the pair correlation of the zeros of $\zeta(s)$. Assuming RH, Goldston shows that

$$\int_0^T |S(t)|^2 \, \mathrm{d}t = \frac{T}{2\pi^2} \log\log T + \frac{aT}{\pi^2} + o(T), \tag{1.3.10}$$

as $T \to \infty$, where the constant a is given by

$$a = \frac{1}{2}\left(\gamma_0 + \sum_{m=2}^{\infty}\sum_p \left(\frac{1}{m^2} - \frac{1}{m}\right)\frac{1}{p^m} + \int_1^{\infty} \frac{F(\alpha)}{\alpha^2}\, \mathrm{d}\alpha\right), \tag{1.3.11}$$

and γ_0 is Euler's constant. Here, the term with $F(\alpha)$ is defined as in (1.3.5), and it captures the information from the zeros of $\zeta(s)$. As initially defined, the constant a actually depends on T. In Lemma 5.13 we show that this dependence is mild (see also [53, Theorem 2]).

1.3.5 The antiderivatives of $S(t)$

Littlewood [76, 77] and Selberg [93, 94] investigated the behavior of $S(t)$ using its antiderivatives $S_n(t)$. Setting $S_0(t) = S(t)$ we define, for $n \geqslant 1$ an integer and $t > 0$,

$$S_n(t) = \int_0^t S_{n-1}(\tau)\, \mathrm{d}\tau + \delta_n \,,$$

where δ_n is a specific constant depending on n (see the full definition in Chapter 4). Assuming the Riemann hypothesis, Littlewood showed that, for $n \geqslant 1$,

$$S_n(t) = O\left(\frac{\log t}{(\log\log t)^{n+1}}\right) \quad \text{and} \quad \int_0^T S_n(t)^2 \, \mathrm{d}t = O(T),$$

revealing a powerful cancellation due to the oscillatory behavior of $S(t)$. Fujii [49] obtained the first-order term in the even moments of $S_n(t)$ using Selberg's method. In the manuscript [A3], we estimate the second moment of $S_n(t)$ up to the second-order term, using Goldston's method.

Theorem 1.3 (c.f. Theorem 4.1). *Assume the Riemann hypothesis. For $n \geqslant 1$, as $T \to \infty$, we have*

$$\int_0^T |S_n(t)|^2 \, \mathrm{d}t = \frac{C_n}{2\pi^2} T + \frac{T}{2\pi^2 \,(\log T)^{2n}} \left[\int_1^{\infty} \frac{F(\alpha)}{\alpha^{2n+2}}\, \mathrm{d}\alpha - \frac{1}{2n}\right] + O\left(\frac{T\sqrt{\log\log T}}{(\log T)^{2n+1/2}}\right).$$

We give expressions for the constants C_n in Chapter 4. While our approach is based on generalizing Goldston's method, there are additional technical challenges involved. In particular, we introduce a family of new auxiliary functions associated to $S_n(t)$ and take advantage of their properties to reveal a surprising cancellation between two of the main terms. Furthermore, there are new difficulties from dealing with both the real and imaginary parts of the logarithm of $\zeta(s)$, which is necessary to model $S_n(t)$ in terms of information from both the primes and the zeros of $\zeta(s)$. We give further details on the manuscript [A3] in Chapter 4.

1.3.6 Number variance of zeta zeros

In the manuscript [A4], we study the number variance of zeta zeros, defined in (1.3.3). Up to a small error, this equals

$$\int_0^T \left[S\left(t+\frac{2\pi\delta}{\log T}\right)-S(t)\right]^2 \mathrm{d}t. \tag{1.3.12}$$

In 1988, Berry [5] conjectured an asymptotic formula for (1.3.12), by using a conjectural model of the imaginary parts of zeros of $\zeta(s)$ as the eigenvalues of a quantum Hamiltonian operator. This model gives more precise predictions than those of GUE matrices: in the *universal regime* of his model, when $\delta = o(\log T)$, his conjectured asymptotic formula for (1.3.12) matches exactly the variance of GUE random matrices; while the *non-universal regime* of his model, when $\delta \gg \log T$, is no longer described by the predictions of GUE, and incorporates additional input from the primes. In 1990, Fujii [46] proved an asymptotic formula for (1.3.12), assuming RH, in the universal regime where $\delta = o(\log T)$. In particular, assuming RH and the strong pair correlation conjecture, he proves Berry's conjecture in the universal regime.

Our main result in the manuscript [A4] is an asymptotic formula for (1.3.12), assuming RH, for any $\delta = o(\log^3 T)$ (see Theorem 5.2 below). In particular, this includes both the universal and non-universal regimes, and allows a better understanding of the behavior for different sizes of δ. To achieve this, we must overcome significant technical challenges, as new main terms arise and we require a more careful consideration of the error terms. Our result relies on finer information from both the primes and the zeros of $\zeta(s)$, requiring information beyond pair correlation. In particular, we require a variation of Montgomery's function $F(\alpha)$ introduced by Chan [23] in his study of the pair correlation of zeros in longer ranges. To the best of our knowledge, this is the first time that information about pair correlation in longer ranges has been rigorously applied to study the number variance of zeta zeros.

In the universal regime where $\delta = o(\log T)$, our result reduces to Fujii's. Moreover, assuming RH and a generalization of the strong pair correlation conjecture due to Chan, our result implies Berry's conjecture in the non-universal regime. In Chapter 5, we will give the details of these results and say more on their history.

1.3.7 The pair correlation of zeros of families of L-functions

In this section, we briefly describe the manuscript [A5], which we will describe in detail in Chapter 6. In [A5], our starting point is the following relation, proved by Goldston [54]:

the pair correlation conjecture (1.3.4) is equivalent to the statement

$$\frac{1}{\ell}\int_b^{b+\ell} F(\alpha, T)\ \mathrm{d}\alpha \sim 1, \tag{1.3.13}$$

as $T \to \infty$, for any fixed $b \geqslant 1$ and $\ell > 0$, where F is defined in (1.3.5).

Recently, Carneiro, Chandee, Chirre, and Milinovich [16] studied these averages of F over bounded intervals, by developing a general theoretical framework that relates them to some extremal problems in Fourier analysis. This was inspired by some constructions of Goldston [53] and Goldston and Gonek [56]. As a corollary of their general theoretical framework, and approximating the solutions of the associated Fourier optimization problems via numerical examples, they showed that, for any $b \geqslant 1$ and for sufficiently large fixed ℓ, as $T \to \infty$, we have

$$0.927818 + o(1) \leqslant \frac{1}{\ell}\int_b^{b+\ell} F(\alpha, T)\ \mathrm{d}\alpha \leqslant 1.330174 + o(1). \tag{1.3.14}$$

Montgomery [81] also suggested the investigation of the pair correlation of zeros of a family of Dirichlet $L-$functions in the q-aspect. One wishes to study the distribution of the low-lying zeros of $L(s, \chi)$, on average over Dirichlet characters $\chi \pmod q$, and over $Q \leqslant q \leqslant 2Q$. Following the framework of [27], we define the q-analogues as follows[2]. Assume the generalized Riemann hypothesis for Dirichlet L-functions (GRH). Let $\Phi : \mathbb{R} \to \mathbb{R}$ be such that

$$\widetilde{\Phi}(s) = \left(\frac{e^s - e^{-s}}{2s}\right)^2,$$

where $\widetilde{\Phi}$ denotes the Mellin transform. Let W be a smooth, non-negative function with compact support in (1, 2). We define the q-analogue of $N(T)$ as

$$N_\Phi(Q) := \sum_q \frac{W(q/Q)}{\phi(q)} \sideset{}{^*}\sum_{\chi \,(\mathrm{mod}\, q)} \sum_{\gamma_\chi} |\widetilde{\Phi}(i\gamma_\chi)|^2,$$

where the second sum (indicated by the superscript *) is over all primitive Dirichlet characters (mod q), and the last sum is over all non-trivial zeros $1/2 + i\gamma_\chi$ of $L(s,\, \chi)$. Define the q-analogue of $F(\alpha, T)$ as

$$F_\Phi(\alpha) = F_\Phi(\alpha, Q) := \frac{1}{N_\Phi(Q)} \sum_q \frac{W(q/Q)}{\phi(q)} \sideset{}{^*}\sum_{\chi \,(\mathrm{mod}\, q)} \sum_{\gamma_\chi} |\widetilde{\Phi}(i\gamma_\chi) Q^{i\alpha\gamma_\chi}|^2.$$

In analogy to Montgomery's results for $F(\alpha)$, Chandee, Lee, Liu and Radziwiłł [27] proved an asymptotic formula for $F_\Phi(\alpha)$ for $|\alpha| < 2$, showing, in particular, that $F_\Phi(\alpha) \sim 1$ when $1 \leqslant |\alpha| < 2$. Moreover, they conjectured that $F_\Phi(\alpha) \sim 1$ for all $|\alpha| \geqslant 1$, in analogy with

[2]For simplicity, here we present a special case of the framework in [27]. In Chapter 6, we present a slightly more general framework

Montgomery's original conjecture for $F(\alpha)$. Our main result in the manuscript [A5] gives evidence for this conjecture.

Theorem 1.4 (c.f. Theorem 6.2)**.** *Let $b \geqslant 1$, and assume GRH for Dirichlet L-functions. For sufficiently large fixed ℓ, as $Q \to \infty$, we have*

$$0.982144 + o(1) < \frac{1}{\ell} \int_b^{b+\ell} F_\Phi(\alpha, Q)\, \mathrm{d}\alpha < 1.077542 + o(1).$$

We highlight that our upper and lower bounds are very close to the conjectured value of 1. To prove our result, we develop a framework for estimating these integrals over bounded intervals via Fourier analysis, extending that of [16]. We take advantage of the new information available when $|\alpha| \in [1, 2)$, from [27]. This leads to slightly different Fourier extremal problems. After arriving at our Fourier extremal problems, we then numerically optimize the bounds. Since the functionals in the associated extremal problems are not smooth, we apply the principal axis method of Brent [13], which is an algorithm for unconstrained non-smooth optimization.

1.4 Integers represented by quadratic forms

In this section, we briefly describe the research article [A2], which we will explore in Chapter 3. Here, we combine tools from Fourier analysis, analytic number theory and algebraic number theory to obtain several new estimates regarding integers and primes represented by quadratic forms. We have two main themes that are ubiquitous in this investigation. First, we use the well-known theme that propositions about quadratic forms can be stated in two other equivalent languages: ideals of number fields and lattices. We use all three points of view to our advantage in different parts of the article. Our second theme is the use of Fourier analysis, in the following way: we begin by finding a summation formula that connects our object of study with an arbitrary function and its Fourier transform; then, we choose an appropriate test function that recovers the desired information in an optimized manner. We give further background on these topics in Chapter 3.

Given a positive-definite quadratic form $f(u, v) = au^2 + buv + cv^2$ and an integer $\ell \geqslant 2$, we first consider the congruence sum

$$\sum_{\substack{n \leqslant x \\ \ell \mid n}} r_f(n), \tag{1.4.1}$$

where $r_f(n)$ is the number of representations of n by the form f. This is motivated by its utility in sieve methods. When $f(u, v) = u^2 + v^2$ and $\ell = 1$, estimating (1.4.1) is the Gauss Circle Problem. We show:

Theorem 1.5 (c.f. Theorem 3.1)**.** *Let $f(u, v) = au^2 + buv + cv^2$ be a positive definite quadratic form of discriminant $-D = b^2 - 4ac < 0$ and let $\ell \geqslant 1$ be an integer. Then, for*

$x \geqslant 3$ *we have*

$$\sum_{\substack{1 \leqslant n \leqslant x \\ \ell | n}} r_f(n) = \frac{2\pi}{\sqrt{D}}\, g(\ell)\, x + O_{f,\ell}\left(x^{1/3}\right),$$

where

$$g(\ell) = \frac{1}{\ell^2}\{u,\, v \in \mathbb{Z} :\, 0 \leqslant u,\, v \leqslant \ell \text{ and } \ell \mid f(u,v)\}.$$

This improves the error term in a result of Zaman [109, Proposition 7.1], who established a similar result with error term $O_{f,\ell}(x^{1/2})$. We also make the dependence on f and ℓ explicit in the error term; see Theorem 3.1 below for the full statement. Higher moments of $r_f(n)$ (with $\ell = 1$) have also been studied by Blomer and Granville [8].

Following the themes above, we first find and prove a summation formula associated with the coefficients $r_f(n)$ over multiples of ℓ, relating it to an arbitrary function and its Fourier transform. These types of Fourier summation formulas are classical, being related to the modularity of a certain theta series associated to f and to a discrete periodic function χ, the latter which allows us to filter the congruence condition $\ell \mid n$. To prove the specific formula we need, we use Poisson summation for the lattice associated to the form f, and the discrete Fourier expansion of the function χ.

Using Theorem 1.5 and Selberg's sieve, we obtain a Brun-Titchmarsh-type upper bound for the number of primes represented by f in short intervals, of the form

$$\pi_f(x) - \pi_f(x-y) \leqslant (C_f + o(1))\frac{y}{\log y}, \tag{1.4.2}$$

in the range $x^{1/3+\varepsilon} \lesssim y \leqslant x^{3/5}$, where $\pi_f(x)$ is the number of primes less than x that are represented by f. Our constants are explicit; for instance, we are especially interested in the following new corollary:

$$\pi_f(x + \sqrt{x}) - \pi_f(x) \leqslant (28 + o(1))\frac{x}{h(-D)\log x}, \tag{1.4.3}$$

where $h(-D)$ is the class number. Our result (1.4.2) improves another result of Zaman [109, Theorem 1.4], which established a similar bound in longer intervals, in the range $x^{1/2+\varepsilon} \lesssim y \leqslant x$. Then, we used our corollary (1.4.3) and a Fourier optimization approach of Carneiro, Milinovich and Soundararajan [22] to obtain a Cramér-type result on the maximum gap between consecutive primes represented by a given form f.

Theorem 1.6 (c.f. Corollary 3.6)**.** *Let $f(u,v) = au^2 + buv + cv^2$ be a positive definite quadratic form of discriminant $-D = b^2 - 4ac < 0$. Let $p_{n,f}$ be the n-th prime number represented by f. Assuming the generalized Riemann hypothesis for Hecke L-functions, we have*

$$\limsup_{n\to\infty} \frac{p_{n+1,f} - p_{n,f}}{\sqrt{p_{n,f}}\log p_{n,f}} < 1.837\, h(-D). \tag{1.4.4}$$

Our corollary (1.4.3) plays a role in optimizing the value of the constant 1.837 above, and here the extended range that comes from (1.4.2) is required. The constant 28 in (1.4.3) plays a role in this optimization, and optimizing this latter constant required obtaining a good explicit dependence on the parameter ℓ in Theorem 1.5 above.

Returning to our two themes, here it is convenient to work in the language of ideals of quadratic fields, to combine the machinery of Hecke characters and Hecke L-functions with the approach of Carneiro, Milinovich and Soundararajan. The approach is based on the explicit formula, which is another Fourier summation formula relating prime numbers with the zeros of an L-function. In our case, we establish a version of the explicit formula that averages over all Hecke characters in a given congruence class group. Then, we take advantage of heuristics from the uncertainty principle discussed above, combined with numerical experimentation, to find a (near) optimal function that establishes Theorem 1.6 (see Section 3.7 for the relation between the uncertainty principle and this problem).

Chapter 2

Uncertainty principles in Fourier analysis

This chapter is comprised of the paper [A1]. Our goal is to formulate a generalized version of the sign uncertainty principle for the Fourier transform, and identify sharp constants where possible. Furthermore, we introduce a new mechanism to establish sign uncertainty principles (see Theorem 2.7), which works in some settings where the previous tools in the literature may not easily apply.

2.1 Introduction

2.1.1 Background

As mentioned in the Introduction, the uncertainty principle roughly states that one cannot have an unrestricted control of a function and its Fourier transform simultaneously. The uncertainty paradigm is directly related to different sorts of Fourier optimization problems. Generically speaking, these are problems in which one imposes suitable conditions on a function and its Fourier transform, and seeks to optimize a certain quantity of interest. There are surprising applications of such problems, for instance, in the theory of the Riemann zeta-function [18, 19, 28], in bounding prime gaps [22] and in the theory of sphere packings [34, 37, 103].

A classical version of Heisenberg's uncertainty principle establishes that a function and its Fourier transform cannot simultaneously have their mass arbitrarily concentrated near the origin. This can be mathematically formulated as (see, for instance, [43, Corollary 2.8])

$$||f||_2^2 \leqslant \frac{4\pi}{d} \big\| |x| f \big\|_2 \cdot \big\| |\xi| \widehat{f} \big\|_2 , \tag{2.1.1}$$

for any $f \in L^2(\mathbb{R}^d)$. One may ask what happens if, instead of the total mass, one considers the *concentration of negative mass* of a function and its Fourier transform near the origin. In [12], Bourgain, Clozel and Kahane introduced a novel uncertainty principle that addresses this question, in connection to the study of real zeros of zeta functions over number fields and bounds for the associated discriminants. In their setup, the trade-off is between the sign of a function at infinity (or more precisely, the last sign change of the function), and a competing local condition for the transform at the origin. This uncertainty principle was later quantitatively refined by Gonçalves, Oliveira e Silva and Steinerberger in [61], who also studied its extremizers. More recently, Cohn and Gonçalves [35] went further in the topic, building on the fact that the original uncertainty principle of Bourgain, Clozel and Kahane [12] is suitably associated to eigenfunctions of the Fourier transform with eigenvalue $+1$, by posing an analogous principle associated to the eigenvalue -1.

The sign uncertainty principles of [12, 35, 61] can be formulated as follows. Recall that for an eventually non-negative function $f : \mathbb{R}^d \to \mathbb{R}$, we defined

$$r(f) := \inf\{r > 0 \;:\; f(x) \geqslant 0 \text{ for all } |x| \geqslant r\}.$$

Let $s \in \{+1, -1\}$ denote a sign, and consider the following family of functions:

$$\mathcal{A}_s(d) = \left\{ \begin{array}{l} f \in L^1(\mathbb{R}^d)\backslash\{\mathbf{0}\} \text{ continuous, even, real-valued and such that } \widehat{f} \in L^1(\mathbb{R}^d); \\ sf(0) \leqslant 0,\ \widehat{f}(0) \leqslant 0; \\ f \text{ and } s\widehat{f} \text{ are eventually non-negative.} \end{array} \right\}. \tag{2.1.2}$$

We then define

$$\mathbb{A}_s(d) := \inf_{f \in \mathcal{A}_s(d)} \sqrt{r(f)\,.\,r\big(s\widehat{f}\,\big)}\,, \tag{2.1.3}$$

which turns out to be a natural object of interest since $r(f)\,.\,r\big(s\widehat{f}\,\big)$ is invariant under rescalings of the function f. The following assertion holds.

Theorem 2.1 (Bourgain, Clozel and Kahane [12] ($s = +1$) ; Cohn and Gonçalves [35] ($s = -1$))**.** *Let $s \in \{+1, -1\}$. Then there exist strictly positive universal constants c and C such that*

$$c\sqrt{d} \leqslant \mathbb{A}_s(d) \leqslant C\sqrt{d}. \tag{2.1.4}$$

In particular note that $\mathbb{A}_s(d) > 0$. Quantitatively speaking, from [12, 35, 61], estimate (2.1.4) holds with $c = (2\pi e)^{-1/2}$ for $s = \pm 1$; $C = (2\pi)^{-1/2} + o_d(1)$ for $s = +1$; and $C = 0.3194\ldots + o_d(1)$ for $s = -1$. An important step in the proof of Theorem 2.1 is the fact that one can reduce the search for the infimum in (2.1.3) to a restricted class $\mathcal{A}_s^{**}(d) \subset \mathcal{A}_s(d)$ given by

$$\mathcal{A}_s^{**}(d) = \left\{ \begin{array}{l} f \in L^1(\mathbb{R}^d)\backslash\{\mathbf{0}\} \text{ continuous, radial and real-valued: } \widehat{f} = sf; \\ f(0) = 0; \\ f \text{ is eventually non-negative.} \end{array} \right\}.$$

This is how the eigenfunctions of the Fourier transform appear in connection to these problems. The existence of extremizers for $\mathbb{A}_s(d)$ (i.e. functions that realize the infimum in

(2.1.3)) in this restricted class was established in [61] for $s = +1$ and in [35] for $s = -1$.

The exact values of $\mathbb{A}_s(d)$ are only known in four particular cases, discovered in some of the most influential works at the interface between analysis and number theory over the last years. Firstly, the celebrated works on the sphere packing problem via linear programming bounds [34, 37, 103] yield the sharp versions of the (-1)-uncertainty principle in dimensions $d = 1, 8$ and 24 as corollaries (see the extended remark at the end of this subsection for the precise connection). In these cases, the optimal lower bound can be established via the classical Poisson summation formula (for the E_8-lattice in dimension $d = 8$, and for the Leech lattice in dimension $d = 24$). The formula then hints on the appropriate interpolating conditions of the extremal functions. In dimension $d = 1$, the function $f(x) = \sin^2(\pi x)/(x^2 - 1)$ is a bandlimited extremizer; see also the earlier work of Logan [78]. In each of the dimensions $d = 8$ and 24, a radial Schwartz extremal eigenfunction (with prescribed values for the function and its radial derivative at the radii $\{\sqrt{2n}\,;\, n \in \mathbb{N}\}$) is constructed via the impressive machinery introduced by Viazovska [103] on Laplace transforms of modular forms; see also the recent work [36]. Secondly, the recent work of Cohn and Gonçalves [35] establishes the sharp version of the $(+1)$-uncertainty principle of Bourgain, Clozel and Kahane in the special dimension $d = 12$, where the optimal lower bound now comes from a Poisson summation formula for radial Schwartz functions on $\mathbb{R}^{12}$ derived from the Eisenstein series E_6, and an explicit radial Schwartz extremal eigenfunction is constructed by further exploring the ideas of Viazovska [103]. We now compile such results.

Theorem 2.2. *Let $s \in \{+1, -1\}$ and let $\mathbb{A}_s(d)$ be defined by* (2.1.3)*. Then*

(i) (Corollaries of Cohn and Elkies [34] ($d = 1$), Viazovska [103] ($d = 8$) and Cohn, Kumar, Miller, Radchenko and Viazovska [37] ($d = 24$)) .

$$\mathbb{A}_{-1}(1) = 1 \; ; \; \mathbb{A}_{-1}(8) = \sqrt{2} \; ; \; \mathbb{A}_{-1}(24) = 2. \tag{2.1.5}$$

(ii) (Cohn and Gonçalves [35]).

$$\mathbb{A}_{+1}(12) = \sqrt{2}. \tag{2.1.6}$$

It is not known in general whether the search for the infimum in (2.1.3) can be restricted to Schwartz functions. This is only known to be true in the cases of Theorem 2.2 and in the additional case $(s, d) = (+1, 1)$, recently established in [60]. It is conjectured that $\mathbb{A}_{-1}(2) = (4/3)^{1/4}$ and that $\mathbb{A}_{+1}(1) = (2\varphi)^{-1/2}$, where $\varphi = (1 + \sqrt{5})/2$ is the golden ratio; see [59, Conjectures 1.6 and 1.7]. The recent work [59] considers extensions of the (± 1)-sign uncertainty principles to a more abstract operator setting, with very interesting applications to Fourier series and spherical harmonics, among others, and it will have important connections to the present paper. In a nutshell, this is the state of the art in this problem.

A natural question that arises is the following: would there be suitable formulations of the sign uncertainty principle associated to the remaining eigenvalues $\pm i$? This was one of the original motivations for this work and, as we shall see, it will drive us to more general versions of such principles in the Euclidean space.

Remark. (Connection between sign Fourier uncertainty and sphere packing). In [34, Theorem 3.2], Cohn and Elkies considered the following Fourier optimization problem, now regarded as the linear programming bound for the sphere packing problem. Consider the class

$$\mathcal{A}_{LP}(d) = \left\{ \begin{array}{l} g \in L^1(\mathbb{R}^d)\backslash\{\mathbf{0}\} \text{ continuous, even, real-valued and such that } \widehat{g} \in L^1(\mathbb{R}^d); \\ g(0) = \widehat{g}(0) = 1; \\ -g \text{ is eventually non-negative;} \\ \widehat{g} \text{ is non-negative;} \end{array} \right\},$$

and define

$$\mathbb{A}_{LP}(d) := \inf_{g \in \mathcal{A}_{LP}(d)} r(-g).$$

They showed that, given any sphere packing $\mathcal{P} \subset \mathbb{R}^d$ of congruent balls, its *upper density* $\Delta(\mathcal{P})$ (i.e. the fraction of the space covered by the balls in the packing; see [34, Appendix A] for details) satisfies

$$\Delta(\mathcal{P}) \leqslant \mathbb{A}_{LP}(d)^d\, |B_{\frac{1}{2}}|.$$

Numerical experiments suggested that this bound was sharp in dimensions $d = 1, 2, 8$ and 24, the latter three for the honeycomb, E_8 and Leech lattices, respectively. It was already pointed out in [34] that $\mathbb{A}_{LP}(1) = 1$. In [37], Viazovska found the extremal function to show that $\mathbb{A}_{LP}(8) = \sqrt{2}$, hence establishing the optimality of the E_8-lattice in $d = 8$. Later, Cohn, Kumar, Miller, Radchenko and Viazovska [37] found the extremal function to show that $\mathbb{A}_{LP}(24) = 2$ and established the optimality of the Leech lattice in $d = 24$. It is a classical theorem, proved by other methods, that the honeycomb lattice is optimal if $d = 2$; see e.g. [67]. Hence, it is conjectured that $\mathbb{A}_{LP}(2) = (4/3)^{1/4}$, but the corresponding extremal function has not yet been discovered. The connection between the (-1)-uncertainty principle and the linear programming bound is simple: if $g \in \mathcal{A}_{LP}(d)$ observe that $f := \widehat{g} - g \in \mathcal{A}_{-1}(d)$ and that $r(f) \leqslant r(-g)$. Hence, one plainly has $\mathbb{A}_{-1}(d) \leqslant \mathbb{A}_{LP}(d)$. It is conjectured that, in fact, one has $\mathbb{A}_{-1}(d) = \mathbb{A}_{LP}(d)$ for all $d \geqslant 1$ (see [34, Conjecture 8.2], [35] and [59]) but, so far, this has only been established in the cases given by (2.1.5).

2.1.2 Generalized sign Fourier uncertainty

In what follows we write $x = (x_1, x_2, \ldots, x_d) \in \mathbb{R}^d$ for our generic variable (from now on used for both f and $\widehat{f}$). Related to (2.1.1), there exist Heisenberg-type principles in the literature that say that f and $\widehat{f}$ cannot be simultaneously concentrated around the zero set of a function $Q : \mathbb{R}^d \to \mathbb{R}$. For instance, when Q is a non-degenerate quadratic form on $\mathbb{R}^d$, a corollary of a theorem of Shubin, Vakilian and Wolff [96] (see also [10, Corollary 2.20]) establishes

$$||f||_2^2 \leqslant C \left\|Qf\right\|_2 \cdot \left\|Q\widehat{f}\right\|_2 \tag{2.1.7}$$

for $f \in L^2(\mathbb{R}^d)$, while Demange [42] establishes (2.1.7) when $Q(x) = |x_1|^{\gamma_1}|x_2|^{\gamma_2}\ldots|x_d|^{\gamma_d}$ with $\gamma_j > 0$ for $1 \leqslant j \leqslant d$. In a vague analogy to such results, we now consider a situation where the signs of f and $\widehat{f}$ at infinity are prescribed by a given generic function P that we now describe.

Throughout the paper we let $P : \mathbb{R}^d \to \mathbb{R}$ be a measurable function, not identically zero on $\mathbb{R}^d\backslash\{0\}$, verifying:

(P1) $P \in L^1_{\text{loc}}(\mathbb{R}^d)$.

(P2) P is either even or odd. We let $\mathfrak{r} \in \{0, 1\}$ be such that

$$P(-x) = (-1)^{\mathfrak{r}} P(x) \tag{2.1.8}$$

for all $x \in \mathbb{R}^d$.

We shall also consider the following pool of additional assumptions. In each of our results below, an appropriate subset of these may be required.

(P3) P is annihilating in the following sense: if $f \in L^1(\mathbb{R}^d)$ is a continuous eigenfunction of the Fourier transform such that Pf is eventually zero then $f = \mathbf{0}$.

(P4) P is homogeneous. That is, there is a real number $\gamma > -d$ such that

$$P(\delta x) = \delta^\gamma P(x) \tag{2.1.9}$$

for all $\delta > 0$ and $x \in \mathbb{R}^d$.

(P5) The sub-level set $A_\lambda = \{x \in \mathbb{R}^d \,:\, |P(x)| \leqslant \lambda\}$ has finite Lebesgue measure for some $\lambda > 0$.

(P6) The sub-level set $A_\lambda = \{x \in \mathbb{R}^d \,:\, |P(x)| \leqslant \lambda\}$ is bounded for some $\lambda > 0$.

(P7) $P \in L^\infty_{\text{loc}}(\mathbb{R}^d)$.

(P8) $P\, e^{-\lambda\pi|\cdot|^2} \in L^1(\mathbb{R}^d)$ for all $\lambda > 0$.

(P9) (Sign density) For each $x \in \mathbb{R}^d\backslash\{0\}$ such that $P(x) \neq 0$ we have

$$\liminf_{\varepsilon\to 0} \frac{\left|\{y \in \mathbb{R}^d : P(y)P(x) > 0\} \cap B_\varepsilon(x)\right|}{\left|B_\varepsilon(x)\right|} > 0.$$

Remark. Condition (P3) above holds in a variety of situations. A simple one would be if the set $\{x \in \mathbb{R}^d : P(x) \neq 0\}$ is dense in $\mathbb{R}^d$ (in this case, Pf eventually zero implies that f has compact support). Another one is if the set $\{x \in \mathbb{R}^d : P(x) = 0\}$ has finite Lebesgue measure (hence (P6) implies (P5) that implies (P3)). In this case, Pf eventually zero implies that f is supported on a set of finite measure, and hence $f = \mathbf{0}$ by Lemma 2.12 below. Note also that (P1) and (P4) imply (P8).

We investigate the sign uncertainty principles in a more general setting as follows. In our formulation, it will be convenient to think of the competing conditions at the origin as weighted integrals over $\mathbb{R}^d$, via the Fourier transform. In this sense, the conditions $sf(0) \leqslant 0$ and $\widehat{f}(0) \leqslant 0$ appearing in (2.1.2) should be viewed as $\int_{\mathbb{R}^d} s\widehat{f} \leqslant 0$ and $\int_{\mathbb{R}^d} f \leqslant 0$, respectively. Assume that our function P verifies properties (P1), (P2), (P3) and (P4) above and let $s \in \{+1, -1\}$ be a sign. Consider the following class of functions, with suitable parity and integrability conditions (note that we move to a slightly different notation to denote the dependence on the function P),

$$\mathcal{A}_s(P;d) = \left\{ \begin{array}{l} f \in L^1(\mathbb{R}^d)\backslash\{\mathbf{0}\} \text{ continuous, real-valued and such that } f(-x) = (-1)^{\mathfrak{r}} f(x); \\ \widehat{f}, Pf, P\widehat{f} \in L^1(\mathbb{R}^d); \\ \int_{\mathbb{R}^d} Pf \leqslant 0 \;,\; \int_{\mathbb{R}^d} s(-i)^{\mathfrak{r}} P\widehat{f} \leqslant 0; \\ Pf,\; s(-i)^{\mathfrak{r}} P\widehat{f} \text{ are eventually non-negative.} \end{array} \right\}. \tag{2.1.10}$$

As before, let us define

$$\mathbb{A}_s(P;d) = \inf_{f \in \mathcal{A}_s(P;d)} \sqrt{r(Pf)\,.\,r\big(s(-i)^{\mathfrak{r}} P\widehat{f}\,\big)}. \tag{2.1.11}$$

Note that if $f \in \mathcal{A}_s(P;d)$, any rescaling $f_\delta(x) := f(\delta x)$, for $\delta > 0$, also belongs to $\mathcal{A}_s(P;d)$, and the product $r(Pf)\,.\,r\big(s(-i)^{\mathfrak{r}} P\widehat{f}\,\big)$ is invariant. This is due to condition (P4).

A particularly interesting case is when P is a homogeneous polynomial of degree $\gamma \in \mathbb{N} \cup \{0\}$ in d variables. In this case, the integral conditions in the definition of $\mathcal{A}_s(P;d)$ are equivalent to conditions given by the differential operator associated to P applied to f and $\widehat{f}$ and evaluated at the origin (provided f and $\widehat{f}$ are sufficiently smooth). Note that, in principle, we do not require in this case that $|x|^\gamma f, |x|^\gamma \widehat{f} \in L^1(\mathbb{R}^d)$, but only the minimal integrability condition $Pf, P\widehat{f} \in L^1(\mathbb{R}^d)$. The class $\mathcal{A}_s(d)$ considered in (2.1.2) corresponds to the case $P = \mathbf{1}$.

The question on whether the uncertainty principle holds for the families $\mathcal{A}_s(P;d)$, and even the question on whether these families are at least non-empty, may possibly depend on the function P; and finding necessary and sufficient conditions seems to be a subtle issue. Before moving into that discussion, let us observe that we can restrict the search to a certain subclass $\mathcal{A}_s^*(P;d) \subset \mathcal{A}_s(P;d)$ of eigenfunctions defined by

$$\mathcal{A}_s^*(P;d) = \left\{ \begin{array}{l} f \in L^1(\mathbb{R}^d)\backslash\{\mathbf{0}\} \text{ continuous, real-valued and such that } \widehat{f} = si^{\mathfrak{r}} f; \\ Pf \in L^1(\mathbb{R}^d); \\ \int_{\mathbb{R}^d} Pf \leqslant 0\,; \\ Pf \text{ is eventually non-negative.} \end{array} \right\}. \tag{2.1.12}$$

We also define

$$\mathbb{A}_s^*(P;d) = \inf_{f \in \mathcal{A}_s^*(P;d)} r(Pf). \tag{2.1.13}$$

Assuming that the class $\mathcal{A}_s(P;d)$ is non-empty, we claim that $\mathcal{A}_s^*(P;d)$ is also non-empty and that

$$\mathbb{A}_s(P;d) = \mathbb{A}_s^*(P;d). \tag{2.1.14}$$

To see this, start with any function $f \in \mathcal{A}_s(P;d)$. By taking an appropriate rescaling $f_\delta(x) := f(\delta x)$, we may assume that $r(Pf) = r\big(s(-i)^{\mathfrak{r}} P\widehat{f}\big)$. Observe that $s(-i)^{\mathfrak{r}}\widehat{f} \in \mathcal{A}_s(P;d)$ and let

$$w = f + s(-i)^{\mathfrak{r}}\widehat{f}.$$

Then $\widehat{w} = si^{\mathfrak{r}} w$, $\int_{\mathbb{R}^d} Pw \leqslant 0$ and $r(Pw) \leqslant r(Pf)$. Note that w is not identically zero. In fact, if $w = \mathbf{0}$, we would have Pf and $s(-i)^{\mathfrak{r}} P\widehat{f} = -Pf$ eventually non-negative, which would make Pf eventually zero. By condition (P3) we would have $f = \mathbf{0}$, a contradiction. Hence $w \in \mathbb{A}_s^*(P;d)$ and does a job at least as good as the original f.

This is how the eigenfunctions of the Fourier transform (now with all possible eigenvalues) play a role in this discussion. Observe that we may consider directly the *eigenfunction extremal problem* described in (2.1.12) - (2.1.13). In this case, *we do not need to assume conditions* (P3) and (P4) for our function $P : \mathbb{R}^d \to \mathbb{R}$, leaving us essentially with the fully generic setup of (P1) and (P2). When we consider the eigenfunction formulation in the results below, the reader should keep in mind the original formulation (2.1.10) - (2.1.11), and identity (2.1.14), if applicable.

Note that all of our conditions (P1) – (P9) are invariant under rotations and reflections. Letting $O(d)$ be the group of linear orthogonal transformations in $\mathbb{R}^d$, if $R \in O(d)$ one can verify that $\mathbb{A}_s^*(P;d) = \mathbb{A}_s^*(P \circ R;d)$ and $\mathbb{A}_s(P;d) = \mathbb{A}_s(P \circ R;d)$ by a suitable change of variables.

It is important to emphasize that we *do not* identify functions P that are equal almost everywhere with respect to the Lebesgue measure. In fact, even if two functions P_1 and P_2 are equal a.e., the two problems (2.1.12) - (2.1.13) that they generate may be very different. Consider for example, in dimension $d = 1$, $P_1 = \mathbf{1}$ and $P_2(x) = 1$ for all $x \in \mathbb{R}\backslash\{a_n\}_{n\in\mathbb{Z}}$, $P_2(a_n) = -1$, where $\{a_n\}_{n\in\mathbb{N}}$ is a given sequence of points with $\lim_{n\to\infty} |a_n| = \infty$. Any function $f \in \mathcal{A}_s^*(P_2;1)$ will necessarily have zeros at a_n for $n \geqslant n_0$. In this regard, even problems where $P(x) = 0$ a.e. are non-trivial, and we quickly realize that we are in a vastly uncharted territory.

We first move in the direction of identifying some important situations when these classes are non-empty and providing reasonable upper bounds.

Theorem 2.3 (Non-empty classes and upper bounds). *Let $P : \mathbb{R}^d \to \mathbb{R}$ be a function verifying properties* (P1), (P2) *and* (P8). *Assume that $P = H\,.\,Q$, where $H : \mathbb{R}^d \to \mathbb{R}$ is a homogeneous and harmonic polynomial of degree $\ell \geqslant 0$, and $Q : \mathbb{R}^d \to \mathbb{R}$ is eventually non-negative. Then $\mathcal{A}_s^*(P; d)$ is non-empty. If, in addition, P verifies* (P4), *letting $\mathfrak{r}$ as in* (2.1.8) *and $\gamma > -d$ as in* (2.1.9) *we have*

$$\mathbb{A}_s^*(P; d) \leqslant \sqrt{\frac{\max\{d + \ell + \gamma\,,\, \ell - \gamma\}}{2\pi}} + O(1),$$

with the implied constant being universal; in fact, when $s\, i^{\ell+\mathfrak{r}} = -1$ and $-d < \gamma \leqslant -\frac{d}{2}$ we have

$$\mathbb{A}_s^*(P; d) = 0.$$

Remark. Note that in Theorem 2.3 we may have $\ell > \gamma$. A simple example would be $P(x) = \operatorname{sgn}(x_1)$, in which $H(x) = x_1$, and $Q(x) = \operatorname{sgn}(x_1)/x_1$ for $x_1 \neq 0$ and zero otherwise. We shall not be particularly interested in more explicit quantitative estimates for the upper bounds here.

There is an interesting relationship between the sign uncertainty principles and other classical uncertainty principles. For our purposes, the relevant inequality would be an analogue of (2.1.7), with L^1-norms on the right-hand side. For instance, a basic application of the Hausdorff-Young inequality yields

$$\|f\|_2^2 \leqslant \|f\|_1\, \|\widehat{f}\|_1$$

for any $f \in L^2(\mathbb{R}^d)$, and similar ideas used to prove (2.1.1), coupled with the Hausdorff-Young inequality, yield

$$\|f\|_2^2 \leqslant 4\pi\, \|x_1 f\|_1\, \|x_1 \widehat{f}\|_1 \tag{2.1.15}$$

for any $f \in L^2(\mathbb{R}^d)$ (see, for instance, [43, Corollary 2.6 and Section 3]). By a change of variables given by any $R \in O(d)$ we see that (2.1.15) holds with the function x_1 replaced by any linear homogeneous polynomial in $x_1, x_2, \ldots, x_d$. Motivated by such examples we now define a class of admissible functions P that will play an important role in our study. As we shall see, this will be an asset (but not the only one) in establishing sign uncertainty principles.

Definition 2.4 (Admissible functions). *A function $P : \mathbb{R}^d \to \mathbb{R}$ verifying properties* (P1) *and* (P2) *is said to be admissible if there exists an exponent q with $1 \leqslant q \leqslant \infty$ and a positive constant $C(P; d; q)$ such that:*

(i) For all $f \in L^1(\mathbb{R}^d)$, with $\widehat{f} = \pm i^{\mathfrak{r}} f$ and $Pf \in L^1(\mathbb{R}^d)$, we have

$$||f||_q \leqslant C(P; d; q)\, \|Pf\|_1. \tag{2.1.16}$$

(ii) If $q > 1$ we have $P \in L^{q'}_{\text{loc}}(\mathbb{R}^d)$. If $q = 1$ we have $\lim_{r\to 0^+} \|P\|_{L^\infty(B_r)} = 0$.[1]

The fact that $\widehat{f} = \pm i^{\mathfrak{r}} f$, together with the Hausdorff-Young inequality, directly implies that $\|f\|_q \leqslant \|f\|_1$ for all $1 \leqslant q \leqslant \infty$. Hence, if (2.1.16) holds for $q = 1$, it holds for any exponent $1 \leqslant q \leqslant \infty$ with $C(P; d; q) \leqslant C(P; d; 1)$. The finiteness of the sub-level sets is related to the concept of admissibility as our next result shows.

Theorem 2.5 (Sufficient conditions for admissibility)**.** *Let $P : \mathbb{R}^d \to \mathbb{R}$ be a function verifying properties* (P1), (P2) *and* (P5). *Then inequality* (2.1.16) *holds with $q = 1$. In particular, P is admissible with respect to $q = \infty$. If, in addition, P verifies property* (P4) *with degree $\gamma \geqslant 0$ in* (2.1.9)*, we can bound the constant $C(P; d; 1)$ as:*

(i) If $\gamma = 0$ then

$$C(P; d; 1) \leqslant \big(\operatorname{ess\,inf}|P|\big)^{-1} < \infty. \tag{2.1.17}$$

(ii) If $\gamma > 0$ then

$$C(P; d; 1) \leqslant \left(1 + \frac{\gamma}{d}\right)\left[\left(1 + \frac{d}{\gamma}\right)|A_1|\right]^{\frac{\gamma}{d}}. \tag{2.1.18}$$

Remark. Note that in the case P homogeneous of degree $\gamma > 0$, the sub-level set A_λ has finite measure (for any $\lambda > 0$) if and only if

$$\int_{\mathbb{S}^{d-1}} |P(\omega)|^{-d/\gamma}\, \mathrm{d}\sigma(\omega) < \infty,$$

where σ denotes the surface measure on the unit sphere $\mathbb{S}^{d-1} \subset \mathbb{R}^d$.

In light of example (2.1.15), note that Theorem 2.5 is not a necessary condition for a function P to be admissible. We are now in position to present a general version of the sign uncertainty principle associated to a function P.

Theorem 2.6 (Sign uncertainty)**.** *Let $P : \mathbb{R}^d \to \mathbb{R}$ be a function verifying properties* (P1) *and* (P2). *Assume that the class $\mathcal{A}^*_s(P; d)$ is non-empty and that P is admissible with respect to an exponent $1 \leqslant q \leqslant \infty$. Then there exists a positive constant $C^*(P; d; q)$ such that*

$$\mathbb{A}^*_s(P; d) \geqslant C^*(P; d; q). \tag{2.1.19}$$

Moreover,

(i) If P verifies properties (P5), (P7) *and* (P9)*, there exist extremizers for $\mathbb{A}^*_s(P; d)$.*

(ii) If P verifies properties (P4) *and* (P7)*, with degree $\gamma \geqslant 0$ in* (2.1.9) *and $K := \|P\|_{L^\infty(B_1)}$,*

$$C^*(P; d; q) \geqslant \left(\frac{(d + \gamma q')\,\Gamma(d/2)}{2\,\pi^{\frac{d}{2}}\,(2KC)^{q'}}\right)^{\frac{1}{(d+\gamma q')}}, \tag{2.1.20}$$

[1] Throughout this chapter $1/q + 1/q' = 1$.

where $C = C(P;d;q)$ as in (2.1.16). If $q = 1$ (and hence $\gamma > 0$), the right-hand side of (2.1.20) should be understood as $(2KC)^{-1/\gamma}$.

Remark. The constant $C^*(P;d;q)$ in (2.1.19) will be described in the proof. In the homogeneous case (ii) above, under (P5), we can use the fact that $C(P;d;q) \leqslant C(P;d;1)$ and (2.1.17) - (2.1.18) to get explicit lower bounds in (2.1.20) (that could be then optimized over q). In the original case $P = \mathbf{1}$ of Theorem 2.1, we can simply choose $q = \infty$ to recover the lower bound $\frac{1}{\sqrt{\pi}}\left(\frac{1}{2}\Gamma\left(\frac{d}{2}+1\right)\right)^{1/d} > \frac{\sqrt{d}}{\sqrt{2\pi e}}$ as in [12, Theorem 3] and [35, Theorem 1.4]. We shall see that, once the non-emptiness and admissibility conditions are in place, the proof of (2.1.19) is rather simple, following the somewhat rigid original scheme of Bourgain, Clozel and Kahane [12]. One then realizes that the crux of the matter here is in fact obtaining such conditions, and that is where results like Theorems 2.3 and 2.5 enter. When $q = \infty$, there is an alternative approach to arrive at the same qualitative conclusion as in (2.1.19) via the operator framework of [59, Theorem 1], as communicated to us by F. Gonçalves. In that statement one could consider $(X,\mu) = (Y,\nu) = (\mathbb{R}^d, |P|\,\mathrm{d}x)$; $p = q = 2$; $b = c = 1$; and $\mathcal{F} = \{(\mathrm{sgn}(P)f,\ s\cdot\mathrm{sgn}(P)f)\,;\ f \in \mathbb{A}_s^*(P;d)\}$. The relevant condition that needs to be checked is that $\|\,\mathrm{sgn}(P)f\|_{L^\infty(\mathbb{R}^d,\nu)} \leqslant a\,\|\,\mathrm{sgn}(P)f\|_{L^1(\mathbb{R}^d,\mu)}$. This follows from the admissibility condition (2.1.16) with $q = \infty$ (which for instance, under (P5), follows from Theorem 2.5) since $\|\,\mathrm{sgn}(P)f\|_{L^\infty(\mathbb{R}^d,\nu)} \leqslant \|f\|_{L^\infty(\mathbb{R}^d)} \leqslant C(P;d;\infty)\|Pf\|_{L^1(\mathbb{R}^d)} = C(P;d;\infty)\|\,\mathrm{sgn}(P)f\|_{L^1(\mathbb{R}^d,\mu)}$. Then, with $r = r(Pf)$, [59, Theorem 1, Eq. (1.4)] yields $\left\|P\mathbb{I}_{B_r}\right\|_1 \geqslant \left(4\,C(P;d;\infty)\right)^{-1}$, qualitatively as in (2.4.2) below. There are also occasions, as exemplified in (2.1.15), where the admissibility exponent q is not, in principle, 1 or ∞.

As already mentioned, Theorems 2.3 and 2.5 can be used to generate a great variety of examples where the hypotheses of Theorem 2.6 are verified. A simple example would be $P(x) = |x|^\gamma$, for $\gamma \geqslant 0$, while a less straightforward one could be $P : \mathbb{R}^3 \to \mathbb{R}$ given by $P(x) = \left(x_1^2+x_2^2-2x_3^2\right)\left(x_1^2+x_2^2+2x_3^2\right)$. The odd functions $P(x) = \mathrm{sgn}(x_1)$ and $P(x) = x_1$ also verify the hypotheses of Theorem 2.6 (the latter is admissible directly from (2.1.15)), and these provide two simple versions of sign uncertainty principles associated to the eigenvalues $\pm i$ in all dimensions. In the case $P(x) = \mathrm{sgn}(x)$ in dimension $d = 1$, the integral conditions defining the class $\mathcal{A}_s(\mathrm{sgn}(x);1)$ can be recast in terms of the sign of the Hilbert transform at the origin. A different sign uncertainty principle for bandlimited functions involving the Hilbert transform appears in [59, Theorem 4.2].

2.1.3 Dimension shifts

There will be occasions where the admissibility inequality (2.1.16), or suitable variants of it, are not, in principle, available (see, for instance, the last remark in Section 2.6). We present now a different tool to obtain the sign uncertainty that may be helpful in such circumstances. The intuitive idea is to allow ourselves some movement between different dimensions in order to fall in a favourable situation as in Theorem 2.6. The classical Bochner's relation will be a crucial ingredient in this process and, therefore, radial functions play an important role. In some special situations we are able to go further and establish a surprising identity connecting the sign uncertainty in different dimensions. The reach of the next result will be exemplified in its two companion corollaries. In what follows, for a function $H : \mathbb{R}^d \to \mathbb{R}$ we denote its orbit under the action of the group $O(d)$ by

$$H \circ O(d) := \{H \circ R : \mathbb{R}^d \to \mathbb{R} \;:\; R \in O(d)\}.$$

Theorem 2.7 (Dimension shifts). *Let $\ell \geqslant 0$ be an integer and let $\mathfrak{r}(\ell) \in \{0,1\}$ be such that $\mathfrak{r}(\ell) \equiv \ell \,(mod\, 2)$. Let $P : \mathbb{R}^{d+2\ell} \to \mathbb{R}$ be a function verifying properties* (P1), (P2) *and* (P3) *that is radial. Write $P(x) = P_0(|x|)$. Let $\widetilde{P} : \mathbb{R}^d \to \mathbb{R}$ be a function verifying properties* (P1) *and* (P2) *of the form*

$$\widetilde{P}(x) = H(x)\, P_0(|x|)\, Q(x), \tag{2.1.21}$$

where $H : \mathbb{R}^d \to \mathbb{R}$ is a non-zero homogeneous and harmonic polynomial of degree ℓ and $Q : \mathbb{R}^d \to \mathbb{R}$ is an even non-negative function, homogeneous of degree 0. If $\mathcal{A}^*_s(P; d+2\ell)$ is non-empty, then $\mathcal{A}^*_{s(-1)^{(\mathfrak{r}(\ell)+\ell)/2}}\big(\widetilde{P}; d\big)$ is also non-empty and

$$\mathbb{A}^*_s(P; d+2\ell) \geqslant \mathbb{A}^*_{s(-1)^{(\mathfrak{r}(\ell)+\ell)/2}}\big(\widetilde{P}; d\big). \tag{2.1.22}$$

If, in addition, P verifies property (P6)*, $Q = \mathbf{1}$ and $H \in (x_1x_2\ldots x_\ell)\circ O(d)$ $(0 \leqslant \ell \leqslant d)$, the converse holds: $\mathcal{A}^*_s(P; d+2\ell)$ is non-empty if and only if $\mathcal{A}^*_{s(-1)^{(\mathfrak{r}(\ell)+\ell)/2}}\big(\widetilde{P}; d\big)$ is non-empty and*

$$\mathbb{A}^*_s(P; d+2\ell) = \mathbb{A}^*_{s(-1)^{(\mathfrak{r}(\ell)+\ell)/2}}\big(\widetilde{P}; d\big). \tag{2.1.23}$$

In general, it is not clear that we can reverse inequality (2.1.22). One of the main obstacles is to show that the search for the infimum on the right-hand side of (2.1.22) can be reduced to functions f of the form Hf_0 with f_0 radial (which may simply not be true in general). In the case presented in (2.1.23) we overcome this and other barriers. Our proof also yields the following fact: if there exist extremizers for either side of (2.1.23), then there exist extremizers for both sides and we have a recipe to explicitly construct one from the other; this is particularly useful to construct explicit extremizers in the situations of Corollary 2.8 below.

We can consider in (2.1.23), for instance, $P(x) = |x|^\gamma$ for $\gamma \geqslant 0$. In the particular case $P = \mathbf{1}$, identity (2.1.23), together with (2.1.5) and (2.1.6), yields the following additional 14 sharp constants (modulo symmetries given by the orthogonal group) in this rough environment of sign uncertainty.

Corollary 2.8 (Sharp constants). *Let $\mathfrak{r}(\ell) \in \{0,1\}$ be such that $\mathfrak{r}(\ell) \equiv \ell \,(mod\, 2)$. Then*

$$\mathbb{A}_{(-1)^{(\mathfrak{r}(\ell)+\ell+2)/2}}\big((x_1\ldots x_\ell)\circ R\,;\, 8-2\ell\big) = \sqrt{2}, \quad \text{for } 0 \leqslant \ell \leqslant 2 \text{ and } R \in O(8-2\ell);$$
$$\mathbb{A}_{(-1)^{(\mathfrak{r}(\ell)+\ell)/2}}\big((x_1\ldots x_\ell)\circ R\,;\, 12-2\ell\big) = \sqrt{2}, \quad \text{for } 0 \leqslant \ell \leqslant 4 \text{ and } R \in O(12-2\ell);$$
$$\mathbb{A}_{(-1)^{(\mathfrak{r}(\ell)+\ell+2)/2}}\big((x_1\ldots x_\ell)\circ R\,;\, 24-2\ell\big) = 2, \quad \text{for } 0 \leqslant \ell \leqslant 8 \text{ and } R \in O(24-2\ell).$$

Remark. *A posteriori*, it is worth reflecting on the difficulties of taking a more classical and direct path (e.g. via Poisson-like summation formulas) to approach the sharp constants in Corollary 2.8. It is also interesting to further investigate the potential connections of this weighted setup and the sharp constants in Corollary 2.8 to other optimization problems in diophantine geometry.

Inequality (2.1.22) is particularly useful in situations where P is singular near the origin (e.g. radially decreasing). In such cases, one can take $Q = |x|^{\ell}\,\mathrm{sgn}(H)/H$ (for $H \neq 0$, and zero otherwise) in (2.1.21) and make $\widetilde{P}$ less singular. Of course, this comes at the expense of lowering the dimension, and there is an intrinsic threshold on how far one can go. For instance, let us come back to the natural power weight $P(x) = |x|^{\gamma}$, where $\gamma > -d$ is a real number. If $\gamma \geqslant 0$, Theorems 2.3, 2.5 and 2.6 can be applied and we are in good shape. Note that, in this case, the integral conditions defining the class $\mathcal{A}_s(|x|^{\gamma}; d)$ can be reformulated in terms of the sign of the fractional Laplacian $(-\Delta)^{\gamma/2}$ of f and $\widehat{f}$, evaluated at the origin. A related sign uncertainty principle for bandlimited functions and powers of the Laplacian was considered by Gorbachev, Ivanov and Tikhonov in [62]. The case $-d < \gamma < 0$ is subtler, and we can bring Theorem 2.7 into play. In fact, in this situation, we are able to prove or disprove the sign uncertainty principle in a set of "full density" as the dimension d grows.

Corollary 2.9 (Power weights). *Let $s \in \{+1, -1\}$ and $\gamma > -d$ be a real number. Let $\varepsilon : \mathbb{N} \to \mathbb{R}$ be defined as: $\varepsilon(d) = 1$ for $d \geqslant 2$ even, $\varepsilon(1) = \varepsilon(3) = \frac{1}{2}$, and $\varepsilon(d) = \frac{3}{2}$ for $d \geqslant 5$ odd.*

(i) If $s = 1$ and $\gamma \notin \big(-\frac{d}{2} - \varepsilon(d), -\frac{d}{2} + \varepsilon(d)\big)$ or if $s = -1$ and $\gamma \notin \big(-d, -\frac{d}{2} + \varepsilon(d)\big)$ we have

$$c\sqrt{\frac{\min\{d, |d + 2\lfloor\gamma\rfloor|, |-d + 2\lfloor-\gamma\rfloor|\}}{2\pi e}} \leqslant \mathbb{A}_s(|x|^{\gamma}; d) \leqslant \sqrt{\frac{\max\{d+\gamma\,,\,-\gamma\}}{2\pi}} + O(1)\,, \tag{2.1.24}$$

where c is a positive universal constant. Moreover, if $\gamma \geqslant 0$, there exists a radial extremizer for $\mathbb{A}_s(|x|^{\gamma}; d)$.

(ii) If $s = -1$ and $\gamma \in \big(-d, -\frac{d}{2}\big]$ then

$$\mathbb{A}_{-1}(|x|^{\gamma}; d) = 0. \tag{2.1.25}$$

The upper bound in (2.1.24) actually holds for all $\gamma > -d$ and $s = \pm 1$. In the proof of this corollary we give a more explicit lower bound in the parameters d and γ (that, in particular, recovers the known bounds in the case $\gamma = 0$; see the remark after Theorem 2.6). The uniform lower bound presented in (2.1.24) holds with constant $c = 0.8595\ldots$ if $d = 1$; or $d = 3$ and $\gamma < 0$; and with constant $c = 1$ in all other cases. Numerical simulations suggest that the sign uncertainty principle should still hold in the small uncovered neighborhood (of size at most 3 when $s = 1$ and size at most $\frac{3}{2}$ when $s = -1$) around the central point $-\frac{d}{2}$ of the negative range.

2.2 Non-empty classes and upper bounds: proof of Theorem 2.3

An important ingredient in this work is the following classical identity.

Lemma 2.10 (Bochner's relation)**.** *Let $H : \mathbb{R}^d \to \mathbb{R}$ be a homogeneous, harmonic polynomial of degree ℓ, and $h : [0, \infty) \to \mathbb{R}$ be a function such that*

$$\int_0^\infty |h(r)|^2 \, r^{d+2\ell-1} \, \mathrm{d}r < \infty.$$

Let $h_d : \mathbb{R}^d \to \mathbb{R}$ be the radial function on $\mathbb{R}^d$ induced by h, that is $h_d(x) := h(|x|)$. Then

$$\mathcal{F}_d[H \cdot h_d](\xi) = (-i)^\ell H(\xi) \cdot \mathcal{F}_{d+2\ell}[h_{d+2\ell}](\xi, 0),$$

where $\xi \in \mathbb{R}^d$ and $(\xi, 0) \in \mathbb{R}^d \times \mathbb{R}^{2\ell}$.

Proof. See [98, Chapter III, Theorem 4 and its corollary]. □

We now move to the proof of Theorem 2.3. From (2.1.8) we have

$$(-1)^{\mathfrak{r}} H(x)Q(x) = H(-x)Q(-x) = (-1)^\ell H(x)Q(-x) \tag{2.2.1}$$

for all $x \in \mathbb{R}^d$.

2.2.1 Non-empty classes

If ℓ and $\mathfrak{r}$ have a different parity, we conclude from (2.2.1) that P must be eventually zero (since Q is assumed to be eventually non-negative). In this case, let $f \in L^1(\mathbb{R}^d)\backslash\{\mathbf{0}\}$ be a continuous and real-valued eigenfunction with $\widehat{f} = s i^{\mathfrak{r}} f$. One plainly sees that either f or $-f$ belongs to $\mathcal{A}_s^*(P; d)$.

If ℓ and $\mathfrak{r}$ have the same parity, we proceed inspired by an example of Bourgain, Clozel and Kahane [12]. We consider functions of the form:

$$g_0(x) = H(x)\left(e^{-\frac{1}{a_0}\pi|x|^2} + a_0^{\frac{d+2\ell}{2}} e^{-a_0\pi|x|^2}\right) \; ; h_0(x) = H(x)\, e^{-\pi|x|^2} \; ; \; f_0(x) = g_0(x) - A_0\, h_0(x), \tag{2.2.2}$$

and

$$g_1(x) = H(x)\left(e^{-\frac{1}{a_1}\pi|x|^2} - a_1^{\frac{d+2\ell}{2}} e^{-a_1\pi|x|^2}\right) \; ; \; h_1(x) = H(x)\left(e^{-\frac{1}{b_1}\pi|x|^2} - b_1^{\frac{d+2\ell}{2}} e^{-b_1\pi|x|^2}\right);$$
$$f_1(x) = g_1(x) - A_1 h_1(x), \tag{2.2.3}$$

with constants $1 < a_0$, $1 < b_1 < a_1$, A_0 and A_1 arbitrary. Using Lemma 2.10 we observe that $\widehat{g}_m = (-1)^m(-i)^\ell g_m$, $\widehat{h}_m = (-1)^m(-i)^\ell h_m$, $\widehat{f}_m = (-1)^m(-i)^\ell f_m$, for $m \in \{0, 1\}$. Since

ℓ and $\mathfrak{r}$ have the same parity, when $(-1)^m = s\, i^{\ell+\mathfrak{r}}$ these are eigenfunctions with the desired eigenvalue $si^{\mathfrak{r}}$. Note that Pg_m, Ph_m and Pf_m are eventually non-negative (and integrable due to property (P8)). If either $\int_{\mathbb{R}^d} Pg_m \leqslant 0$ or $\int_{\mathbb{R}^d} Ph_m \leqslant 0$, that function will belong to the class $\mathcal{A}_s^*(P;d)$. If both of these integrals are positive, we adjust the constant A_m to make $\int_{\mathbb{R}^d} Pf_m \leqslant 0$ and hence $f_m \in \mathcal{A}_s^*(P;d)$. This shows that $\mathcal{A}_s^*(P;d)$ is non-empty.

2.2.2 Homogeneous case

Assume now that P verifies (P4). As discussed in §2.2.1, in this situation we must have ℓ and $\mathfrak{r}$ with the same parity.

Case $si^{\ell+\mathfrak{r}} = 1$

In this case we work with the function f_0 in (2.2.2) and let

$$A_0 = a_0^{\frac{d+\ell+\gamma}{2}} + a_0^{\frac{\ell-\gamma}{2}}.$$

From the homogeneity of P and H one can check that this choice of A_0 yields $\int_{\mathbb{R}^d} Pf_0 = 0$. Note from (2.2.2) that

$$Pf_0 \geqslant PH\, e^{-\pi|x|^2}\left(e^{(1-\frac{1}{a_0})\pi|x|^2} - A_0\right)$$

for $x \neq 0$ (recall that $PH = H^2Q$ being homogeneous and eventually non-negative is actually non-negative outside the origin). This plainly implies that

$$r(Pf_0) \leqslant \sqrt{\frac{a_0 \log A_0}{\pi(a_0-1)}}\ .$$

Let $\rho := \max\{d+\ell+\gamma\,,\, \ell-\gamma\} \geqslant \frac{d}{2}$, and let $a_0 = 1+\alpha$, with $0<\alpha\leqslant\sqrt{2}$ to be chosen. Using that $1 \leqslant A_0 \leqslant 2a_0^{\rho/2}$ and that

$$\frac{a_0 \log a_0}{(a_0-1)} = 1 + O(\alpha)\ \ ;\ \ \frac{a_0}{(a_0-1)} = \frac{1}{\alpha}+1,$$

we find

$$r(Pf_0) \leqslant \sqrt{\frac{a_0\big((\rho/2)\log a_0 + \log 2\big)}{\pi(a_0-1)}} = \sqrt{\frac{\rho}{2\pi}\big(1+O(\alpha)\big) + O\left(\frac{1}{\alpha}\right)}. \tag{2.2.4}$$

We now choose $\alpha = \frac{1}{\sqrt{\rho}}$. Then (2.2.4) reads

$$r(Pf_0) \leqslant \sqrt{\frac{\rho}{2\pi} + O(\sqrt{\rho})} = \sqrt{\frac{\rho}{2\pi}} + O(1),$$

as we wanted.

Case $si^{\ell+\mathfrak{r}} = -1$ and $-d < \gamma \leqslant -\frac{d}{2}$

In this situation we consider the function g_1 in (2.2.3). Using the homogeneity we note that

$$\int_{\mathbb{R}^d} P(x)\, g_1(x)\, \mathrm{d}x = \left(\int_{\mathbb{R}^d} P(x)\, H(x)\, e^{-\pi|x|^2}\, \mathrm{d}x\right)\left(a_1^{\frac{d+\ell+\gamma}{2}} - a_1^{\frac{\ell-\gamma}{2}}\right) \leqslant 0$$

for $a_1 > 1$. From (2.2.3) we plainly see that

$$r(Pg_1) \leqslant \sqrt{\frac{(d+2\ell)\log a_1}{2\pi\big(a_1 - \frac{1}{a_1}\big)}} \;\to\; 0$$

as $a_1 \to \infty$. Hence, in this case, $\mathbb{A}_s^*(P;d) = 0$.

Case $si^{\ell+\mathfrak{r}} = -1$ and $-\frac{d}{2} < \gamma$

We now consider f_1 in (2.2.3) with the choice

$$A_1 = \frac{a_1^{\frac{d+\ell+\gamma}{2}} - a_1^{\frac{\ell-\gamma}{2}}}{b_1^{\frac{d+\ell+\gamma}{2}} - b_1^{\frac{\ell-\gamma}{2}}}.$$

Observe that $\int_{\mathbb{R}^d} Pf_1 = 0$. We consider $a_1 = 1 + 2\alpha$ and $b_1 = 1 + \alpha$ with $0 < \alpha \leqslant \sqrt{2}$ to be chosen. Using the expansion

$$\frac{a_1 \log a_1}{(a_1^2 - 1)} = \frac{1}{2} + O(\alpha),$$

we note that the inequality

$$a_1^{\frac{d+2\ell}{2}}\, e^{-a_1\pi|x|^2} \leqslant \frac{1}{2}\, e^{-\frac{1}{a_1}\pi|x|^2} \tag{2.2.5}$$

holds for all $|x| \geqslant r_1$, where

$$r_1 = \sqrt{\frac{(d+2\ell)}{2\pi}\left(\frac{1}{2} + O(\alpha)\right) + O\left(\frac{1}{\alpha}\right)}. \tag{2.2.6}$$

Assuming that (2.2.5) holds, we have that

$$Pf_1 \geqslant PH\, e^{-\frac{1}{b_1}\pi|x|^2}\left(\frac{1}{2}\, e^{(\frac{1}{b_1} - \frac{1}{a_1})\pi|x|^2} - A_1\right) \quad (x \neq 0).$$

This tells us that $r(Pf_1) \leqslant \max\{r_1, r_2\}$, with r_1 as in (2.2.6) and

$$r_2 := \sqrt{\frac{\log 2A_1}{\pi}\frac{a_1 b_1}{(a_1 - b_1)}}. \tag{2.2.7}$$

As before, let $\rho := \max\{d+\ell+\gamma\,,\,\ell-\gamma\} = d+\ell+\gamma$ in this case. Observe that we can write A_1 as

$$A_1 = \left(\frac{a_1}{b_1}\right)^{\rho/2}\left(\frac{1-a_1^{-\frac{(d+2\gamma)}{2}}}{1-b_1^{-\frac{(d+2\gamma)}{2}}}\right).$$

Since $1 < b_1 < a_1$, one can verify that the function

$$t \mapsto \left(\frac{1-a_1^{-t}}{1-b_1^{-t}}\right)$$

is non-increasing for $t > 0$, with the limit being $\log a_1/\log b_1$ as $t \to 0^+$. Hence

$$1 \leqslant A_1 \leqslant \left(\frac{a_1}{b_1}\right)^{\rho/2}\left(\frac{\log a_1}{\log b_1}\right). \tag{2.2.8}$$

Now we plug in the upper bound (2.2.8) in (2.2.7) and use the expansions

$$\frac{a_1b_1(\log a_1 - \log b_1)}{(a_1-b_1)} = 1+O(\alpha)\,;\; \frac{a_1b_1(\log(\log a_1/\log b_1))}{(a_1-b_1)} = O\left(\frac{1}{\alpha}\right)\;;\; \frac{a_1b_1}{(a_1-b_1)} = O\left(\frac{1}{\alpha}\right)$$

to find that

$$r_2 \leqslant \sqrt{\frac{\rho}{2\pi}\big(1+O(\alpha)\big)+O\left(\frac{1}{\alpha}\right)}\,.$$

This is the same as (2.2.4). We have seen that the choice $\alpha = \frac{1}{\sqrt{\rho}}$ leads to $r_2 \leqslant \sqrt{\frac{\rho}{2\pi}}+O(1)$. Since $(d+2\ell)/2 \leqslant \rho$, we also have $r_1 \leqslant \sqrt{\frac{\rho}{2\pi}}+O(1)$. This concludes the proof of Theorem 2.3.

2.2.3 An additional reduction

We briefly present a related result that may be helpful in some situations. This is inspired in similar reductions in [12, 35].

Proposition 2.11. *Let $P : \mathbb{R}^d \to \mathbb{R}$ be a function verifying properties* (P1), (P2), (P3) *and* (P4). *Assume that $P = H\,.\,Q$, where $H : \mathbb{R}^d \to \mathbb{R}$ is a homogeneous and harmonic polynomial of degree $\ell \geqslant 0$, and $Q : \mathbb{R}^d \to \mathbb{R}$ is a non-negative function. Let $\mathfrak{r}$ as in* (2.1.8). *If $s\,i^{\ell+\mathfrak{r}} = 1$, or if $s\,i^{\ell+\mathfrak{r}} = -1$ and $\gamma \geqslant \ell$, we can reduce the search in* (2.1.12) - (2.1.13) *to functions verifying $\int_{\mathbb{R}^d} Pf = 0$.*

Proof. Assume that $f \in \mathcal{A}_s^*(P;d)$ is such that $\int_{\mathbb{R}^d} Pf < 0$. Note, in particular, that we cannot have $P(x) = 0$ a.e. in this situation. Let us show how we can adjust the function f.

Case 1: $si^{\ell+\mathfrak{r}} = 1$

Let $\varphi(x) = H(x)\, e^{-\pi|x|^2}$. By Lemma 2.10 we have $\widehat{\varphi} = (-i)^{\ell}\varphi = si^{\mathfrak{r}}\varphi$. Then $\int_{\mathbb{R}^d} P\varphi > 0$ and we may consider

$$g(x) = f(x) - \frac{\int_{\mathbb{R}^d} Pf}{\int_{\mathbb{R}^d} P\varphi}\, \varphi(x).$$

One can verify that $g \neq \mathbf{0}$ (otherwise Pf is eventually zero and from (P3) we get a contradiction), $\widehat{g} = si^{\mathfrak{r}} g$, $r(Pg) \leqslant r(Pf)$ and $\int_{\mathbb{R}^d} Pg = 0$.

Case 2: $si^{\ell+\mathfrak{r}} = -1$ **and** $\gamma \geqslant \ell$

Let $t > 0$ be a parameter to be chosen later, and define

$$\psi_t(x) := H(x) \left(e^{-t\pi|x|^2} - 2^{-\frac{(\gamma-\ell)}{2}}\, e^{-2t\pi|x|^2} \right).$$

Then, by Lemma 2.10,

$$\widehat{\psi}_t(x) = (-i)^{\ell} H(x) \left(t^{-\frac{(d+2\ell)}{2}} e^{-\frac{\pi|x|^2}{t}} - 2^{-\frac{(\gamma-\ell)}{2}}\, (2t)^{-\frac{(d+2\ell)}{2}} e^{-\frac{\pi|x|^2}{2t}} \right).$$

Observe that ψ_t is a Schwartz function that satisfies $P\psi_t \geqslant 0$ and $\int_{\mathbb{R}^d} P\psi_t > 0$. Using the homogeneity, a change of variables shows that $\int_{\mathbb{R}^d} P\widehat{\psi}_t = 0$. Observe also that

$$i^{\ell} P(x)\, \widehat{\psi}_t(x) < 0 \quad \text{for} \quad |x| > \sqrt{\frac{(d+\ell+\gamma)\, t \log 2}{\pi}}.$$

We choose $t > 0$ such that

$$r(Pf) = \sqrt{\frac{(d+\ell+\gamma)\, t \log 2}{\pi}}$$

and consider

$$g(x) = f(x) - \frac{\int_{\mathbb{R}^d} Pf}{\int_{\mathbb{R}^d} P\psi_t} \big(\psi_t(x) - i^{\ell}\, \widehat{\psi}_t(x)\big).$$

One can verify that $g \neq \mathbf{0}$ (otherwise Pf is eventually zero and from (P3) we get a contradiction), $\widehat{g} = si^{\mathfrak{r}} g$, $r(Pg) \leqslant r(Pf)$ and $\int_{\mathbb{R}^d} Pg = 0$. $\square$

2.3 Sufficient conditions for admissibility: proof of Theorem 2.5

For $E \subset \mathbb{R}^d$, recall that $|E|$ denotes its Lebesgue measure, and we let $E^c = \mathbb{R}^d \backslash E$. The following classical result will be useful.

Lemma 2.12 (Amrein-Berthier [2])**.** *Let $E, F \subset \mathbb{R}^d$ be sets of finite measure. Then there exists a constant $C = C(E, F; d) > 0$ such that for all $g \in L^2(\mathbb{R}^d)$ we have*

$$\int_{\mathbb{R}^d} |g(x)|^2 \, \mathrm{d}x \leqslant C \left(\int_{E^c} |g(x)|^2 \, \mathrm{d}x + \int_{F^c} |\widehat{g}(x)|^2 \, \mathrm{d}x \right). \tag{2.3.1}$$

Remark. Later works of Nazarov [87] and Jaming [70] show that (2.3.1) holds with

$$C(E, F; d) \leqslant c\, e^{c|E||F|},$$

for some $c = c(d)$.

2.3.1 Proof of Theorem 2.5: general case

Let $f \in L^1(\mathbb{R}^d)$ with $\widehat{f} = \pm i^{\mathfrak{r}} f$, and let $A = A_\lambda = \{x \in \mathbb{R}^d : |P(x)| \leqslant \lambda\}$ be of finite Lebesgue measure. For a set $E \subset \mathbb{R}^d$, let $f_E := f \cdot \mathbb{I}_E$, where $\mathbb{I}_E$ is the characteristic function of E. By the triangle inequality and the Cauchy-Schwarz inequality we have

$$\|f\|_1 \leqslant \|f_A\|_1 + \|f_{A^c}\|_1 \leqslant |A|^{1/2} \|f_A\|_2 + \|f_{A^c}\|_1. \tag{2.3.2}$$

In the terminology of Lemma 2.12, let $E = F = A$ and let $C = C(A, A; d)$ in (2.3.1). Letting $g = f_A$ in (2.3.1) we plainly get

$$\int_A |f(x)|^2 \,\mathrm{d}x \leqslant C \int_{A^c} \left|\widehat{f_A}(x)\right|^2 \,\mathrm{d}x = C \left(\int_A |f(x)|^2 \,\mathrm{d}x - \int_A \left|\widehat{f_A}(x)\right|^2 \,\mathrm{d}x \right),$$

and then

$$\int_A \left|\widehat{f_A}(x)\right|^2 \,\mathrm{d}x \leqslant \frac{(C-1)}{C} \int_A |f(x)|^2 \,\mathrm{d}x. \tag{2.3.3}$$

The fact that f is an eigenfunction yields $f = \pm(-i)^{\mathfrak{r}} \widehat{f} = \pm(-i)^{\mathfrak{r}} \big(\widehat{f_A} + \widehat{f_{A^c}}\big)$ and hence

$$f_A = \pm(-i)^{\mathfrak{r}} \left(\big(\widehat{f_A}\big)_A + \big(\widehat{f_{A^c}}\big)_A \right).$$

A basic triangle inequality then yields

$$\|f_A\|_2 \leqslant \left\| \big(\widehat{f_A}\big)_A \right\|_2 + \left\| \big(\widehat{f_{A^c}}\big)_A \right\|_2. \tag{2.3.4}$$

We bound the last term in (2.3.4) as follows:

$$\left\| \big(\widehat{f_{A^c}}\big)_A \right\|_2 \leqslant \left\| \big(\widehat{f_{A^c}}\big) \right\|_\infty |A|^{1/2} \leqslant \|f_{A^c}\|_1 \, |A|^{1/2}. \tag{2.3.5}$$

From (2.3.3), (2.3.4) and (2.3.5) we get

$$\|f_A\|_2 \leqslant \left(\frac{C-1}{C} \right)^{1/2} \|f_A\|_2 + |A|^{1/2} \|f_{A^c}\|_1,$$

which implies that

$$\|f_A\|_2 \leqslant \frac{|A|^{1/2}}{\left(1 - \left(\frac{C-1}{C}\right)^{1/2}\right)} \|f_{A^c}\|_1. \tag{2.3.6}$$

Finally, plugging (2.3.6) into (2.3.2) yields

$$\|f\|_1 \leqslant \left(1 + \frac{|A|}{\left(1 - \left(\frac{C-1}{C}\right)^{1/2}\right)}\right)\|f_{A^c}\|_1 \leqslant \left(1 + \frac{|A|}{\left(1 - \left(\frac{C-1}{C}\right)^{1/2}\right)}\right)\lambda^{-1}\,\|Pf\|_1,$$

as we wanted.

2.3.2 Homogeneous case

If P is homogeneous of degree $\gamma = 0$, inequality (2.1.17) is clear. In this case, $|A_\lambda|$ is either 0 or ∞, and therefore (P5) implies that $\operatorname{essinf}|P| > 0$. Assume then that P is homogeneous of degree $\gamma > 0$. In this case, $A_\lambda = \lambda^{1/\gamma}A_1$, and hence $|A_\lambda| = \lambda^{d/\gamma}|A_1|$. Let us write again $A = A_\lambda$ for some $\lambda > 0$ to be properly chosen later, with the condition that $|A_\lambda| < 1$. By the Hausdorff-Young and Cauchy-Schwarz inequalities we have

$$\big\|\widehat{f_A}\big\|_\infty \leqslant \big\|f_A\big\|_1 \leqslant \big\|f_A\big\|_2\,|A|^{1/2},$$

from which we obtain

$$\int_A \big|\widehat{f_A}(x)\big|^2\,\mathrm{d}x \leqslant |A|^2\int_A |f(x)|^2\,\mathrm{d}x. \tag{2.3.7}$$

We let estimate (2.3.7) replace (2.3.3) in the proof of the general case in §2.3.1. If we repeat all the other steps we get

$$\|f\|_1 \leqslant \left(1 + \frac{|A|}{(1-|A|)}\right)\big\|f_{A^c}\big\|_1 = \frac{1}{1-|A|}\big\|f_{A^c}\big\|_1 \leqslant \frac{1}{(1-\lambda^{d/\gamma}|A_1|)}\,\lambda^{-1}\,\|Pf\|_1.$$

We are now free to choose $\lambda > 0$ in order to minimize the function

$$\varphi(t) = \frac{1}{t\,(1 - t^{d/\gamma}|A_1|)},$$

subject to the condition $|A_\lambda| = \lambda^{d/\gamma}|A_1| < 1$. The minimum occurs when

$$\lambda^{d/\gamma}|A_1| = \frac{\frac{\gamma}{d}}{1+\frac{\gamma}{d}},$$

which gives

$$\varphi(\lambda) = \left(1 + \frac{\gamma}{d}\right)\left[\left(1 + \frac{d}{\gamma}\right)|A_1|\right]^{\frac{\gamma}{d}}.$$

2.4 Sign uncertainty: proof of Theorem 2.6

Throughout this proof we let $\omega_{d-1} = 2\,\pi^{d/2}\,\Gamma(d/2)^{-1}$ be the surface area of the unit sphere $\mathbb{S}^{d-1} \subset \mathbb{R}^d$. For $y \in \mathbb{R}$ we denote $y_+ = \max\{y, 0\}$ and $y_- = \max\{-y, 0\}$.

2.4.1 Lower bound

Let $f \in \mathcal{A}_s^*(P;d)$ and let r be arbitrary with $r > r(Pf)$. Then

$$\int_{\mathbb{R}^d} P(x)\, f(x)\, \mathrm{d}x = \int_{\mathbb{R}^d} [P(x)f(x)]_+ \,\mathrm{d}x - \int_{\mathbb{R}^d} [P(x)f(x)]_- \,\mathrm{d}x \;\leqslant\; 0.$$

Let $B_r = \{x \in \mathbb{R}^d \,:\, |x| < r\}$. By definition, $[Pf]_-$ is supported on $\overline{B_r}$ and $[Pf]_- \leqslant |Pf|$. Since P is admissible with respect to an exponent $1 \leqslant q \leqslant \infty$, by Hölder's inequality we have

$$\|Pf\|_1 = \int_{\mathbb{R}^d} [Pf]_+ + \int_{\mathbb{R}^d} [Pf]_- \;\leqslant\; 2\int_{\mathbb{R}^d} [Pf]_- \;\leqslant\; 2\int_{B_r} |Pf| \;\leqslant\; 2\left\|P\mathbb{I}_{B_r}\right\|_{q'} \|f\|_q. \tag{2.4.1}$$

From (2.1.16) and (2.4.1) we get

$$\|f\|_q \leqslant C(P;d;q)\, \|Pf\|_1 \leqslant 2\, C(P;d;q) \left\|P\mathbb{I}_{B_r}\right\|_{q'} \|f\|_q\,,$$

and we conclude that

$$\left\|P\mathbb{I}_{B_r}\right\|_{q'} \geqslant \frac{1}{2\, C(P;d;q)}. \tag{2.4.2}$$

From (2.4.2) we deduce that r is bounded below by a constant, since, by assumption (ii) in the definition of admissible function, we have $\lim_{r\to 0^+} \left\|P\mathbb{I}_{B_r}\right\|_{q'} = 0$.

2.4.2 Homogeneous case

In this case observe that $|P(x)| \leqslant K|x|^\gamma$ and we can directly compute

$$\left\|P\mathbb{I}_{B_r}\right\|_{q'} \leqslant K\left(\int_{B_r} |x|^{\gamma q'}\, \mathrm{d}x\right)^{1/q'} = K\left(\frac{\omega_{d-1}\, r^{d+\gamma q'}}{d+\gamma q'}\right)^{1/q'} \tag{2.4.3}$$

if $q > 1$. If $q = 1$ (and hence $\gamma > 0$ from the admissibility hypotheses) we simply have

$$\left\|P\mathbb{I}_{B_r}\right\|_{\infty} \leqslant K r^\gamma. \tag{2.4.4}$$

Plugging (2.4.3) - (2.4.4) into (2.4.2) yields, for $q > 1$,

$$r \geqslant \left(\frac{(d+\gamma q')\, \Gamma(d/2)}{2\,\pi^{\frac{d}{2}}\, (2\,K\,C(P;d;q))^{q'}}\right)^{\frac{1}{(d+\gamma q')}}, \tag{2.4.5}$$

If $q = 1$, the right-hand side of (2.4.5) becomes $(2\,K\,C(P;d;1))^{-1/\gamma}$.

2.4.3 Existence of extremizers

The argument to establish the existence of extremizers in certain Fourier optimization problems generally involves showing that a suitable weak limit is a viable candidate. Examples of such methods can be found in [22, 35, 61].

Let $\{f_n\} \subset \mathcal{A}_s^*(P;d)$ be an extremizing sequence. This implies that $r(Pf_n) \to \mathbb{A}^* := \mathbb{A}_s^*(P;d)$, and we may assume that $r(Pf_n)$ is non-increasing. We normalize the sequence so that $\|f_n\|_2 = 1$. From the reflexivity of $L^2(\mathbb{R}^d)$, passing to a subsequence if necessary, we may assume that $f_n \rightharpoonup f$ weakly, for some $f \in L^2(\mathbb{R}^d)$. By Plancherel's theorem, note that $\widehat{f_n} \rightharpoonup \widehat{f}$ and therefore $\widehat{f} = si^{\mathrm{r}} f$. We now prove that f is equal a.e. to our desired extremizer.

Let $r_1 = r(Pf_1)$. Then $r_1 \geqslant r(Pf_n) \geqslant \mathbb{A}^*$ for all $n \in \mathbb{N}$. Since we are assuming property (P5), Theorem 2.5 tells us that (2.1.16) holds with $q = 1$, and hence also with $q = 2$. Estimate (2.4.1) also holds for $q = 1$ and $q = 2$, and under conditions (P1) and (P7) we then have

$$\|f_n\|_1 \simeq \|f_n\|_2 \simeq \|Pf_n\|_1, \tag{2.4.6}$$

with implied constants only depending on d, P and r_1. By Mazur's lemma [14, Corollary 3.8 and Exercise 3.4], we can find g_n a finite convex combination of $\{f_n, f_{n+1}, \ldots\}$ such that $g_n \to f$ strongly in $L^2(\mathbb{R}^d)$. Passing to a subsequence, if necessary, we may also assume that $g_n \to f$ almost everywhere. Observe that g_n is not identically zero (since each Pf_k must be strictly positive somewhere in $\{x \in \mathbb{R}^d : |x| > r_1\}$ due to condition (P3) which is implied by (P5)) and hence $g_n \in \mathcal{A}_s^*(P;d)$ with

$$r_1 \geqslant r(Pf_n) \geqslant r(Pg_n) \geqslant \mathbb{A}^* \tag{2.4.7}$$

for all $n \in \mathbb{N}$. By the triangle inequality, we have $\|g_n\|_2 \leqslant 1$. The norm equivalences as in (2.4.6) continue to hold for g_n. In particular, by Fatou's lemma,

$$\|f\|_1 \leqslant \liminf_{n\to\infty} \|g_n\|_1 \lesssim \|g_n\|_2 \leqslant 1 \quad \text{and} \quad \|Pf\|_1 \leqslant \liminf_{n\to\infty} \|Pg_n\|_1 \lesssim \|g_n\|_2 \leqslant 1. \tag{2.4.8}$$

By the Hausdorff-Young inequality, $\|g_n\|_\infty \leqslant \|g_n\|_1 \lesssim |\|g_n\|_2 \leqslant 1$, and we may then use dominated convergence to get

$$\int_{B_{r_1}} Pf = \lim_{n\to\infty} \int_{B_{r_1}} Pg_n. \tag{2.4.9}$$

Fatou's lemma again gives us

$$\int_{B_{r_1}^c} Pf \leqslant \liminf_{n\to\infty} \int_{B_{r_1}^c} Pg_n, \tag{2.4.10}$$

and if we add up (2.4.9) and (2.4.10) we get

$$\int_{\mathbb{R}^d} Pf \leqslant \liminf_{n\to\infty} \int_{\mathbb{R}^d} Pg_n \leqslant 0,$$

since $g_n \in \mathcal{A}_s^*(P;d)$. By (2.4.8), since f is an integrable eigenfunction, it is equal a.e. to a continuous function, and we make this identification. Once we establish that $f \neq \mathbf{0}$, we will have that $f \in \mathcal{A}_s^*(P;d)$. In fact, assume that $g_n(x) \to f(x)$ for all $x \in E$, where $\left|\mathbb{R}^d \backslash E\right| = 0$. Then, if $x \in E \cap \overline{B}^c_{\mathbb{A}*}$, from (2.4.7) we get $P(x)f(x) \geqslant 0$. Now consider $x \in E^c \cap \overline{B}^c_{\mathbb{A}*}$ such that $P(x) \neq 0$. From the sign density property (P9) we can find a sequence $x_j \to x$ with $x_j \in E \cap \overline{B}^c_{\mathbb{A}*}$ and $P(x_j)P(x) > 0$. Since $P(x_j)f(x_j) \geqslant 0$, we have $P(x)f(x_j) \geqslant 0$ and, by the continuity of f, we arrive at $P(x)f(x) \geqslant 0$. The conclusion is that $P(x)f(x) \geqslant 0$ for all $|x| > \mathbb{A}^*$. Hence $r(Pf) = \mathbb{A}^*$ and f will be our desired extremizer.

It remains to show that $f \neq \mathbf{0}$. Under (P5), let $A = A_\lambda = \{x \in \mathbb{R}^d \,:\, |P(x)| \leqslant \lambda\}$ be of finite measure. From Lemma 2.12 (with $E = F = A \cup B_{r_1}$), the Hausdorff-Young inequality, and (2.4.6) we get

$$
\begin{aligned}
1 = \|f_n\|_2^2 &\lesssim \int_{B^c_{r_1} \cap A^c} |f_n(x)|^2 \, \mathrm{d}x \leqslant \|f_n\|_\infty \int_{B^c_{r_1} \cap A^c} |f_n(x)| \, \mathrm{d}x \\
&\lesssim \int_{B^c_{r_1} \cap A^c} P(x)\, f_n(x) \, \mathrm{d}x \\
&\leqslant \int_{B^c_{r_1}} P(x)\, f_n(x) \, \mathrm{d}x.
\end{aligned} \tag{2.4.11}
$$

Since $\int_{\mathbb{R}^d} Pf_n \leqslant 0$ and Pf_n is non-negative in $\overline{B}^c_{r_1}$, estimate (2.4.11) tells us that there is a positive constant C depending only on d, P and r_1 such that

$$
\int_{B_{r_1}} Pf_n \leqslant -C.
$$

The weak convergence directly implies that (note properties (P1) and (P7))

$$
\int_{B_{r_1}} Pf \leqslant -C.
$$

In particular, this shows that $f \neq \mathbf{0}$ and the proof is concluded.

2.5 Dimension shifts: proof of Theorem 2.7

2.5.1 Dropping the dimension

Let us first prove inequality (2.1.22) in the generic case. We are assuming that $\mathcal{A}_s^*(P; d+2\ell)$ is non-empty. We first observe that the search can be further restricted to radial functions. For this, let $SO(d+2\ell)$ be the group of rotations in $\mathbb{R}^{d+2\ell}$ (linear orthogonal transformations of determinant 1) with its Haar measure μ, normalized so that $\mu(SO(d+2\ell)) = 1$. For $f \in \mathcal{A}_s^*(P; d+2\ell)$ we define

$$
f^{\mathrm{rad}}(x) := \int_{SO(d+2\ell)} f(Rx) \, \mathrm{d}\mu(R). \tag{2.5.1}
$$

One can readily check that f^{rad} is continuous, that $f^{\mathrm{rad}}, Pf^{\mathrm{rad}} \in L^1(\mathbb{R}^{d+2\ell})$, $\int_{\mathbb{R}^{d+2\ell}} Pf^{\mathrm{rad}} \leqslant 0$, $\widehat{f^{\mathrm{rad}}} = sf^{\mathrm{rad}}$, and that $r(Pf^{\mathrm{rad}}) \leqslant r(Pf)$. To see that $f^{\mathrm{rad}} \neq \mathbf{0}$ we argue as follows. Let

$r = r(Pf)$. From condition (P3), there exists a certain $x_0 \in \mathbb{R}^{d+2\ell}$, with $|x_0| > r$ such that $P(x_0)f(x_0) > 0$. As P is radial, we have $P(x_0)f(Rx_0) \geqslant 0$ for all $R \in SO(d+2\ell)$, with strict inequality if R is in a suitable neighborhood of the identity, since f is continuous. Then $P(x_0)f^{\mathrm{rad}}(x_0) > 0$. The conclusion is that in fact $f^{\mathrm{rad}} \in \mathcal{A}_s^*(P; d+2\ell)$ (and does a job at least as good as the original f).

Now let us start with $f \in \mathcal{A}_s^*(P; d+2\ell)$ radial. Write $f(x) = f_0(|x|)$ for some continuous $f_0 : [0,\infty) \to \mathbb{R}$. The conditions $f, Pf \in L^1(\mathbb{R}^{d+2\ell})$ can be rewritten as

$$\int_0^\infty |f_0(r)|\, r^{d+2\ell-1}\, \mathrm{d}r < \infty \quad \text{and} \quad \int_0^\infty |f_0(r)|\, |P_0(r)|\, r^{d+2\ell-1}\, \mathrm{d}r < \infty. \tag{2.5.2}$$

Define $f^\flat : \mathbb{R}^d \to \mathbb{R}$ by

$$f^\flat(x) := H(x)\, f_0(|x|). \tag{2.5.3}$$

Then $|f^\flat(x)| \leqslant C|x|^\ell |f_0(|x|)|$ and (2.5.2) gives us that $|x|^\ell\, f^\flat$, $|x|^\ell |P_0(|x|)|\, f^\flat \in L^1(\mathbb{R}^d)$. This plainly implies that $f^\flat, \widetilde{P} f^\flat \in L^1(\mathbb{R}^d)$. The latter is obvious if $P_0 = 0$ a.e. in $[0,\infty)$ and, if not, observe that property (P1) for $\widetilde{P}$ implies that $HQ \in L^1(\mathbb{S}^{d-1})$. In this second case we also have

$$\begin{aligned}\int_{\mathbb{R}^d} \widetilde{P}(x)\, f^\flat(x)\, \mathrm{d}x &= \int_{\mathbb{R}^d} H(x)^2 Q(x) P_0(|x|) f_0(|x|)\, \mathrm{d}x \\ &= \left(\int_{\mathbb{S}^{d-1}} H(\omega)^2 Q(\omega)\, \mathrm{d}\sigma(\omega)\right) \int_0^\infty P_0(r)\, f_0(r)\, r^{d+2\ell-1}\, \mathrm{d}r \;\leqslant\; 0,\end{aligned}$$

since the quantity in parentheses is non-negative (and finite) and $\int_{\mathbb{R}^{d+2\ell}} Pf \leqslant 0$.

From Bochner's relation (Lemma 2.10) and the fact that $\widehat{f} = sf$ we have

$$\widehat{f^\flat}(x) = (-i)^\ell\, H(x)\, \mathcal{F}_{d+2\ell}[f](x_1, x_2, \ldots, x_d, 0, \ldots, 0) = s(-i)^\ell\, f^\flat(x).$$

Note also that $r(\widetilde{P} f^\flat) \leqslant r(Pf)$. The fact that $f^\flat \neq \mathbf{0}$ follows from the assumption that $f_0 \neq \mathbf{0}$ and the fact that H cannot be identically zero in any open set of $\mathbb{R}^d$. Then $f^\flat \in \mathcal{A}^*_{s(-1)^{(\mathfrak{r}(\ell)+\ell)/2}}\big(\widetilde{P}; d\big)$ and (2.1.22) plainly follows.

2.5.2 Lifting the dimension

We now work under the additional assumption (P6) for P, and consider the case $Q = \mathbf{1}$. In case $\ell = 0$, we have H being a non-zero constant and (2.1.23) plainly follows. Hence, from now on, let us assume that $1 \leqslant \ell \leqslant d$. By a change of variables given by an element $R \in O(d)$ we may assume without loss of generality that $H(x) = x_1 x_2 \ldots x_\ell$. Hence,

$$\widetilde{P}(x) = x_1 x_2 \ldots x_\ell\, P_0(|x|) \qquad (x \in \mathbb{R}^d).$$

Let us first argue that we have property (P3) for $\widetilde{P}$. In fact, if $f \in L^1(\mathbb{R}^d)$ is a continuous eigenfunction of the Fourier transform such that

$$\widetilde{P}(x)f(x) = x_1 x_2 \dots x_\ell \, P_0(|x|)f(x) = 0 \quad \text{for} \quad |x| > r,$$

the continuity of f implies that

$$P_0(|x|)f(x) = 0 \quad \text{for} \quad |x| > r.$$

Property (P6) holds also for $x \mapsto P_0(|x|)$ ($x \in \mathbb{R}^d$), and we have seen that this implies (P3) for $x \mapsto P_0(|x|)$ ($x \in \mathbb{R}^d$). Hence $f = \mathbf{0}$, establishing (P3) for $\widetilde{P}$.

Now let $s' = s(-1)^{(\mathfrak{r}(\ell)+\ell)/2}$ and assume that $\mathcal{A}^*_{s'}\big(\widetilde{P}; d\big)$ is non-empty. Let $f \in \mathcal{A}^*_{s'}\big(\widetilde{P}; d\big)$. We start by considering an important reduction.

Symmetrization with respect to $x_1, x_2, \dots, x_\ell$

Throughout the rest of this proof let us write $x = (x_1, \dots, x_\ell, \widetilde{x})$ with $\widetilde{x} \in \mathbb{R}^{d-\ell}$. Let

$$w(x_1, x_2, \dots, x_\ell, \widetilde{x}) = f(x_1, x_2, \dots, x_\ell, \widetilde{x}) - f(-x_1, x_2, \dots, x_\ell, \widetilde{x}).$$

Note that $\int_{\mathbb{R}^d} \widetilde{P}w = 2\int_{\mathbb{R}^d} \widetilde{P}f \leqslant 0$. Observe also that $w \neq \mathbf{0}$, otherwise $\widetilde{P}f$ would be eventually zero and from condition (P3) we would have $f = \mathbf{0}$, a contradiction. It is clear that $r(\widetilde{P}w) \leqslant r(\widetilde{P}f)$, and hence $w \in \mathcal{A}^*_{s'}\big(\widetilde{P}; d\big)$. Moreover, w is odd with respect to the variable x_1. We apply the same symmetrization procedure $\ell - 1$ times, to the variables $x_2, \dots, x_\ell$. One then arrives at a function in $\mathcal{A}^*_{s'}\big(\widetilde{P}; d\big)$ that is odd with respect to each of the variables $x_1, \dots, x_\ell$ independently.

Remark. As far as radial symmetrization goes, at this point one could proceed as in (2.5.1) and integrate over $SO(d-\ell)$ to symmetrize f with respect to the variable $\widetilde{x}$, but this is not particularly necessary for our argument below.

Main argument

Let us now assume that $f \in \mathcal{A}^*_{s'}\big(\widetilde{P}; d\big)$ has the symmetries above. Define $g : \mathbb{R}^d \to \mathbb{R}$ by

$$g(x) = \begin{cases} \dfrac{f(x)}{x_1 x_2 \dots x_\ell}, & \text{if } x_1 x_2 \dots x_\ell \neq 0; \\ 0, & \text{if } x_1 x_2 \dots x_\ell = 0. \end{cases} \tag{2.5.4}$$

Then $f(x) = x_1 x_2 \dots x_\ell \, g(x)$ for all $x \in \mathbb{R}^d$, and g is even with respect to each of the variables $x_1, x_2, \dots, x_\ell$ independently. Observe that $P_0(|\cdot|)g$ is eventually non-negative and that

$$r(P_0(|\cdot|)g) = r\big(\widetilde{P}f\big). \tag{2.5.5}$$

For each $1 \leqslant k \leqslant \ell$ let $y_k \in \mathbb{R}^3$ and let $\widetilde{y} \in \mathbb{R}^{d-\ell}$. We now work with the variable $y = (y_1, \ldots, y_\ell, \widetilde{y}) \in \mathbb{R}^{d+2\ell}$. Define the function $g^\# : \mathbb{R}^{d+2\ell} \to \mathbb{R}$ by

$$g^\#(y) = g^\#(y_1, \ldots, y_\ell, \widetilde{y}) := g\big(|y_1|, \ldots, |y_\ell|, \widetilde{y}\big). \tag{2.5.6}$$

Note that $Pg^\#$ is eventually non-negative with

$$r(Pg^\#) = r(P_0(|\cdot|)g). \tag{2.5.7}$$

We first observe that $g^\# \in L^1(\mathbb{R}^{d+2\ell})$. In fact, with changes to polar coordinates in each of the first ℓ variables on $\mathbb{R}^3$, we get

$$\begin{aligned}\int_{\mathbb{R}^{d+2\ell}} \left|g^\#(y)\right| \,\mathrm{d}y &= \omega_2^\ell \int_{\mathbb{R}^{d-\ell}} \int_{(\mathbb{R}^+)^\ell} x_1^2 \ldots x_\ell^2 \left|g(x_1, \ldots, x_\ell, \widetilde{y})\right| \,\mathrm{d}x_1 \ldots \mathrm{d}x_\ell \,\mathrm{d}\widetilde{y} \\ &= \omega_2^\ell \int_{\mathbb{R}^{d-\ell}} \int_{(\mathbb{R}^+)^\ell} x_1 \ldots x_\ell \left|f(x_1, \ldots, x_\ell, \widetilde{y})\right| \,\mathrm{d}x_1 \ldots \mathrm{d}x_\ell \,\mathrm{d}\widetilde{y} \\ &< \infty.\end{aligned} \tag{2.5.8}$$

The last integral is finite since f is continuous, $\widetilde{P}f \in L^1(\mathbb{R}^d)$ and we have property (P6) for P (or equivalently, for P_0). Similarly, $Pg^\# \in L^1(\mathbb{R}^{d+2\ell})$ since

$$\begin{aligned}&\int_{\mathbb{R}^{d+2\ell}} |P(y)| \left|g^\#(y)\right| \,\mathrm{d}y \\ &\quad= \omega_2^\ell \int_{\mathbb{R}^{d-\ell}} \int_{(\mathbb{R}^+)^\ell} x_1 \ldots x_\ell \left|P_0\Big(\big(x_1^2 + \ldots + x_\ell^2 + |\widetilde{y}|^2\big)^{1/2}\Big)\, f(x_1, \ldots, x_\ell, \widetilde{y})\right| \,\mathrm{d}x_1 \ldots \mathrm{d}x_\ell \,\mathrm{d}\widetilde{y} \\ &\quad= \frac{\omega_2^\ell}{2^\ell} \int_{\mathbb{R}^d} \big|\widetilde{P}f\big| < \infty.\end{aligned} \tag{2.5.9}$$

By recalculating (2.5.9) without the absolute value, and using that $\int_{\mathbb{R}^d} \widetilde{P}f \leqslant 0$, we find also that $\int_{\mathbb{R}^{d+2\ell}} Pg^\# \leqslant 0$.

Observe that, for each $1 \leqslant k \leqslant \ell$, the functions

$$\begin{aligned}x_k &\mapsto x_k\, g(x_1, \ldots, x_k, \ldots, x_\ell, \widetilde{x}) \\ x_k &\mapsto x_k^2\, g(x_1, \ldots, x_k, \ldots, x_\ell, \widetilde{x}) \\ x_k &\mapsto x_k^2\, g(x_1, \ldots, x_k, \ldots, x_\ell, \widetilde{x})^2\end{aligned}$$

are absolutely integrable for a.e. $(x_1, \ldots, x_{k-1}, x_{k+1}, \ldots x_\ell, \widetilde{x}) \in \mathbb{R}^{d-1}$ (the second one follows from (2.5.8) and the latter follows from the fact that $f \in L^2(\mathbb{R}^d)$). In the computation below let us denote $x_k^* = (x_k, 0, 0) \in \mathbb{R}^3$ and $y_k = (y_{k1}, y_{k2}, y_{k3}) \in \mathbb{R}^3$ for $1 \leqslant k \leqslant \ell$. By a repeated use of Fubini's theorem and Bochner's relation (Lemma 2.10, with $d = \ell = 1$ in that statement) we find

$$
\begin{aligned}
&s' i^{\mathfrak{r}(\ell)} x_1 x_2 \dots x_\ell \, g^{\#}(x_1^*, \dots, x_\ell^*, \widetilde{x}) = s' i^{\mathfrak{r}(\ell)} x_1 x_2 \dots x_\ell \, g(x) = s' i^{\mathfrak{r}(\ell)} f(x) = \widehat{f}(x) \\
&= \int_{\mathbb{R}^{d-1}} \left(\int_{\mathbb{R}} z_1 \, g(z_1, z_2, \dots, z_\ell, \widetilde{z}) \, e^{-2\pi i x_1 z_1} \, \mathrm{d}z_1 \right) z_2 \dots z_\ell \, e^{-2\pi i (x_2 z_2 + \dots + x_\ell z_\ell + \widetilde{x} \cdot \widetilde{z})} \, \mathrm{d}z_2 \dots \mathrm{d}z_\ell \, \mathrm{d}\widetilde{z} \\
&= (-i) \, x_1 \int_{\mathbb{R}^{d-1}} \left(\int_{\mathbb{R}^3} g(|y_1|, z_2, \dots, z_\ell, \widetilde{z}) \, e^{-2\pi i x_1 y_{11}} \, \mathrm{d}y_1 \right) \\
&\qquad\qquad\qquad\qquad z_2 \dots z_\ell \, e^{-2\pi i (x_2 z_2 + \dots + x_\ell z_\ell + \widetilde{x} \cdot \widetilde{z})} \, \mathrm{d}z_2 \dots \mathrm{d}z_\ell \, \mathrm{d}\widetilde{z} \\
&= (-i) \, x_1 \int_{\mathbb{R}^{d+1}} \left(\int_{\mathbb{R}} z_2 \, g(|y_1|, z_2, \dots, z_\ell, \widetilde{z}) \, e^{-2\pi i x_2 z_2} \, \mathrm{d}z_2 \right) \\
&\qquad\qquad\qquad\qquad z_3 \dots z_\ell \, e^{-2\pi i (x_1 y_{11} + x_3 z_3 + \dots + x_\ell z_\ell + \widetilde{x} \cdot \widetilde{z})} \, \mathrm{d}y_1 \, \mathrm{d}z_3 \dots \mathrm{d}z_\ell \, \mathrm{d}\widetilde{z} \\
&= (-i)^2 \, x_1 x_2 \int_{\mathbb{R}^{d+1}} \left(\int_{\mathbb{R}^3} g(|y_1|, |y_2|, z_3, \dots, z_\ell, \widetilde{z}) \, e^{-2\pi i x_2 y_{21}} \, \mathrm{d}y_2 \right) \\
&\qquad\qquad\qquad\qquad z_3 \dots z_\ell \, e^{-2\pi i (x_1 y_{11} + x_3 z_3 + \dots + x_\ell z_\ell + \widetilde{x} \cdot \widetilde{z})} \, \mathrm{d}y_1 \, \mathrm{d}z_3 \dots \mathrm{d}z_\ell \, \mathrm{d}\widetilde{z} \\
&= \dots \\
&= (-i)^\ell \, x_1 \dots x_\ell \int_{\mathbb{R}^{d+2\ell}} g(|y_1|, \dots, |y_\ell|, \widetilde{z}) \, e^{-2\pi i (x_1 y_{11} + x_2 y_{21} + \dots + x_\ell y_{\ell 1} + \widetilde{x} \cdot \widetilde{z})} \, \mathrm{d}y_1 \dots \mathrm{d}y_\ell \, \mathrm{d}\widetilde{z} \\
&= (-i)^\ell \, x_1 \dots x_\ell \, \widehat{g^{\#}}(x_1^*, \dots, x_\ell^*, \widetilde{x}).
\end{aligned}
$$

Since $y \mapsto g^{\#}(y)$ is radial on each of the first ℓ variables $y_k \in \mathbb{R}^3$, the same is valid for $\widehat{g^{\#}}$ and therefore, if $|y_1| \dots |y_\ell| \neq 0$, we find that

$$
\widehat{g^{\#}}(y_1, \dots, y_\ell, \widetilde{y}) = s \, g^{\#}(y_1, \dots, y_\ell, \widetilde{y}).
$$

In particular, by the Riemann-Lebesgue lemma, $g^{\#}$ is equal a.e. to a continuous function, that we now call $\overline{g^{\#}}$. All the integrability properties defining the class $\mathcal{A}_s^*(P; d+2\ell)$ automatically transfer from $g^{\#}$ to $\overline{g^{\#}}$. We must pay a bit of attention when it comes to (2.5.7). Note that by definitions (2.5.4) and (2.5.6), $g^{\#}$ is already continuous on the set $Y = \{y = (y_1, \dots, y_\ell, \widetilde{y}) \in \mathbb{R}^{d+2\ell} \ : \ |y_1| \dots |y_\ell| \neq 0\}$. So, $\overline{g^{\#}}$ is potentially redefining the values of $g^{\#}$ at the set Y^c. We claim that we continue to have

$$
r\big(P\overline{g^{\#}}\big) = r(Pg^{\#}). \tag{2.5.10}
$$

In fact, let $r = r(Pg^{\#})$. Taking $y \in \mathbb{R}^{d+2\ell}$ with $|y| > r$, we want to show that $P(y)\overline{g^{\#}}(y) \geqslant 0$. If $|y_1| \dots |y_\ell| \neq 0$ then $P(y)\overline{g^{\#}}(y) = P(y)g^{\#}(y) \geqslant 0$. If $|y_1| \dots |y_\ell| = 0$, we have two options. If $P(y) = 0$ we are done. If not, assume without loss of generality that $P(y) > 0$. In this case, we can take a sequence of points $\{y^{(j)}\}_{j \in \mathbb{N}} \subset Y$ such that $\big|y^{(j)}\big| = |y| > r$ and $y^{(j)} \to y$ as $j \to \infty$. Since P is radial, then $P\big(y^{(j)}\big)\overline{g^{\#}}\big(y^{(j)}\big) = P(y)\overline{g^{\#}}\big(y^{(j)}\big) = P(y)g^{\#}\big(y^{(j)}\big) = P\big(y^{(j)}\big)g^{\#}\big(y^{(j)}\big) \geqslant 0$, and we conclude that $\overline{g^{\#}}\big(y^{(j)}\big) \geqslant 0$ and by continuity $\overline{g^{\#}}(y) \geqslant 0$. This shows that $r\big(P\overline{g^{\#}}\big) \leqslant r(Pg^{\#})$. The reverse inequality is simpler, proceeding along the same lines.

The conclusion is that $\overline{g^{\#}} \in \mathcal{A}_s^*(P; d+2\ell)$ and from (2.5.5), (2.5.7) and (2.5.10) we have

$$\mathbb{A}^*_{s(-1)^{(\mathfrak{r}(\ell)+\ell)/2}}\big(\widetilde{P}; d\big) \geqslant \mathbb{A}_s^*(P; d+2\ell).$$

This inequality, together with (2.1.22), leads to the identity (2.1.23). This concludes the proof.

Remark. It is interesting to notice that if we start with $f \in \mathcal{A}^*_{s'}\big(\widetilde{P}; d\big)$ as in §2.5.2, run the procedure of §2.5.2 to arrive at the function $\overline{g^{\#}} \in \mathcal{A}_s^*(P; d+2\ell)$, and then run the radialization and dropping procedure of §2.5.1 with this $\overline{g^{\#}}$, we end up with a new function $f_1 = \big(\overline{g^{\#}}\big)^{\flat} \in \mathcal{A}^*_{s'}\big(\widetilde{P}; d\big)$ that does a job at least as good as the original f and has the form $f_1(x) = x_1 \ldots x_\ell f_0(x)$, with f_0 radial. Such a reduction is not obvious from the start. Since we have explicit radial extremizers for (2.1.5) and (2.1.6) in [35, 37, 103], one can construct explicit extremizers for all the other 14 situations in Corollary 2.8 by formula (2.5.3).

2.6 Power weights: proof of Corollary 2.9

Although we call this a corollary, it requires a brief proof, that will essentially be a collage of passages from our previous results. For instance, using Theorem 2.3 with $H = \mathbf{1}$ and $Q = |x|^\gamma$ we have: that $\mathcal{A}_s^*(|x|^\gamma; d)$ is non-empty for all $\gamma > -d$; that the upper bound in (2.1.24) holds for all $\gamma > -d$ and $s = \pm 1$; and that the identity (2.1.25) holds. From Theorem 2.6 (i) we have the existence of extremizers for $\mathbb{A}_s(|x|^\gamma; d)$ when $\gamma \geqslant 0$, and the fact that they can be taken to be radial follows as in (2.5.1) (from Proposition 2.11 we can even assume that $\int_{\mathbb{R}^d} f|x|^\gamma = 0$). This leaves us with the task of proving the lower bound in (2.1.24), which is the actual sign uncertainty principle. We consider below the different regimes.

2.6.1 The case $\gamma \geqslant 0$

The case $\gamma = 0$ is known (see Theorem 2.1 or the remark after Theorem 2.6). Let us assume that $\gamma > 0$. Recall that the volume of the unit ball $B = B_1 \subset \mathbb{R}^d$ is given by $|B| = \pi^{d/2}/\Gamma\big(\frac{d}{2}+1\big)$. Using (2.1.18) and (2.1.20) we find that

$$\mathbb{A}_s(|x|^\gamma; d) \geqslant \left(\frac{(d+\gamma q')}{d} \frac{1}{|B|} \frac{1}{\left(2\left(1+\frac{\gamma}{d}\right)\left[\left(1+\frac{d}{\gamma}\right)|B|\right]^{\frac{\gamma}{d}}\right)^{q'}} \right)^{\frac{1}{(d+\gamma q')}} = \frac{1}{|B|^{\frac{1}{d}}}\, F(q')\,, \quad (2.6.1)$$

where

$$F(q') = \left(\frac{d+\gamma q'}{d}\right)^{\frac{1}{(d+\gamma q')}} \left(\frac{d}{2(d+\gamma)}\right)^{\frac{q'}{(d+\gamma q')}} \left(\frac{\gamma}{d+\gamma}\right)^{\frac{\gamma q'}{d(d+\gamma q')}}.$$

Let us briefly indicate why the choice $q' = 1$ indeed maximizes $F(q')$ for all d and γ in this case. Write $\gamma = \lambda d$, with $\lambda > 0$. Then $\log F(x) = \frac{1}{d}\, H(x)$, with

$$H(x) = \left(\frac{1}{1+\lambda x}\right)\left(\log(1+\lambda x) - x\log(2(1+\lambda)) + \lambda x \log\left(\frac{\lambda}{1+\lambda}\right)\right).$$

Routine calculus arguments lead to $H'(x) < 0$ for all $x \geqslant 1$. We then plug $q' = 1$ in (2.6.1) to get

$$\mathbb{A}_s(|x|^\gamma; d) \geqslant \left(\frac{\Gamma\left(\frac{d}{2}+1\right)}{\pi^{d/2}}\right)^{\frac{1}{d}} \left(\frac{1}{2}\right)^{\frac{1}{d+\gamma}} \left(\frac{\gamma}{d+\gamma}\right)^{\frac{\gamma}{d(d+\gamma)}}. \tag{2.6.2}$$

This is an explicit lower bound in which the parameters d and $\gamma > 0$ may vary independently. If one is interested in bounds that are uniform on the parameter $\gamma > 0$, we call $x = \gamma/(d+\gamma)$ and note that the function

$$\gamma \mapsto \left(\frac{1}{2}\right)^{\frac{1}{d+\gamma}} \left(\frac{\gamma}{d+\gamma}\right)^{\frac{\gamma}{d(d+\gamma)}}$$

is minimized when $x = 1/2e$, with value $2^{-\frac{1}{d}}\, e^{-\frac{1}{2ed}}$. Then

$$\mathbb{A}_s(|x|^\gamma; d) \geqslant \left(\frac{\Gamma\left(\frac{d}{2}+1\right)}{2\,\pi^{d/2}\, e^{\frac{1}{2e}}}\right)^{\frac{1}{d}}. \tag{2.6.3}$$

Using the inequality $\Gamma(x+1) > (\frac{x}{e})^x\sqrt{2\pi x}$ for all $x > 0$ we see that the right-hand side of (2.6.3) is greater than $\sqrt{\frac{d}{2\pi e}}$ for all $d \geqslant 2$, and we can actually take $c = 1$ in (2.1.24). If $d = 1$ then the right-hand side of (2.6.3) is equal to $c\sqrt{\frac{1}{2\pi e}}$ for $c = 0.8595\ldots$.

2.6.2 The case $-\frac{d}{2} + \varepsilon(d) \leqslant \gamma < 0$

Here we use inequality (2.1.22) in Theorem 2.7 (note that the dimension d here shall correspond to the dimension $d + 2\ell$ in (2.1.22)). If $d = 3$, we let $H(x) = x_1$ (of degree $\ell = 1$). If $d \geqslant 4$, we let H be a homogeneous and harmonic polynomial of two variables and degree $\ell = -\lfloor\gamma\rfloor$ (e.g. we can take $H(x_1, x_2) = \Re((x_1 + ix_2)^\ell)$). Having defined H, we let $Q(x) = |x|^\ell \cdot \frac{\operatorname{sgn}(H(x))}{H(x)}$ for $H(x) \neq 0$, and zero otherwise. Then (2.1.22) yields

$$\mathbb{A}_s(|x|^\gamma; d) \geqslant \mathbb{A}_{s(-1)^{(\mathfrak{r}(\ell)+\ell)/2}}\big(\operatorname{sgn}(H(x))|x|^{\gamma+\ell}; d-2\ell\big). \tag{2.6.4}$$

Note that the final dimension $d - 2\ell$ is at least equal to the number of variables we need to construct our harmonic polynomial H (this is how we define the function $\varepsilon : \mathbb{N} \to \mathbb{R}$), and on the right-hand side of (2.6.4) we now have a homogeneous function $\operatorname{sgn}(H(x))|x|^{\gamma+\ell}$ of degree $0 \leqslant \gamma + \ell < 1$. Note that $|\operatorname{sgn}(H(x))|\,|x|^{\gamma+\ell} = |x|^{\gamma+\ell}$ for a.e. $x \in \mathbb{R}^{d-2\ell}$, and hence the volume of their sub-level sets are the same. We may then proceed as in §2.6.1, using (2.1.18) and (2.1.20) to arrive at the exact same bounds as in (2.6.2) and (2.6.3), with $\gamma + \ell$ in the place of γ and $d - 2\ell$ in the place of d. This leads to (2.1.24) in this case.

2.6.3 The case $s = 1$ and $-d < \gamma \leqslant -\frac{d}{2} - \varepsilon(d)$

Recall that for any Schwartz function f we have the identity (see [98, Chapter V, §1, Lemma 2])

$$\Gamma\left(\frac{d+\gamma}{2}\right)\pi^{\frac{-d-\gamma}{2}}\int_{\mathbb{R}^d}|x|^{-d-\gamma}\widehat{f}(x)\,\mathrm{d}x = \Gamma\left(-\frac{\gamma}{2}\right)\pi^{\frac{\gamma}{2}}\int_{\mathbb{R}^d}|x|^{\gamma}f(x)\,\mathrm{d}x. \tag{2.6.5}$$

Standard approximation arguments show that (2.6.5) remains valid for $f \in L^1(\mathbb{R}^d)$ such that $\widehat{f} \in L^1(\mathbb{R}^d)$. In particular, this implies that

$$\mathbb{A}_{+1}(|x|^{\gamma}; d) = \mathbb{A}_{+1}(|x|^{-d-\gamma}; d). \tag{2.6.6}$$

Using this symmetry we fall in the case $-\frac{d}{2} + \varepsilon(d) \leqslant -d - \gamma < 0$ treated in §2.6.2. This leads again to (2.1.24) and concludes the proof.

Remark. The symmetry (2.6.6) is not valid in the case $s = -1$ as we have (2.1.24) and (2.1.25). In particular, in light of (2.6.5), this implies that one cannot reduce the search in $\mathbb{A}_{-1}(|x|^{\gamma}; d)$, when $\gamma \leqslant -\frac{d}{2} - \varepsilon(d)$ to functions satisfying $\int_{\mathbb{R}^d} f|x|^{\gamma} = 0$. Proposition 2.11 already pointed in this direction.

Remark. Establishing the sign uncertainty for $P(x) = |x|^{\gamma}$, with $-d < \gamma < 0$, in a more direct way seems to be subtle. For instance, one could try to prove (2.1.16), or even a suitable weaker variation of it that would still make the Hölder's inequality argument in (2.4.1) work. For instance, it would be natural and sufficient to consider an inequality of the type, for $f \in L^1(\mathbb{R}^d)$ with $\widehat{f} = \pm f$,

$$\left\| f|x|^{\alpha} \right\|_q \leqslant C \left\| f|x|^{\gamma} \right\|_1, \tag{2.6.7}$$

for some α and q verifying the conditions: (i) if $q = 1$ then $-d < \alpha < \gamma$; or (ii) if $1 < q < \infty$ then $-\frac{d}{q} < \alpha < \gamma + \frac{d}{q'}$. However, the inequality (2.6.7) is simply not true. The following counterexample in dimension $d = 1$ was communicated to us by F. Nazarov. Choose a small $\delta > 0$ and consider a real-valued, radially non-increasing Schwartz function g supported on $[-\delta, \delta]$ with $g \equiv 1$ on $[-\delta/2, \delta/2]$. Let $h_t(x) = g(x)\cos(2\pi t x)$ for large t and put $f_t = h_t + \widehat{h}_t$. Then $f_t = \widehat{f}_t$. Noting that $\limsup_{t\to\infty} \left\| \widehat{h}_t|x|^{\gamma} \right\|_1 = 0$, by the triangle inequality,

$$\limsup_{t\to\infty} \left\| f_t|x|^{\gamma} \right\|_1 \leqslant \limsup_{t\to\infty} \left\| h_t|x|^{\gamma} \right\|_1 + \limsup_{t\to\infty} \left\| \widehat{h}_t|x|^{\gamma} \right\|_1 \leqslant \left\| g|x|^{\gamma} \right\|_1 \lesssim \delta^{\gamma+1}. \tag{2.6.8}$$

Similarly, noting that $\limsup_{t\to\infty} \left\| \widehat{h}_t|x|^{\alpha} \right\|_{L^q([-\delta,\delta])} = 0$,

$$\begin{aligned} \liminf_{t\to\infty} \left\| f_t|x|^{\alpha} \right\|_{L^q([-\delta,\delta])} &\geqslant \liminf_{t\to\infty} \left\| h_t|x|^{\alpha} \right\|_{L^q([-\delta,\delta])} - \limsup_{t\to\infty} \left\| \widehat{h}_t|x|^{\alpha} \right\|_{L^q([-\delta,\delta])} \\ &\geqslant \liminf_{t\to\infty} \left\| h_t|x|^{\alpha} \right\|_{L^q([-\delta,\delta])} \\ &\gtrsim \delta^{\alpha+\frac{1}{q}}. \end{aligned} \tag{2.6.9}$$

If (2.6.7) were true, (2.6.8) and (2.6.9) would imply that $\alpha \geqslant \gamma + \frac{1}{q'}$, a contradiction. It should be noted that the functions in the counterexample above are eigenfunctions but do not necessarily belong to the class $\mathcal{A}_s^*(|x|^\gamma; d)$. Hence, one may still try to find suitable admissibility inequalities like (2.1.16) or (2.6.7) imposing this additional constraint on f (and even assuming that $r(f)$ is small). Several other types of weighted norm inequalities related to uncertainty are considered in [3].

Chapter 3

Integers represented by quadratic forms

This chapter is comprised of the paper [A2]. In this chapter, we combine tools from Fourier analysis, analytic number theory, and algebraic number theory to prove a number of new estimates related to integers represented by positive definite quadratic forms. In particular, we improve some results given by Zaman [109, Proposition 7.1 and Theorem 1.4], concerning these types of estimates. As an application, assuming the generalized Riemann hypothesis, we establish a Cramér-type result, extending the method developed by Carneiro, Milinovich, and Soundararajan [22].

3.1 Introduction

3.1.1 Background

A classical problem in number theory is to understand the distribution of primes represented by positive definite quadratic forms. The survey [39] by D. A. Cox is the classical reference on the subject, describing some of the historical milestones of its study and showing how it leads to class field theory.

An integral quadratic form in two variables is a function defined by

$$f(u,v) = au^2 + buv + cv^2,$$

where $a, b, c \in \mathbb{Z}$. Its discriminant $-D$ is given by $-D = b^2 - 4ac$. For simplicity, we refer to a form (or quadratic form) as a function f defined in this way. We say that f is positive definite if $D > 0$, and f is primitive if its coefficients a, b, and c are relatively prime. In the set of primitive forms, we define an equivalence relation in the following way: f and g are properly equivalent if there are integers p, q, r, s such that

$$f(u,v) = g(pu + qv, ru + sv), \text{ and } ps - qr = 1.$$

Note that two properly equivalent forms have the same discriminant. A primitive positive definite form f is reduced if $|b| \leqslant a \leqslant c$ and if, in addition, when $|b| = a$ or $a = c$, then $b \geqslant 0$. Classical theorems in the theory of quadratic forms (see [39, Theorem 2.8 and Theorem 2.13]) establish that every primitive positive definite form is properly equivalent to a unique reduced form. Moreover, for each $D > 0$, the number of classes of primitive positive definite forms of discriminant $-D$ is finite, and it is equal to the number of reduced forms of discriminant $-D$. This number is called the class number and it is denoted by $h(-D)$.

3.1.2 Congruence sums

An integer n is represented by the quadratic form f if there is $(u, v) \in \mathbb{Z}^2$ such that $n = f(u, v)$. For $n \geqslant 0$ an integer, define

$$r_f(n) = \#\{(u, v) \in \mathbb{Z}^2 : f(u, v) = n\},$$

that is, the number of representations of n by f. Motivated by applications using sieve theory, we are interested in estimating the congruence sums

$$\sum_{\substack{n \leqslant x \\ \ell | n}} r_f(n), \tag{3.1.1}$$

where $x \geqslant 1$ is a real number and $\ell \geqslant 1$ is an integer. In the case $\ell = 1$ and $f(u, v) = u^2 + v^2$, the congruence sum (3.1.1) corresponds to the classical Gauss circle problem.[1] Here, Gauss used a lattice point counting argument to prove that (3.1.1) has the asymptotic formula $\pi x + O(x^{1/2})$. Later, Sierpiński improved the error term to $O(x^{1/3})$ using ideas from Voronoi's work on the Dirichlet divisor problem. Afterward, Landau [75, Treatise I] extended this asymptotic formula to positive definite quadratic forms (still in the case $\ell = 1$), with error term $O(x^{1/3})$, but without making explicit the dependence on f in this error term. For the case where $\ell \geqslant 1$ is a squarefree[2] integer, we prove the following result.

Theorem 3.1. *Let $f(u, v) = au^2 + buv + cv^2$ be a reduced positive definite quadratic form of discriminant $-D$ and let $\ell \geqslant 1$ be a squarefree integer. Then, for $x \geqslant D^2$ we have*

$$\sum_{\substack{1 \leqslant n \leqslant x \\ \ell | n}} r_f(n) = \frac{2\pi}{\sqrt{D}} g(\ell)\, x + O\left(\frac{\tau(\ell)\, \ell}{D^{1/6}} x^{1/3} + \frac{\tau(\ell)\, \ell^{5/2} D^{3/4}}{a^{7/4}} x^{1/4} \right), \tag{3.1.2}$$

where g is the multiplicative function defined by

$$g(p) = \frac{1}{p}\left(1 + \chi(p) - \frac{\chi(p)}{p} \right)$$

[1] For a survey of this problem, see [66, Section 2.7] and [4].

[2] As we shall see in (3.3.7), our result also holds for an arbitrary integer $\ell \geqslant 1$, with an adequate function $g(\ell)$ and perhaps a modification in the error term.

for all primes p, $\chi = \chi_{-D} = \left(\frac{-D}{\cdot}\right)$ is the corresponding Kronecker symbol, and τ is the divisor function.

Theorem 3.1 improves a result of Zaman [109, Proposition 7.1], whose error term is of magnitude $x^{1/2}$. Note that, when $\ell = 1$, we recover Landau's result, with an explicit dependence on f in the error term.

As we shall see in the next section, a direct application of Selberg's sieve allows us to use Theorem 3.1 to obtain upper bounds for the number of primes represented by f, in short intervals.

3.1.3 Brun-Titchmarsh-type result

Assume that f is a primitive positive definite quadratic form. For $x \geqslant 1$, let $\pi_f(x)$ be the number of primes represented by f up to x, i.e.,

$$\pi_f(x) = \#\{p \leqslant x : p = f(u,v) \text{ for some } (u,v) \in \mathbb{Z}^2\}.$$

The classical result for $\pi_f(x)$ goes back to de la Vallée Poussin (see, for instance [86]), and establishes that, as $x \to \infty$,

$$\pi_f(x) \sim \frac{\delta_f\, x}{h(-D)\log x},$$

where

$$\delta_f = \begin{cases} \frac{1}{2}, & \text{if } f(u,v) \text{ is properly equivalent to } f(u,-v); \\ 1 & \text{otherwise.} \end{cases} \tag{3.1.3}$$

Assuming the generalized Riemann hypothesis (GRH), we also have (see [74])

$$\pi_f(x) = \frac{\delta_f \operatorname{Li}(x)}{h(-D)} + O\big(x^{1/2}\log(Dx)\big), \tag{3.1.4}$$

for $x \geqslant 2$, where

$$\operatorname{Li}(x) = \int_2^x \frac{1}{\log t}\, \mathrm{d}t.$$

Recently, Thorner and Zaman [100, Corollary 1.3] established a Brun-Titchmarsh result, improving upon the Chebotarev version given by Lagarias-Montgomery-Odlyzko [73]. Unconditionally, they showed that, for D sufficiently large,

$$\pi_f(x) < \frac{2\,\delta_f \operatorname{Li}(x)}{h(-D)}, \quad \text{for } x \geqslant D^{700}. \tag{3.1.5}$$

We want to establish a result similar to (3.1.5) for primes in short intervals.[3] For instance, if we assume GRH, from (3.1.4) we get that

$$\pi_f(x) - \pi_f(x-y) \ll \frac{\delta_f\, y}{h(-D)\log y},$$

for $(Dx)^{1/2+\varepsilon} \leqslant y \leqslant x$. Unconditionally, Zaman used his asymptotic formula for the congruence sum (3.1.1) and Selberg's sieve to establish a similar Brun-Titchmarsh-type result in short intervals [109, Theorem 1.4], with the same order of magnitude.

Theorem 3.2 (Zaman [109])**.** *Let $f(u,v) = au^2 + buv + cv^2$ be a reduced positive definite quadratic form of discriminant $-D$, and let $\varepsilon > 0$ be arbitrary. Suppose that*

$$\left(\frac{D^2}{a}\right)^{1/2+\varepsilon} x^{1/2+\varepsilon} \leqslant y \leqslant x. \tag{3.1.6}$$

Then,

$$\pi_f(x) - \pi_f(x-y) < \frac{2}{(1-\theta')} \cdot \frac{\delta_f\, y}{h(-D)\log y}\left(1 + O_\varepsilon\left(\frac{\log\log y}{\log y}\right)\right),$$

where

$$\theta' = \frac{\log x}{2\log y} + \left(\frac{3}{4} + \frac{\varepsilon}{4}\right)\frac{\log D}{\log y} - \frac{\log a}{2\log y}.$$

Using Theorem 3.1, we are able to establish an analogous result to Theorem 3.2, for a range beyond (3.1.6).

Theorem 3.3. *Let $f(u,v) = au^2 + buv + cv^2$ be a reduced[4] positive definite quadratic form of discriminant $-D$. Then, the following statements hold.*

1. *Let $0 < \varepsilon < 1/20$ be arbitrary, and suppose that*

$$\frac{D^2}{a} x^{1/3+\varepsilon} \leqslant y \leqslant x^{4/9}. \tag{3.1.7}$$

Then,

$$\pi_f(x) - \pi_f(x-y) < \frac{4}{(1-\theta_1)} \cdot \frac{\delta_f\, y}{h(-D)\log y}\left(1 + O_\varepsilon\left(\frac{\log\log y}{\log y}\right)\right),$$

where

$$\theta_1 = \frac{\log x}{3\log y} + \left(\frac{4}{3} + \varepsilon\right)\frac{\log D}{\log y} - \frac{\log a}{\log y}.$$

[3] Montgomery and Vaughan [82, Theorem 2] gave a classical version for primes in arithmetic progressions, in short intervals.

[4] The hypothesis of being reduced can be removed, and Theorem 3.3 holds for any primitive positive definite quadratic form, by considering $a = 1$ in the range (3.1.7) and in the values of θ_1 and θ_2. A similar situation occurs in Theorem 3.2 (see Remark (ii) in [109, Theorem 1.4]).

2. Suppose that

$$x^{4/9} \leqslant y \leqslant x^{3/5} \quad \textit{and} \quad x \geqslant D^{18}. \tag{3.1.8}$$

Then,

$$\pi_f(x) - \pi_f(x-y) < \frac{7}{(1-\theta_2)} \cdot \frac{\delta_f\, y}{h(-D)\log y}\left(1 + O\left(\frac{\log\log y}{\log y}\right)\right),$$

where

$$\theta_2 = \frac{\log x}{4\log y} + \frac{31\log D}{12\log y} - \frac{7\log a}{4\log y}.$$

Theorem 3.3 states a Brun-Titchmarsh-type inequality in short intervals, for $x^{1/3+\varepsilon} \lesssim y \leqslant x^{3/5}$, extending the range (3.1.6) in Theorem 3.2. This also improves the constant in the range $x^{1/2+\varepsilon} \leqslant y \leqslant x^{3/5}$, since we have that

$$\frac{7}{1-\theta_2} < \frac{2}{1-\theta'} < \frac{2}{\varepsilon}.$$

The associated constants in our results can be estimated, uniformly, by

$$16 < \frac{4}{1-\theta_1} < \frac{16}{9\varepsilon}, \quad \text{and} \quad 12 < \frac{7}{1-\theta_2} \leqslant \frac{672}{11}.$$

We highlight that, unlike in Theorem 3.2, even under the assumption of GRH, the order of magnitude of the bounds in Theorem 3.3 cannot be obtained using (3.1.4).[5]

As we shall see, the special case $y = x^{1/2}$ will be useful in the following form:

Corollary 3.4. *Let $f(u,v) = au^2 + buv + cv^2$ be a fixed primitive positive definite quadratic form of discriminant $-D$. Then,*

$$\pi_f(x+\sqrt{x}) - \pi_f(x) \leqslant \frac{28\,\delta_f\sqrt{x}}{h(-D)\log x}(1+o(1)),$$

as $x \to \infty$.

3.1.4 Cramér-type result

Let $\pi(x)$ denote be the number of primes up to x. A classical theorem of Cramér [40] states that, assuming RH, there are constants $c, \alpha > 0$ such that

$$\frac{\pi(x + c\sqrt{x}\log x) - \pi(x)}{\sqrt{x}} > \alpha$$

[5]Assuming GRH for quadratic Dirichlet L-functions modulo D, Theorem 3.3 can be stated with slight changes in the power of D on the ranges, and in the definition of θ_1 and θ_2. A similar situation occurs in Theorem 3.2 (see [109, Theorem 1.4]).

for all x sufficiently large. Recently, using a Fourier analysis approach, Carneiro, Milinovich and Soundararajan [22, Theorem 1.3] established this estimate in an optimized explicit form. They proved that, under RH, for $\alpha \geqslant 0$ we have

$$\inf\left\{c>0;\ \liminf_{x\to\infty}\frac{\pi(x+c\sqrt{x}\log x)-\pi(x)}{\sqrt{x}}>\alpha\right\}<\frac{21}{25}(1+2\alpha).$$

This was slighlty improved by Chirre, Pereira and de Laat [33], replacing $21/25 = 0.84$ by 0.8358. Furthermore, they obtained an analogous result for primes in arithmetic progressions. Our next result extends these techniques for primes represented by quadratic forms.

Theorem 3.5. *Let f be a primitive positive definite quadratic form of discriminant $-D$. Assume the generalized Riemann hypothesis for Hecke L-functions. Then, for $\alpha \geqslant 0$,*

$$\inf\left\{c>0;\ \liminf_{x\to\infty}\frac{\pi_f\left(x+c\sqrt{x}\log x\right)-\pi_f(x)}{\sqrt{x}}>\alpha\right\}<1.837\,\frac{(\delta_f+\alpha)\,h(-D)}{\delta_f}.$$

In particular, for a fixed primitive positive definite quadratic form f of discriminant $-D$, there is always a prime number represented by f in the interval $[x,\ x+1.837\,h(-D)\sqrt{x}\log x]$, for x sufficiently large. Then, we deduce the following conditional estimate for large gaps between primes represented by a quadratic form.[6]

Corollary 3.6. *Let f be a primitive positive definite quadratic form of discriminant $-D$, and let $p_{n,f}$ be the n-th prime represented by f. Assume the generalized Riemann hypothesis for Hecke L-functions. Then,*

$$\limsup_{n\to\infty}\frac{p_{n+1,f}-p_{n,f}}{\sqrt{p_{n,f}}\,\log p_{n,f}}<1.837\,h(-D). \tag{3.1.9}$$

Remark. Consider the quadratic form $f(u,v) = u^2 + mv^2$, where m is a positive integer. It is known that there are at most 66 positive integers m, such that f represents a prime p if and only if p belongs to a certain union of arithmetic progressions (see [39]). For instance, when $m = 1$, a classical theorem of Fermat states that a prime p is represented by f, if and only if $p \equiv 1 \pmod 4$. In this case, $D = 4$, $h(-D) = 1$, and we can recover the estimate (3.1.9) from [33, Corollary 2], with the better constant 1.7062. However, in general, the characterization of such primes is more subtle. For instance, consider the case $m = 27$, where $D = 108$ and $h(-D) = 3$. A conjecture of Euler, proven by Gauss, states that p has the form $u^2 + 27v^2$ if and only if both $p \equiv 1 \pmod 3$, and 2 is a cubic residue $\pmod p$. This cannot be described by just unions of arithmetic progressions, so the results of [33] no longer apply.

[6] To the best of our knowledge, there is no other explicit result of this type in the literature.

3.1.5 Outline of the proof

There are two main themes that will be ubiquitous throughout this chapter. The first theme is the use of Fourier analysis, in the following way. We begin by finding a summation formula that connects our object of study with an arbitrary function and its Fourier transform. Then, we choose an appropriate test function that recovers the desired information in an optimized manner. The second is the well-known theme that propositions about quadratic forms can be stated in two other equivalent languages: ideals of number fields and lattices. We now discuss the main ideas in each theorem.

Congruence sums

The first step is obtaining a summation formula associated with the coefficients $r_f(n)$, relating it to an arbitrary test function and its Fourier transform. These types of formulas are well-known, and are equivalent to the modularity of certain theta series associated with a quadratic form f and a discrete periodic function χ (see, for instance, [69, p. 83] and [106, p. 32]), the latter which, in this case, allows us to filter out the congruence condition $\ell \,|\, n$. Since we were unable to find an explicit statement in the literature, we provide a proof of the specific summation formula that we require. In Section 3.2, we obtain the desired expression from an application of the classical Poisson summation formula for the lattice associated with the quadratic form f, combined with the discrete Fourier expansion of the periodic function χ. In Section 3.3, we prove Theorem 3.1 following an approach outlined in [69, Section 4.4], which was applied to the Gauss circle problem in [69, Corollary 4.9]. By choosing an appropriate test function in our summation formula and carrying out an asymptotic analysis (for instance, see Lemma 7.1 in Appendix A), we arrive at our new estimate for (3.1.1). We highlight that a good explicit dependence on ℓ and the parameters of f is required. This imposes significant technical difficulties when compared to the argument in [69], and requires a careful analysis and delicate manipulations with a reduced quadratic form.

Remark. Higher moments of $r_f(n)$ have also been studied by Blomer and Granville [8]. Later, Xu [104] gave some improvements in their error terms. Additionally, he proved that, when $\ell = 1$ in Theorem 3.1, the optimal error term in (3.1.2) satisfies $\Omega(D^{1/4}x^{1/4})$, which generalizes the classical omega result given originally by Hardy and Landau (see [66]).

Brun-Titchmarsh-type result

In Section 3.4 we prove Theorem 3.3, following Zaman's general outline in [109]. Here the main strategy is an application of Selberg's sieve [44, Theorem 7.1], which transforms the problem of obtaining an upper bound for primes represented by f in short intervals, into the problem of estimating the associated congruence sums (3.1.1). We remark that our extended range in Theorem 3.3 comes from the improved error term in our estimate of the congruence sums (3.1.1), of the form $O_{f,\ell}(x^{1/3})$, given in Theorem 3.1. When x is large compared to ℓ, this improves the estimate $O_{f,\ell}(x^{1/2})$ given in [109, Proposition 7.1], and it allows us to take intervals around x of size as small as roughly $x^{1/3}$.

Cramér-type result

We follow the argument of Carneiro, Milinovich, and Soundararajan in [22, Section 5], to prove Theorem 3.5. Here, we work with the language of ideals in imaginary quadratic fields. This allows us to use the machinery of Hecke characters and Hecke L-functions to obtain information about prime ideals in a given ideal class, and therefore, about prime numbers represented by a given quadratic form f. We first give some necessary background on Hecke L-functions, and their relation to quadratic forms, in Section 3.5. The main ingredients in Theorem 3.5 are our version of the Brun-Titchmarsh inequality in Corollary 3.4, and the Guinand-Weil explicit formula for L-functions (see, for instance, [69, Theorem 5.12] and [21, Lemma 5]). Then, we establish a version for Hecke L-functions that averages over all Hecke characters in a given congruence class group. We finish the proof of Theorem 3.5 in Section 3.6. Following [22], we start with an arbitrary function F in our version of the Guinand-Weil formula. The strategy then consists of taking a suitable dilation and modulation of F, so that we emphasize, in our explicit formula, intervals containing few prime numbers represented by f. We must then carry out an asymptotic analysis, and choose an appropriate function F at the end, to conclude the desired result. In Section 3.7, we discuss some qualitative aspects of the problem of choosing an optimal function F, related to the uncertainty principle.

3.1.6 Remarks

Throughout this chapter, let $f(u,v) = au^2 + buv + cv^2$ be a positive definite quadratic form of discriminant $-D$, and without loss of generality assume that $a, c \geqslant 1$. In the case when f is reduced, since $|b| \leqslant a \leqslant c$, we have that $a \ll \sqrt{D}$ and $D \geqslant 3$. We will use these frequently. Moreover, we have that $r_f(0) = 1$, and a is the smallest positive integer represented by f.

3.2 Summation formula for $r_f(n)$

Let $f(u,v) = au^2 + buv + cv^2$ be a positive definite quadratic form of discriminant $-D$. We recall that, for $n \geqslant 0$,

$$r_f(n) = \#\left\{(u,v) \in \mathbb{Z}^2 : f(u,v) = n\right\}.$$

Lemma 3.7. *Let $G \in L^1(\mathbb{R}^2)$ be a radial continuous function. Suppose that*

$$|G(x)| \ll \frac{1}{(1+|x|^2)^{1+\delta}} \quad \text{and} \quad |\widehat{G}(\xi)| \ll \frac{1}{(1+|\xi|^2)^{1+\delta}}, \tag{3.2.1}$$

for some $\delta > 0$. Then, for an integer $\ell \geqslant 1$, we have

$$\sum_{\substack{n=0\\ \ell|n}}^{\infty} r_f(n)\, G(\sqrt{n}) = \frac{2\,\widetilde{g}(\ell)}{\sqrt{D}} \sum_{n=0}^{\infty} r_f(n)\, \widehat{G}\left(\sqrt{\frac{4n}{D}}\right)$$
$$+ O\left(\frac{\widetilde{g}(\ell)\,\ell^2}{\sqrt{D}} \max_{\substack{0\leqslant r,\, s<\ell\\ (r,s)\in\mathbb{Z}^2\setminus(0,0)}} \sum_{(u,v)\in\mathbb{Z}^2} \left|\widehat{G}\left(\sqrt{\frac{4f(u-r/\ell, v-s/\ell)}{D}}\right)\right|\right), \tag{3.2.2}$$

where

$$\widetilde{g}(\ell) = \frac{1}{\ell^2}\,\#\left\{(u,v)\in\mathbb{Z}^2 : 0 \leqslant u, v < \ell, \textit{ and } \ell\,|\,f(u,v)\right\}. \tag{3.2.3}$$

Proof. We start associating a lattice $\Lambda \subset \mathbb{R}^2$, defined by the basis $\{\omega_1, \omega_2\}$, to the quadratic form f in such a way that $a = |\omega_1|^2$, $b = 2\,\omega_1 \cdot \omega_2$ and $c = |\omega_2|^2$. This implies that

$$|u\,\omega_1 + v\,\omega_2|^2 = f(u,v), \text{ and } r_f(n) = \#\{\omega \in \Lambda : |\omega|^2 = n\}, \text{ for } n \geqslant 0. \tag{3.2.4}$$

Let us consider the abelian group[7] $(\Lambda/\ell\Lambda, +)$ of order ℓ^2, and let $\chi : \Lambda/\ell\Lambda \to \mathbb{C}$ be the function defined by

$$\chi(\overline{\omega}) = \begin{cases} 1, & \text{if } \ell\,|\,|\omega|^2;\\ 0 & \text{otherwise.}\end{cases}$$

Then, since G satisfies (3.2.1), we have

$$\sum_{\substack{\omega\in\Lambda\\ \ell\,|\,|\omega|^2}} G(\omega) = \sum_{\omega\in\Lambda} \chi(\overline{\omega}) G(\omega). \tag{3.2.5}$$

On the other hand, we consider the dual lattice $\Lambda^* = \{\omega^* \in \mathbb{R}^2 : \omega \cdot \omega^* \in \mathbb{Z}, \text{ for all } \omega \in \Lambda\}$. It has a basis $\{\omega_1^*, \omega_2^*\}$, given by $\omega_1^* = 4c\,\omega_1/D - 2b\,\omega_2/D$ and $\omega_2^* = 2b\,\omega_1/D - 4a\,\omega_2/D$. This implies that

$$|u\,\omega_1^* + v\,\omega_2^*|^2 = 4f(v,u)/D, \text{ and } r_f(n) = \#\{\omega^* \in \Lambda^* : |\omega^*|^2 = 4n/D\}, \text{ for } n \geqslant 0. \tag{3.2.6}$$

For each λ^* in the set $P = \{sw_1^* + rw_2^* : 0 \leqslant s, r < \ell \text{ and } s, r \in \mathbb{Z}\}$, we define a character e_{λ^*} in the group $(\Lambda/\ell\Lambda, +)$ by $e_{\lambda^*}(\overline{w}) = e^{2\pi i\,\omega\cdot\lambda^*/\ell}$. Since the cardinality of P is ℓ^2, we conclude that $\{e_{\lambda^*}\}_{\lambda^*\in P}$ are all the characters in the group $(\Lambda/\ell\Lambda, +)$ (see [99, Theorem 2.5 in Chapter 7]). Now, we define the Fourier coefficient of χ with respect to e_{λ^*}, by

$$\widehat{\chi}(e_{\lambda^*}) = \frac{1}{\ell^2} \sum_{\overline{\omega}\in\Lambda/\ell\Lambda} \chi(\overline{\omega})\, e^{-2\pi i\,\omega\cdot\lambda^*/\ell}.$$

[7] We recall that the set $\Lambda/\ell\Lambda$ is defined by the equivalence classes in Λ given by $\overline{\omega} = \{\omega + \ell\lambda : \lambda \in \Lambda\}$.

Then, the Fourier inversion formula (see [99, Theorem 2.7 in Chapter 7]) yields

$$\chi(\overline{w}) = \sum_{\lambda^* \in P} \widehat{\chi}(e_{\lambda^*})\, e^{2\pi i\, \omega \cdot \lambda^*/\ell}. \tag{3.2.7}$$

Combining (3.2.5), (3.2.7) and Fubini's theorem, we get

$$\sum_{\substack{\omega\in\Lambda \\ \ell \,|\, |\omega|^2}} G(\omega) = \sum_{\lambda^* \in P} \widehat{\chi}(e_{\lambda^*}) \left(\sum_{w\in\Lambda} G(w)\, e^{2\pi i\, \omega \cdot \lambda^*/\ell} \right).$$

Recalling that $vol(\Lambda^*) = \sqrt{4/D}$, we use the Poisson summation formula for lattices in the above inner sum (since G satisfies (3.2.1)) to find that

$$\sum_{\substack{\omega\in\Lambda \\ \ell \,|\, |\omega|^2}} G(\omega) = \sqrt{\frac{4}{D}} \sum_{\lambda^* \in P} \widehat{\chi}(e_{\lambda^*}) \sum_{w^* \in \Lambda^*} \widehat{G}\left(w^* - \frac{\lambda^*}{\ell} \right). \tag{3.2.8}$$

On the other hand, if we define

$$\widetilde{g}(\ell) = \frac{1}{\ell^2} \# \left\{ \overline{\omega} \in \Lambda/\ell\Lambda : \ell \mid |\omega|^2 \right\},$$

it is clear that $\widehat{\chi}(e_{0^*}) = \widetilde{g}(\ell)$ and $|\widehat{\chi}(e_{\lambda^*})| \leqslant \widetilde{g}(\ell)$. Therefore, isolating the point $\lambda^* = 0$ in (3.2.8) gives us

$$\begin{aligned}
\sum_{\substack{\omega\in\Lambda \\ \ell \,|\, |\omega|^2}} G(\omega) &= \frac{2\,\widetilde{g}(\ell)}{\sqrt{D}} \sum_{\omega^* \in \Lambda^*} \widehat{G}(\omega^*) + \frac{2}{\sqrt{D}} \sum_{\lambda^* \in P \setminus \{0^*\}} \widehat{\chi}(e_{\lambda^*}) \sum_{w^* \in \Lambda^*} \widehat{G}\left(w^* - \frac{\lambda^*}{\ell} \right) \\
&= \frac{2\,\widetilde{g}(\ell)}{\sqrt{D}} \sum_{n=0}^{\infty} r_f(n)\, \widehat{G}\left(\sqrt{\frac{4n}{D}} \right) \\
&\qquad + O\left(\frac{\widetilde{g}(\ell)\, \ell^2}{\sqrt{D}} \max_{\substack{0 \leqslant r,\, s < \ell \\ (r,s)\in\mathbb{Z}^2 \setminus (0,0)}} \sum_{(u,v)\in\mathbb{Z}^2} \left| \widehat{G}\left(\sqrt{\frac{4f(u - r/\ell, v - s/\ell)}{D}} \right) \right| \right),
\end{aligned}$$

where we have used (3.2.6) and the fact that $\widehat{G}$ is radial. We conclude the proof using (3.2.4). □

The following technical lemma will help us estimate the error term. We compare a small translation of f with the untranslated value, outside of a finite number of exceptions.

Lemma 3.8. *Suppose that f is reduced. Let ℓ, r, s be integers such that $\ell \geqslant 1$ and $0 \leqslant r, s < \ell$. Then,*

$$\#\left\{ (u,v) \in \mathbb{Z}^2 : f\left(u - \frac{r}{\ell}, v - \frac{s}{\ell} \right) < \frac{f(u,v)}{2} \right\} \ll \frac{\sqrt{D}}{a}.$$

Proof. Define the set

$$A = \left\{ (u,v) \in \mathbb{Z}^2 : f\left(u - \frac{2r}{\ell}, v - \frac{2s}{\ell} \right) < 6c \right\}.$$

First we show that

$$\left\{ (u,v) \in \mathbb{Z}^2 : f\left(u - \frac{r}{\ell}, v - \frac{s}{\ell} \right) < \frac{f(u,v)}{2} \right\} \subset A. \tag{3.2.9}$$

Indeed, if $(u,v) \in A^c$, using that f is reduced, we have

$$\frac{2\,f(r,s)}{\ell^2} \leqslant 6c \leqslant f\left(u - \frac{2r}{\ell}, v - \frac{2s}{\ell} \right). \tag{3.2.10}$$

Applying the identity

$$f(u-x, v-y) = f(u,v) + f(x,y) - 2aux - buy - bxv - 2cvy \tag{3.2.11}$$

in (3.2.10) yields

$$\frac{2\,f(r,s)}{\ell^2} \leqslant f(u,v) + \frac{4\,f(r,s)}{\ell^2} - \frac{4aur + 2bus + 2bvr + 4cvs}{\ell}.$$

Then,

$$-\frac{f(r,s)}{\ell^2} + \frac{2aur + bus + bvr + 2cvs}{\ell} \leqslant \frac{f(u,v)}{2}.$$

Using this inequality and identity (3.2.11), we see that

$$f\left(u - \frac{r}{\ell}, v - \frac{s}{\ell} \right) = f(u,v) + \frac{f(r,s)}{\ell^2} - \frac{2aur + bus + bvr + 2cvs}{\ell} \geqslant \frac{f(u,v)}{2}.$$

This shows (3.2.9), and it now suffices to obtain an upper bound for the cardinality of A. Observe that

$$\begin{aligned} \#A &= \#\{(u,v) \in \mathbb{Z}^2 : f(u\ell - 2r, v\ell - 2s) < 6c\ell^2\} \\ &\leqslant \#\{(u,v) \in \mathbb{Z}^2 :\ f(u,v) \leqslant 6c\ell^2,\ u \equiv -2r \pmod{\ell},\ v \equiv -2s \pmod{\ell}\}. \end{aligned}$$

We now proceed with the well-known argument in [8, Lemma 3.1] as follows. Rewriting $f(u,v)$, we must bound the number of integer solutions to the inequality $(2au+bv)^2 + Dv^2 \leqslant 24ac\ell^2$. A solution (u,v) must satisfy that $|v| \ll \ell$ (where we used that $ac \ll D$), and that

$$\frac{-\sqrt{24ac\ell^2 - Dv^2} - bv}{2a} \leqslant u \leqslant \frac{\sqrt{24ac\ell^2 - Dv^2} - bv}{2a}.$$

Therefore, v belongs to an interval of size at most $\ll \ell$, and u belongs to an interval of size at most $\ll \sqrt{D}\,\ell/a$ (once again using that $ac \ll D$). Hence, the number of solutions (u,v) with the desired congruences modulo ℓ is at most $\ll \sqrt{D}/a$. □

3.3 Proof of Theorem 3.1

In [109, Proposition 7.1], Zaman used a lattice point counting argument, via geometry of numbers methods, to estimate (3.1.1). He established the following: for a primitive positive definite quadratic form f of discriminant $-D$, and a squarefree integer $\ell \geqslant 1$, we have

$$\sum_{\substack{n\leqslant x\\ \ell\mid n}} r_f(n) = \frac{2\pi}{\sqrt{D}}\, g(\ell)\, x + O\left(\frac{\tau_3(\ell)\, a^{1/2}}{D^{1/2}} x^{1/2} + \frac{\tau(\ell)\,\tau_3(\ell)\,\ell^{1/2}\, D^{1/4}}{a^{3/4}} x^{1/4} + 1\right), \tag{3.3.1}$$

for $x \geqslant 1$. Here, g is a multiplicative function satisfying

$$g(p) = \frac{1}{p}\left(1 + \chi(p) - \frac{\chi(p)}{p}\right) \tag{3.3.2}$$

for all primes p, $\chi = \chi_{-D}$ is the corresponding Kronecker symbol, and τ_3 is the 3-divisor function. The main goal here is to improve the error term in (3.3.1), reducing $x^{1/2}$ to $x^{1/3}$.

3.3.1 Proof of Theorem 3.1

We partially follow the approach outlined in [69, Corollary 4.9]. Assume that $x \geqslant 1$ is a real number and $\ell \geqslant 1$ is an integer. Let $1 \leqslant y \leqslant x^{1/2}$ be a parameter to be chosen. We will apply Lemma 3.7 to the radial function $G : \mathbb{R}^2 \to \mathbb{R}$ supported in $0 \leqslant r \leqslant (x+y)^{1/2}$, and defined by

$$G_{x,y}(r) = G(r) := \min\left\{r^2, 1, \frac{x+y-r^2}{y}\right\}.$$

By Lemma 7.1, the function G satisfies the conditions (3.2.1), with the bounds

$$\left|\widehat{G}(\sqrt{\xi})\right| \ll \frac{x^{1/4}}{|\xi|^{3/4}} \text{ for } |\xi| \neq 0, \text{ and } \left|\widehat{G}(\sqrt{\xi})\right| \ll \frac{x^{3/4}}{y|\xi|^{5/4}} \text{ for } |\xi| \geqslant 1. \tag{3.3.3}$$

Now, let us analyze the right-hand side of (3.2.2). We recall that $r_f(0) = 1$, and by Lemma 7.1, we know that $\widehat{G}(0) = \pi x + O(y)$. Letting $z = Dx/y^2$ (note that $4z/D \geqslant 1$), and using the estimates in (3.3.3) we obtain

$$\begin{aligned}\left|\sum_{n=1}^{\infty} r_f(n)\,\widehat{G}\left(\sqrt{\frac{4n}{D}}\right)\right| &= \left|\sum_{a\leqslant n\leqslant z} r_f(n)\,\widehat{G}\left(\sqrt{\frac{4n}{D}}\right) + \sum_{n>z} r_f(n)\,\widehat{G}\left(\sqrt{\frac{4n}{D}}\right)\right| \\ &\ll D^{3/4}x^{1/4}\sum_{a\leqslant n\leqslant z}\frac{r_f(n)}{n^{3/4}} + \frac{D^{5/4}x^{3/4}}{y}\sum_{n>z}\frac{r_f(n)}{n^{5/4}}.\end{aligned}$$

To estimate the sums above, we use integration by parts and the well-known result (see [8, Lemma 3.1])

$$\sum_{a\leqslant n\leqslant x} r_f(n) = \frac{2\pi x}{\sqrt{D}} + O\left(\sqrt{\frac{x}{a}}\right),$$

for $x \geqslant a$. Therefore,

$$\left|\sum_{n=1}^{\infty} r_f(n)\,\widehat{G}\left(\sqrt{\frac{4n}{D}}\right)\right| \ll \frac{D^{3/4}x^{1/4}}{a^{3/4}} + \frac{D^{1/2}x^{1/2}}{y^{1/2}}.$$

We now estimate the translated terms in (3.2.2). Let r, s be integers such that $0 \leqslant r,\, s < \ell$ and $(r,s) \neq (0,0)$. Let

$$B := \left\{(u,v) \in \mathbb{Z}^2 : f\left(u - \frac{r}{\ell}, v - \frac{s}{\ell}\right) < \frac{f(u,v)}{2}\right\} \cup \{(0,0)\}$$

be the set in the statement of Lemma 3.8 (with the point $(0,0)$ included). First, let us bound the sum over $(u,v) \in B$. We will use the fact that $f(u - r/\ell, v - s/\ell) \geqslant a/\ell^2$ for all $(u,v) \in \mathbb{Z}^2$, and Lemma 3.8. Then, recalling that $a \ll D^{1/2}$ and using (3.3.3), we see that

$$\sum_{(u,\,v)\in B}\left|\widehat{G}\left(\sqrt{\frac{4f(u-r/\ell, v-s/\ell)}{D}}\right)\right| \ll (\#B) \max_{(u,v)\in\mathbb{Z}^2}\left\{\frac{x^{1/4}D^{3/4}}{f(u-r/\ell, v-s/\ell)^{3/4}}\right\} \ll \frac{\ell^{3/2}D^{5/4}x^{1/4}}{a^{7/4}}.$$

We analyze the sum over $(u,v) \in B^c$, by splitting it once more into the sets $B^c \cap \{f(u,v) \leqslant z\}$ and $B^c \cap \{f(u,v) > z\}$. We estimate it using (3.3.3) as follows:

$$\begin{aligned}
&\sum_{(u,\,v)\in B^c}\left|\widehat{G}\left(\sqrt{\frac{4f(u-r/\ell, v-s/\ell)}{D}}\right)\right| \\
&\quad \ll \sum_{(u,\,v)\in B^c\cap\{f(u,v)\leqslant z\}} \frac{D^{3/4}x^{1/4}}{f(u-r/\ell, v-s/\ell)^{3/4}} + \sum_{(u,\,v)\in B^c\cap\{f(u,v)>z\}} \frac{D^{5/4}x^{3/4}}{y\, f(u-r/\ell, v-s/\ell)^{5/4}} \\
&\quad \ll D^{3/4}x^{1/4} \sum_{(u,\,v)\in B^c\cap\{f(u,v)\leqslant z\}} \frac{1}{f(u,v)^{3/4}} + \frac{D^{5/4}x^{3/4}}{y} \sum_{\{f(u,v)>z\}} \frac{1}{f(u,v)^{5/4}} \\
&\quad \ll D^{3/4}x^{1/4} \sum_{a\leqslant n\leqslant z} \frac{r_f(n)}{n^{3/4}} + \frac{D^{5/4}x^{3/4}}{y} \sum_{n>z} \frac{r_f(n)}{n^{5/4}} \ll \frac{D^{3/4}x^{1/4}}{a^{3/4}} + \frac{D^{1/2}x^{1/2}}{y^{1/2}}.
\end{aligned}$$

Therefore, since $G(0) = 0$, we combine all the terms in (3.2.2) to find, for $1 \leqslant y \leqslant x^{1/2}$,

$$\sum_{\substack{n=1\\ \ell\mid n}}^{\infty} r_f(n)\, G_{x,y}(\sqrt{n}) = \frac{2\pi}{\sqrt{D}}\,\widetilde{g}(\ell)\, x + O\left(\widetilde{g}(\ell)\left(\frac{\ell^{7/2}D^{3/4}x^{1/4}}{a^{7/4}} + \frac{\ell^2 x^{1/2}}{y^{1/2}} + \frac{y}{D^{1/2}}\right)\right), \tag{3.3.4}$$

where $\widetilde{g}(\ell)$ was defined in (3.2.3). Since $G_{x,y}(r) \geqslant 0$, we truncate the sum on the left-hand side of (3.3.4) over $1 \leqslant n \leqslant x$. Using the definition of G, this implies that

$$\sum_{\substack{1\leqslant n\leqslant x\\ \ell\mid n}} r_f(n) \leqslant \frac{2\pi}{\sqrt{D}}\,\widetilde{g}(\ell)\, x + O\left(\widetilde{g}(\ell)\left(\frac{\ell^{7/2}D^{3/4}x^{1/4}}{a^{7/4}} + \frac{\ell^2 x^{1/2}}{y^{1/2}} + \frac{y}{D^{1/2}}\right)\right). \tag{3.3.5}$$

To obtain the inverse inequality, we replace x by $x-y$ (in this case $1 \leqslant y \leqslant (x-y)^{1/2}$) in (3.3.4) and use the fact that

$$\sum_{\substack{n=1\\ \ell|n}}^{\infty} r_f(n)\, G_{x-y,y}(\sqrt{n}) = \sum_{\substack{1\leqslant n\leqslant x\\ \ell|n}} r_f(n)\, G_{x-y,y}(\sqrt{n}) \leqslant \sum_{\substack{1\leqslant n\leqslant x\\ \ell|n}} r_f(n).$$

This yields

$$\sum_{\substack{1\leqslant n\leqslant x\\ \ell|n}} r_f(n) \geqslant \frac{2\pi}{\sqrt{D}}\,\widetilde{g}(\ell)\,x + O\left(\widetilde{g}(\ell)\left(\frac{\ell^{7/2}D^{3/4}(x-y)^{1/4}}{a^{7/4}} + \frac{\ell^2(x-y)^{1/2}}{y^{1/2}} + \frac{y}{D^{1/2}}\right)\right). \tag{3.3.6}$$

Then, choosing $y = D^{1/3}x^{1/3}/2^{1/2}$ in (3.3.5) and (3.3.6), we conclude[8] that, for $x \geqslant D^2$

$$\sum_{\substack{1\leqslant n\leqslant x\\ \ell|n}} r_f(n) = \frac{2\pi}{\sqrt{D}}\,\widetilde{g}(\ell)\,x + O\left(\frac{\widetilde{g}(\ell)\,\ell^2 x^{1/3}}{D^{1/6}} + \frac{\widetilde{g}(\ell)\,\ell^{7/2}D^{3/4}x^{1/4}}{a^{7/4}}\right). \tag{3.3.7}$$

Now, if we compare the main terms in (3.3.1) and (3.3.7), we plainly see that $\widetilde{g}(\ell) = g(\ell)$ for any ℓ squarefree integer. Also note that, for each prime p, (3.3.2) implies that $|g(p)| \leqslant 2/p$. Since g is a multiplicative function, for a squarefree integer $\ell = p_1 \dots p_k$, we have

$$|\widetilde{g}(\ell)| = |g(\ell)| = |g(p_1 \dots p_k)| \leqslant \frac{2^k}{p_1 \dots p_k} = \frac{\tau(\ell)}{\ell}.$$

Inserting this estimate in the error term of (3.3.7), we conclude. □

Remark. We highlight that the asymptotic formula (3.1.2) in Theorem 3.1 holds for $x \geqslant D^2$. We can establish a similar result for $x \geqslant 3$, if we choose $y = x^{1/3}/2^{1/2}$ in the previous proof. Then, for $x \geqslant 3$,

$$\sum_{\substack{1\leqslant n\leqslant x\\ \ell|n}} r_f(n) = \frac{2\pi}{\sqrt{D}}\,g(\ell)\,x + O\left(\tau(\ell)\,\ell\,x^{1/3} + \frac{\tau(\ell)\,\ell^{5/2}D^{3/4}}{a^{7/4}}x^{1/4}\right).$$

Also note that the above formula can be extended to any primitive positive definite quadratic form, not necessarily reduced, by considering $a = 1$ in the error term.

3.4 Proof of Theorem 3.3

Let $f(u,v) = au^2+buv+cv^2$ be a reduced positive definite quadratic form of discriminant $-D$, and fix $0 < \varepsilon < 1/20$. To prove Theorem 3.3, we follow the idea developed in [109]. Let $\chi = \chi_{-D}(\cdot) := \left(\frac{-D}{\cdot}\right)$ denote the corresponding Kronecker symbol, which is a quadratic

[8] Note that, so far, $\ell \geqslant 1$ is not necessarily a squarefree integer. Using the estimate $|\widetilde{g}(\ell)| \leqslant 1$, we obtain a general version of Theorem 3.1.

Dirichlet character, and let $L(s,\chi)$ be the associated L-function. We remark that, in the ranges (3.1.7) and (3.1.8), using the fact that f is reduced, we have that $x \geqslant x-y \geqslant D^2$.

Let us define $w = \#\{(p,q,r,s) \in \mathbb{Z}^4 : ps-qr = 1 \text{ and } f(u,v) = f(pu+qv, ru+sv)\}$. By [105, p. 63 Satz 2], we have that $w=6$ when $D=3$, $w=4$ when $D=4$, and $w=2$ otherwise. This implies that, if p is a prime represented by f, then it is represented with multiplicity $\delta_f^{-1}w$, where δ_f is defined in (3.1.3). The number w is related to the class number $h(-D)$ through the class number formula (see [105, p. 72, Staz 5]):

$$h(-D) = \frac{w\sqrt{D}}{2\pi} L(1,\chi). \tag{3.4.1}$$

We start by dividing into cases, depending on the size of $L(1,\chi)$.

3.4.1 The case $L(1,\chi) \geqslant (\log y)^{-2}$

Let $z \geqslant 2$ be a parameter to be chosen later, and define $P = \prod_{p\leqslant z} p$. Then, one can see that

$$\frac{w}{\delta_f}\big(\pi_f(x) - \pi_f(x-y)\big) \leqslant \sum_{\substack{x-y<n\leqslant x\\(n,P)=1}} r_f(n) + \frac{w}{\delta_f}\pi(z). \tag{3.4.2}$$

Let us bound the sieved sum on the right-hand side of (3.4.2). For a squarefree integer $\ell \geqslant 1$, Theorem 3.1 gives us

$$\sum_{\substack{x-y<n\leqslant x\\ \ell | n}} r_f(n) = \frac{2\pi\, y}{\sqrt{D}}\, g(\ell) + E_\ell, \tag{3.4.3}$$

where

$$|E_\ell| \ll \frac{\tau(\ell)\,\ell}{D^{1/6}} x^{1/3} + \frac{\tau(\ell)\,\ell^{5/2} D^{3/4}}{a^{7/4}} x^{1/4}. \tag{3.4.4}$$

Then, (3.4.3) and a direct application of Selberg's upper bound sieve (see [44, Theorem 7.1 and Eq. (7.32)] with level of distribution z^2 give us

$$\sum_{\substack{x-y<n\leqslant x\\(n,P)=1}} r_f(n) \leqslant \frac{2\pi\, y}{\sqrt{D}}\, J^{-1} + \sum_{\substack{\ell | P\\ \ell<z^2}} \tau_3(\ell)|E_\ell|, \tag{3.4.5}$$

where $J = \sum_{\ell<z,\, \ell|P} h(\ell)$, and h is a multiplicative function defined by

$$h(\ell) = \prod_{p|\ell} \frac{g(p)}{1-g(p)}.$$

To bound the main term in (3.4.5), we treat g as a completely multiplicative function, to obtain (see [109, Eq. (8.8)])

$$J \geqslant \sum_{\ell<z} g(\ell). \tag{3.4.6}$$

To bound the sum on the right-hand side of (3.4.5), we use (3.4.4), and integration by parts with the estimate (see [79, Theorem 1])

$$\sum_{n\leqslant x} \tau_3(n)\tau(n) \ll x(\log x)^5.$$

It follows that

$$\begin{aligned}\sum_{\substack{\ell|P\\ \ell<z^2}} \tau_3(\ell)|E_\ell| &\ll \frac{x^{1/3}}{D^{1/6}} \sum_{\ell<z^2} \tau_3(\ell)\tau(\ell)\,\ell + \frac{D^{3/4}x^{1/4}}{a^{7/4}} \sum_{\ell<z^2} \tau_3(\ell)\tau(\ell)\,\ell^{5/2}\\ &\ll \frac{x^{1/3}z^4(\log z)^5}{D^{1/6}} + \frac{D^{3/4}x^{1/4}z^7(\log z)^5}{a^{7/4}}. \end{aligned}\tag{3.4.7}$$

We now combine (3.4.2), (3.4.5), (3.4.6), (3.4.7), the prime number theorem, and the fact that $x \geqslant D^2$. We obtain

$$\frac{w}{\delta_f}\big(\pi_f(x) - \pi_f(x-y)\big) \leqslant \frac{2\pi\, y}{\sqrt{D}\sum_{\ell<z} g(\ell)} + O\bigg(\frac{x^{1/3}z^4(\log z)^5}{D^{1/6}} + \frac{D^{3/4}x^{1/4}z^7(\log z)^5}{a^{7/4}}\bigg). \tag{3.4.8}$$

To analyze the main term in the right-hand side of (3.4.8), we use some bounds given in [109]. Combining Lemma 4.3, Lemma 4.4 and Lemma 8.2 of [109], for any fixed $0 < \varepsilon < 1/20$, it follows that

$$\sum_{\ell<z} g(\ell) \geqslant L(1,\chi)\log z - \left(\frac{1}{8} + \varepsilon\right)L(1,\chi)\log D + O\big(L(1,\chi) + z^{-\varepsilon^2/2}\big), \tag{3.4.9}$$

for any $z \geqslant 1$ such that $z \gg D^{1/4+\varepsilon}$.

The first range (3.1.7)

We recall that, in the range

$$\frac{D^2}{a}\,x^{1/3+\varepsilon} \leqslant y \leqslant x^{4/9},$$

we have $x \geqslant D^{18}/a^9 \geqslant D^{13}$, since f is reduced. Now, we choose

$$z = \frac{a^{1/4}y^{1/4}(\log y)^{-2}}{D^{5/24}x^{1/12}} + 2.$$

Note that $\log z \simeq \log y$. Then, from (3.4.8) we see that

$$\frac{w}{\delta_f}\big(\pi_f(x) - \pi_f(x-y)\big) \leqslant \frac{2\pi\, y}{\sqrt{D}\sum_{\ell<z} g(\ell)} + O\bigg(\frac{y}{\sqrt{D}(\log y)^3}\bigg).$$

Using the class number formula (3.4.1) and the well-known estimate $L(1,\chi) \ll \log D \ll \log y$, we get

$$\pi_f(x) - \pi_f(x-y) \leqslant \frac{\delta_f\, y}{h(-D)(L(1,\chi))^{-1}\sum_{\ell<z} g(\ell)} + O\bigg(\frac{\delta_f\, y}{h(-D)(\log y)^2}\bigg). \tag{3.4.10}$$

On the other hand, since $z \geqslant 1$ and $z \gg D^{1/4+\varepsilon/4}$, from (3.4.9) it follows that

$$\begin{aligned}
(L(1,\chi))^{-1}\sum_{\ell<z} g(\ell) &\geqslant \log z - \left(\frac{1}{8} + \frac{\varepsilon}{4}\right)\log D + O\big(1 + (\log y)^2 z^{-\varepsilon^2/32}\big)\\
&\geqslant \frac{1}{4}\log y - \frac{1}{12}\log x - \left(\frac{1}{3} + \frac{\varepsilon}{4}\right)\log D + \frac{1}{4}\log a + O(\log\log y)\\
&= \frac{1-\theta_1}{4}\log y + O(\log\log y),
\end{aligned}$$

where θ_1 is defined as

$$\theta_1 = \frac{\log x}{3\log y} + \left(\frac{4}{3} + \varepsilon\right)\frac{\log D}{\log y} - \frac{\log a}{\log y}.$$

One can see that $9\varepsilon/4 < 1 - \theta_1 < 1/4$. Therefore,

$$\frac{1}{(L(1,\chi))^{-1}\sum_{\ell<z} g(\ell)} \leqslant \frac{4}{(1-\theta_1)\log y}\bigg(1 + O\bigg(\frac{\log\log y}{\log y}\bigg)\bigg).$$

Inserting this in (3.4.10), we obtain the desired result.

The second range (3.1.8)

We recall that, in the range

$$x^{4/9} \leqslant y \leqslant x^{3/5},$$

we are assuming that $x \geqslant D^{18}$. Now, we choose

$$z = \frac{a^{1/4}\, y^{1/7}(\log y)^{-2}}{D^{5/24}x^{1/28}} + 2.$$

Note that $z \geqslant 1$, $z \gg D^{1/4+1/28}$ and $\log z \simeq \log y$. We proceed as in the previous case to obtain (3.4.10). Using (3.4.9), it follows that

$$
\begin{aligned}
(L(1,\chi))^{-1} \sum_{\ell<z} g(\ell) &\geqslant \frac{1}{7}\log y - \frac{1}{28}\log x - \frac{31}{84}\log D + \frac{1}{4}\log a + O(\log\log y) \\
&= \frac{1-\theta_2}{7}\log y + O(\log\log y),
\end{aligned}
$$

where θ_2 is defined by

$$
\theta_2 = \frac{\log x}{4\log y} + \frac{31}{12}\frac{\log D}{\log y} - \frac{7}{4}\frac{\log a}{\log y}.
$$

Then, $11/96 \leqslant 1-\theta_2 < 7/12$, and we obtain

$$
\frac{1}{(L(1,\chi))^{-1}\sum_{\ell<z} g(\ell)} \leqslant \frac{7}{(1-\theta_2)\log y}\left(1 + O\left(\frac{\log\log y}{\log y}\right)\right).
$$

Inserting this in (3.4.10), we obtain the desired result.

3.4.2 The case $L(1,\chi) < (\log y)^{-2}$

Applying Theorem 3.1 with $\ell = 1$, we have that

$$
\frac{w}{\delta_f}\big(\pi_f(x) - \pi_f(x-y)\big) \leqslant \sum_{x-y<n\leqslant x} r_f(n) = \frac{2\pi\, y}{\sqrt{D}} + O\left(\frac{x^{1/3}}{D^{1/6}} + \frac{D^{3/4}x^{1/4}}{a^{7/4}}\right).
$$

Then, using the class number formula (3.4.1) and the bound $L(1,\chi) < (\log y)^{-2}$, it follows that, in both ranges,

$$
\pi_f(x) - \pi_f(x-y) \leqslant \left\{1 + O\left(\frac{D^{1/3}x^{1/3}}{y}\right) + O\left(\frac{D^{5/4}x^{1/4}}{a^{7/4}y}\right)\right\}\frac{\delta_f\, y}{h(-D)}\, L(1,\chi) \ll \frac{y}{h(-D)(\log y)^2}.
$$

This implies our desired result in this case, and we conclude the proof of Theorem 3.3. $\square$

3.5 Hecke characters and Hecke L-functions

In this section, we will review the necessary background on Hecke L-functions, and their relation to quadratic forms, to prove Theorem 3.5.

3.5.1 From quadratic forms to ideals of quadratic fields

It is well-known that there is a bijection between equivalence classes of positive definite quadratic forms, and equivalence classes of certain ideals in imaginary quadratic fields (see [39, Section 7] and [105] for expositions). More precisely, let f be a positive definite primitive form of discriminant $-D$, and let $K = \mathbb{Q}(\sqrt{-D})$ be the associated imaginary quadratic field.

We can write

$$D = q^2 D_K, \tag{3.5.1}$$

where q is some positive integer and D_K is the absolute discriminant of K over $\mathbb{Q}$. To describe the classes of ideals that correspond to quadratic forms, we must first introduce some notation.[9] We follow Zaman's notation in [107] and [108].

Denote by N be the norm in K over $\mathbb{Q}$, and let $\mathfrak{q}$ be an integral ideal of K. Let $I(\mathfrak{q})$ be the group of fractional ideals of K relatively prime to $\mathfrak{q}$, and let $P_{\mathfrak{q}}$ be the group of principal ideals (α) of K such that α is positive and $\alpha \equiv 1 \,(\mathrm{mod}\, \mathfrak{q})$. Let

$$Cl(\mathfrak{q}) := I(\mathfrak{q})/P_{\mathfrak{q}} \tag{3.5.2}$$

be the narrow ray class group of K modulo $\mathfrak{q}$. Additionally, let H be a subgroup of $I(\mathfrak{q})$ such that

$$P_{\mathfrak{q}} \subset H \subset I(\mathfrak{q}). \tag{3.5.3}$$

For such an H, we call the quotient $I(\mathfrak{q})/H$ a congruence class group, and we denote by $h_H := |I(\mathfrak{q})/H|$ its cardinality. Note that $I(\mathfrak{q})/H \subset Cl(\mathfrak{q})$. In our setting for quadratic forms, we will mainly need the above with the principal ideal $\mathfrak{q} = (q)$, where q is given in (3.5.1); and with H_0 the group of principal ideals (α) of K such that $\alpha \equiv a \,(\mathrm{mod}\, \mathfrak{q})$, for some $a \in \mathbb{Z}$ with $((a), \mathfrak{q}) = 1$ (that is, with (a) and $\mathfrak{q}$ coprime). Note that $P_{\mathfrak{q}} \subset H_0 \subset I(\mathfrak{q})$. With this notation, we can state the equivalence between ideals and forms.

Lemma 3.9. *For each equivalence class of primitive positive definite quadratic forms $[f]$, there is a unique $A = A_f \in I(\mathfrak{q})/H_0$ such that, for any integer m, m is represented by f if and only if there is an integral ideal $\mathfrak{a} \in A$, with $\mathrm{N}\mathfrak{a} = m$. This correspondence is bijective.*

Proof. This follows from Theorem 7.7 and Proposition 7.22 of [39]. See also [39, pp. 144-145] for the slightly more general framework of congruence class groups that we use here. □

In particular, note that $h(-D) = h_{H_0} = |I(\mathfrak{q})/H_0|$, where $h(-D)$ is the number of proper equivalence classes of primitive quadratic forms of discriminant $-D$.

3.5.2 Hecke characters

We define a Hecke character $\chi \,(\mathrm{mod}\, \mathfrak{q})$ to be a character of the group $Cl(\mathfrak{q})$, which we defined in (3.5.2). Additionally, a character $\chi \,(\mathrm{mod}\, H)$ is a character of a congruence class group $I(\mathfrak{q})/H$. Given a Hecke character $\chi \,(\mathrm{mod}\, \mathfrak{q})$, abusing notation, we can extend the definition of χ to a multiplicative function over all integral ideals of K, such that $\chi(\mathfrak{n}) = 0$ when $(\mathfrak{n}, \mathfrak{q}) \neq 1$, and $\chi(\mathfrak{n}) = 1$ when $\mathfrak{n} \in P_{\mathfrak{q}}$. With this correspondence, the characters $\chi \,(\mathrm{mod}\, H)$ of a congruence class group correspond exactly to the Hecke characters mod $\mathfrak{q}$

[9] This notation and some of our subsequent results in this section, could be given for arbitrary algebraic number fields, as in [107]. However, for simplicity, we will only state the definitions and results in the case of imaginary quadratic fields, which is the case relevant to positive definite quadratic forms.

such that $\chi(\mathfrak{h}) = 1$, for all $\mathfrak{h} \in H$. From now on, we will work with this extended definition of Hecke characters, as functions over all integral ideals.

We denote the trivial character mod $\mathfrak{q}$ by χ_0, so that $\chi_0(\mathfrak{n}) = 1$ when $(\mathfrak{n}, \mathfrak{q}) = 1$, and 0 otherwise. Given a character $\chi \,(\mathrm{mod}\, \mathfrak{q})$, there is a unique $\mathfrak{f}_\chi \mid \mathfrak{q}$, the conductor of χ, such that χ is induced by a primitive character $\chi^* \,(\mathrm{mod}\, \mathfrak{f}_\chi)$. This implies that $\chi(\mathfrak{n}) = \chi^*(\mathfrak{n})\chi_0(\mathfrak{n})$. See, for instance, [107] for further background on Hecke characters. For any congruence class group, we also have the orthogonality relations (see [69, p. 44]): for all $A \in I(\mathfrak{q})/H$,

$$\sum_{\chi \,(\mathrm{mod}\, H)} \chi(A) = \begin{cases} h_H, & \text{if } A = H, \\ 0, & \text{if } A \neq H. \end{cases}$$

In particular, for an integral ideal $\mathfrak{a}$, we have that

$$\sum_{\chi \,(\mathrm{mod}\, H)} \overline{\chi(A)}\chi(\mathfrak{a}) = \begin{cases} h_H, & \text{if } \mathfrak{a} \in A, \\ 0, & \text{if } \mathfrak{a} \notin A. \end{cases} \tag{3.5.4}$$

3.5.3 The family of Hecke L-functions

Here, we describe the family of Hecke L-functions in the framework of [69, Chapter 5]. Below, we adopt the notation

$$\Gamma_{\mathbb{R}}(z) := \pi^{-z/2}\,\Gamma\left(\frac{z}{2}\right),$$

where Γ is the usual Gamma function. For a character $\chi \,(\mathrm{mod}\, \mathfrak{q})$, we define the function

$$L(s, \chi) := \sum_{\mathfrak{a}} \frac{\chi(\mathfrak{a})}{(N\mathfrak{a})^s} = \prod_{\mathfrak{p}} \left(1 - \frac{\chi(\mathfrak{p})}{(N\mathfrak{p})^s}\right)^{-1},$$

where the sum and the product runs over all integral ideals $\mathfrak{a}$ and prime ideals $\mathfrak{p}$ of K, respectively, and both converge absolutely to $L(s, \chi)$ on $\{s \in \mathbb{C}\,;\, \mathrm{Re}\, s > 1\}$. When χ is primitive, it is known that $L(s, \chi)$ satisfies the following conditions (see [69, p. 129] and [107, Section 2]):

(i) There exists a sequence $\{\lambda_\chi(n)\}_{n \geqslant 1}$ of complex numbers ($\lambda_\chi(1) = 1$), such that the series

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

converges absolutely to $L(s, \chi)$ on $\{s \in \mathbb{C}\,;\, \mathrm{Re}\, s > 1\}$. In fact, the sequence $\{\lambda_\chi(n)\}_{n \geqslant 1}$ is defined by

$$\lambda_\chi(n) = \sum_{\substack{\mathfrak{a} \\ \mathrm{N}\mathfrak{a} = n}} \chi(\mathfrak{a}).$$

(ii) For each prime number p, there exist $\alpha_{1,\chi}(p)$ and $\alpha_{2,\chi}(p)$ in $\mathbb{C}$, such that $|\alpha_{j,\chi}(p)| \leqslant 1$

and[10]

$$L(s,\chi) = \prod_p \left(1 - \frac{\alpha_{1,\chi}(p)}{p^s}\right)^{-1} \left(1 - \frac{\alpha_{2,\chi}(p)}{p^s}\right)^{-1}.$$

The product converges absolutely on the half plane $\{s \in \mathbb{C}; \operatorname{Re} s > 1\}$.

(iii) Denote $D_\chi := D_K \, \mathrm{N}\mathfrak{f}_\chi$. The completed L-function

$$\Lambda(s,\chi) := D_\chi^{s/2}\, \Gamma_{\mathbb{R}}(s)\, \Gamma_{\mathbb{R}}(s+1)\, L(s,\chi)$$

is a meromorphic function of order 1. It has no poles other than 0 and 1, which have the same order $r(\chi) \in \{0,1\}$. Additionally, $r(\chi) = 1$ if χ is the trivial character mod $\mathfrak{q}$, and 0 otherwise. Furthermore, the function $\Lambda(s,\chi)$ satisfies the the functional equation

$$\Lambda(s,\chi) = \epsilon(\chi)\Lambda(1-s,\overline{\chi}),$$

where $\epsilon(\chi)$ is a complex number of absolute value 1. In particular, when $\mathfrak{q} = (1)$ and $\chi = \chi_0$, the function $L(s,\chi_0)$ is the Dedekind zeta function $\zeta_K(s)$ of K, defined as in [69, Section 5.10]. Moreover, we have that

$$\frac{L'}{L}(s,\chi) = -\sum_{n=2}^{\infty} \frac{\Lambda_\chi(n)}{n^s}$$

converges absolutely for $\operatorname{Re} s > 1$, where[11]

$$\Lambda_\chi(n) = \sum_{\substack{\mathfrak{a} \\ \mathrm{N}\mathfrak{a}=n}} \chi(\mathfrak{a})\Lambda_K(\mathfrak{a}), \tag{3.5.5}$$

and

$$\Lambda_K(\mathfrak{a}) = \begin{cases} \log \mathrm{N}\mathfrak{p}, & \text{if } \mathfrak{a} = \mathfrak{p}^r \text{ for some integer } r \geqslant 1, \\ 0, & \text{otherwise.} \end{cases} \tag{3.5.6}$$

Logarithmically differentiating the Euler product, it can be shown that $|\Lambda_\chi(n)| \leqslant 2\Lambda(n)$, where $\Lambda(n)$ is the usual von Mangoldt function. In particular, one can see that

$$\sum_{\substack{\mathfrak{a} \\ \mathrm{N}\mathfrak{a}=n}} \Lambda_K(\mathfrak{a}) \leqslant 2\Lambda(n). \tag{3.5.7}$$

Remark. If $\chi \pmod{\mathfrak{q}}$ is a non-primitive character induced by the primitive character χ^* $\pmod{\mathfrak{f}_\chi}$, we have the relation

$$L(s,\chi) = L(s,\chi^*) \prod_{\mathfrak{p}|\mathfrak{q}} \left(1 - \frac{\chi^*(\mathfrak{p})}{(\mathrm{N}\mathfrak{p})^s}\right). \tag{3.5.8}$$

[10] This follows from the factorization law of primes in imaginary quadratic fields (see, for instance [69, p. 57]).

[11] We also extend this definition of Λ_χ to any function defined over integral ideals, in place of χ.

In particular, $L(s,\chi)$ also extends to a meromorphic function, such that $L(s,\chi)$ and $L(s,\chi^*)$ have the same set of zeros in the strip $0 < \operatorname{Re} s < 1$.

3.5.4 The Guinand-Weil formula

The classical Guinand-Weil explicit formula establishes a relationship between the zeros of an L-function, the associated coefficients $\Lambda_\chi(n)$ (given in this case in (3.5.5)), an arbitrary function G, and its Fourier transform $\widehat{G}$. In the case of a Hecke L-function $L(s,\chi)$, the coefficients $\Lambda_\chi(n)$ contain information about prime ideals, twisted by the character χ.

We will use the version of this formula in [21, Lemma 5]. However, this only applies to the case of a primitive Hecke character mod $\mathfrak{q}$, and we will need a version that averages over all characters, primitive and non-primitive, in a given congruence class group. The result is the following, which could be of independent interest for further applications.[12]

Lemma 3.10. *Let $\mathfrak{q}$ be an integral ideal of the imaginary quadratic field K. Let $I(\mathfrak{q})/H$ be a congruence class group as in* (3.5.3)*, and let $A \in I(\mathfrak{q})/H$. Let $G(s)$ be analytic in the strip $|\operatorname{Im} s| \leqslant \frac{1}{2} + \varepsilon$, for some $\varepsilon > 0$. Assume that $|G(s)| \ll (1+|s|)^{-(1+\delta)}$ for some $\delta > 0$, when $|\operatorname{Re} s| \to \infty$. Then*

$$\begin{aligned}
\sum_{\chi \,(\mathrm{mod}\, H)} \overline{\chi(A)} \sum_{\rho_\chi} G\left(\frac{\rho_\chi - \frac{1}{2}}{i}\right) &= G\left(\frac{1}{2i}\right) + G\left(-\frac{1}{2i}\right) \\
&\quad + \frac{h_H \kappa_H(A)}{\pi} \int_{-\infty}^{\infty} G(u) \left\{ \operatorname{Re} \frac{\Gamma'_{\mathbb{R}}}{\Gamma_{\mathbb{R}}} \left(\tfrac{1}{2} + iu\right) + \operatorname{Re} \frac{\Gamma'_{\mathbb{R}}}{\Gamma_{\mathbb{R}}} \left(\tfrac{3}{2} + iu\right) \right\} \mathrm{d}u \\
&\quad - \frac{h_H}{2\pi} \sum_{n=2}^{\infty} \frac{1}{\sqrt{n}} \widehat{G}\left(\frac{\log n}{2\pi}\right) \left\{ \sum_{\substack{\mathfrak{a} \in A \\ \mathrm{N}\mathfrak{a} = n}} \Lambda_K(\mathfrak{a}) \right\} \\
&\quad - \frac{1}{2\pi} \sum_{n=2}^{\infty} \frac{1}{\sqrt{n}} \widehat{G}\left(\frac{-\log n}{2\pi}\right) \left\{ \sum_{\chi \,(\mathrm{mod}\, H)} \overline{\chi(A) \Lambda_\chi(n)} \right\} \\
&\quad + O\left(h_H \log(D_K \mathrm{N}\mathfrak{q}) \|\widehat{G}\|_\infty\right),
\end{aligned}$$

where the sum over ρ_χ runs over all zeros of $L(s,\chi)$ in the strip $0 < \operatorname{Re} s < 1$. The coefficients $\Lambda_\chi(n)$ and $\Lambda_K(\mathfrak{a})$ are defined in (3.5.5)*; $\kappa_H(A) = 1$ when $A = H$, and 0 otherwise.*

Proof. We follow the approach used in [33, Lemma 3] for Dirichlet characters modulo $q \geqslant 3$. The Guinand-Weil formula in [21, Lemma 5], when specialized to $L(s,\chi)$ for a primitive

[12] Like the rest of this section, the previous lemma is only stated for the case of imaginary quadratic fields, to simplify the technical details of some of the definitions. However, a similar statement holds true for families of Hecke L-functions of arbitrary algebraic number fields, with a similar proof.

Hecke character $\chi\,(\mathrm{mod}\,\mathfrak{q})$, states the following:

$$\begin{aligned}\sum_{\rho_\chi} G\left(\frac{\rho_\chi-\frac{1}{2}}{i}\right) &= r(\chi)\left\{G\left(\frac{1}{2i}\right)+G\left(-\frac{1}{2i}\right)\right\}+\frac{\log D_\chi}{2\pi}\,\widehat{G}(0)\\ &\quad+\frac{1}{\pi}\int_{-\infty}^{\infty}G(u)\left\{\,\mathrm{Re}\,\frac{\Gamma_{\mathbb{R}}'}{\Gamma_{\mathbb{R}}}\left(\tfrac{1}{2}+iu\right)+\,\mathrm{Re}\,\frac{\Gamma_{\mathbb{R}}'}{\Gamma_{\mathbb{R}}}\left(\tfrac{3}{2}+iu\right)\right\}\mathrm{d}u \qquad (3.5.9)\\ &\quad-\frac{1}{2\pi}\sum_{n=2}^{\infty}\frac{1}{\sqrt{n}}\left\{\Lambda_\chi(n)\,\widehat{G}\left(\frac{\log n}{2\pi}\right)+\overline{\Lambda_\chi(n)}\,\widehat{G}\left(\frac{-\log n}{2\pi}\right)\right\},\end{aligned}$$

where the sum on the left-hand side runs over the zeros of $\Lambda(s,\chi)$, which coincide with the zeros of $L(s,\chi)$ in $0<\mathrm{Re}\,s<1$. Now, let χ be a non-primitive character mod $\mathfrak{q}$. Let $\chi^*\,(\mathrm{mod}\,\mathfrak{f}_\chi)$ be the unique primitive character that induces χ, where $\mathfrak{f}_\chi\,|\,\mathfrak{q}$, so that $\chi=\chi^*\chi_0$, where χ_0 is the trivial character mod $\mathfrak{q}$. We can then write $\chi^*(\mathfrak{a})=\chi(\mathfrak{a})+\chi^*(\mathfrak{a})\tilde{\chi}_0(\mathfrak{a})$, where $\tilde{\chi}_0(\mathfrak{a})=1-\chi_0(\mathfrak{a})$. Applying (3.5.9) for χ^*, it follows that

$$\begin{aligned}\sum_{\rho_{\chi^*}} G\left(\frac{\rho_{\chi^*}-\frac{1}{2}}{i}\right) &= r(\chi)\left\{G\left(\frac{1}{2i}\right)+G\left(-\frac{1}{2i}\right)\right\}+\frac{\log D_{\chi^*}}{2\pi}\,\widehat{G}(0)\\ &\quad+\frac{1}{\pi}\int_{-\infty}^{\infty}G(u)\left\{\,\mathrm{Re}\,\frac{\Gamma_{\mathbb{R}}'}{\Gamma_{\mathbb{R}}}\left(\tfrac{1}{2}+iu\right)+\,\mathrm{Re}\,\frac{\Gamma_{\mathbb{R}}'}{\Gamma_{\mathbb{R}}}\left(\tfrac{3}{2}+iu\right)\right\}\mathrm{d}u\\ &\quad-\frac{1}{2\pi}\sum_{n=2}^{\infty}\frac{1}{\sqrt{n}}\left\{\Lambda_\chi(n)\,\widehat{G}\left(\frac{\log n}{2\pi}\right)+\overline{\Lambda_\chi(n)}\,\widehat{G}\left(\frac{-\log n}{2\pi}\right)\right\}\\ &\quad-\frac{1}{2\pi}\sum_{n=2}^{\infty}\frac{1}{\sqrt{n}}\left\{\Lambda_{\chi^*\tilde{\chi}_0}(n)\,\widehat{G}\left(\frac{\log n}{2\pi}\right)+\overline{\Lambda_{\chi^*\tilde{\chi}_0}(n)}\,\widehat{G}\left(\frac{-\log n}{2\pi}\right)\right\}.\end{aligned}$$

Since $\tilde{\chi}_0(\mathfrak{a})=0$ when $\mathfrak{a}$ and $\mathfrak{q}$ are coprime, by Lemma 7.2, the last sum can be bounded by

$$\begin{aligned}\left|\frac{1}{2\pi}\sum_{n=2}^{\infty}\frac{1}{\sqrt{n}}\left\{\Lambda_{\chi^*\tilde{\chi}_0}(n)\,\widehat{G}\left(\frac{\log n}{2\pi}\right)+\overline{\Lambda_{\chi^*\tilde{\chi}_0}(n)}\,\widehat{G}\left(\frac{-\log n}{2\pi}\right)\right\}\right| &\ll \|\widehat{G}\|_\infty\sum_{\mathfrak{p}|\mathfrak{q},\,k\geqslant 1}\frac{\log \mathrm{N}\mathfrak{p}}{(\mathrm{N}\mathfrak{p})^{k/2}}\\ &\ll \|\widehat{G}\|_\infty\sqrt{\log(\mathrm{N}\mathfrak{q}+1)}.\end{aligned}$$

Letting $Q_H:=\max\{\mathrm{N}\mathfrak{f}_\chi:\,\chi\,(\mathrm{mod}\,H)\}$, note that

$$\log D_\chi\leqslant\log(D_K\,Q_H)\leqslant\log(D_K\,\mathrm{N}\mathfrak{q}).$$

By (3.5.8), $L(s,\chi)$ and $L(s,\chi^*)$ have the same zeros in $0<\mathrm{Re}\,s<1$. Then, for any non-primitive character $\chi\,(\mathrm{mod}\,H)$, we obtain that[13]

$$\begin{aligned}\sum_{\rho_\chi} G\left(\frac{\rho_\chi-\frac{1}{2}}{i}\right) &= r(\chi)\left\{G\left(\frac{1}{2i}\right)+G\left(-\frac{1}{2i}\right)\right\}\\ &\quad+\frac{1}{\pi}\int_{-\infty}^{\infty}G(u)\left\{\,\mathrm{Re}\,\frac{\Gamma_{\mathbb{R}}'}{\Gamma_{\mathbb{R}}}\left(\tfrac{1}{2}+iu\right)+\,\mathrm{Re}\,\frac{\Gamma_{\mathbb{R}}'}{\Gamma_{\mathbb{R}}}\left(\tfrac{3}{2}+iu\right)\right\}\mathrm{d}u\end{aligned}$$

[13]In fact, in this step we have the slightly better error term $\ll\big(\log(D_K\,Q_H)+\sqrt{\log\,(N\mathfrak{q}+1)}\big)\|\widehat{G}\|_\infty$.

$$
\begin{aligned}
&- \frac{1}{2\pi} \sum_{n=2}^{\infty} \frac{1}{\sqrt{n}} \left\{ \Lambda_\chi(n)\, \widehat{G}\left(\frac{\log n}{2\pi}\right) + \overline{\Lambda_\chi(n)}\, \widehat{G}\left(\frac{-\log n}{2\pi}\right) \right\} \\
&+ O\left(\log(D_K\, \mathrm{N}\mathfrak{q}) \|\widehat{G}\|_\infty\right).
\end{aligned}
$$

We now multiply by $\chi(A)$ and sum over all $\chi \,(\mathrm{mod}\, H)$. Using that $r(\chi) = 1$ if χ is the trivial character, and 0 otherwise, we get that

$$
\begin{aligned}
\sum_{\chi \,(\mathrm{mod}\, H)} \overline{\chi(A)} \sum_{\rho_\chi} G\left(\frac{\rho_\chi - \frac{1}{2}}{i}\right) &= G\left(\frac{1}{2i}\right) + G\left(-\frac{1}{2i}\right) \\
&+ \sum_{\chi \,(\mathrm{mod}\, H)} \overline{\chi(A)} \frac{1}{\pi} \int_{-\infty}^{\infty} G(u) \left\{ \mathrm{Re}\, \frac{\Gamma_{\mathbb{R}}'}{\Gamma_{\mathbb{R}}}\left(\tfrac{1}{2} + iu\right) + \mathrm{Re}\, \frac{\Gamma_{\mathbb{R}}'}{\Gamma_{\mathbb{R}}}\left(\tfrac{3}{2} + iu\right) \right\} du \\
&- \frac{1}{2\pi} \sum_{n=2}^{\infty} \frac{1}{\sqrt{n}} \widehat{G}\left(\frac{\log n}{2\pi}\right) \left\{ \sum_{\chi \,(\mathrm{mod}\, H)} \overline{\chi(A)} \Lambda_\chi(n) \right\} \\
&- \frac{1}{2\pi} \sum_{n=2}^{\infty} \frac{1}{\sqrt{n}} \widehat{G}\left(\frac{-\log n}{2\pi}\right) \left\{ \sum_{\chi \,(\mathrm{mod}\, H)} \overline{\chi(A) \Lambda_\chi(n)} \right\} \\
&+ O\left(h_H \log(D_K \mathrm{N}\mathfrak{q})\, \|\widehat{G}\|_\infty\right).
\end{aligned}
$$

Using (3.5.5), Fubini's theorem, and the orthogonality relations (3.5.4), we obtain the desired result. □

3.6 Proof of Theorem 3.5

We follow the argument of Carneiro, Milinovich, and Soundararajan in [22, Section 5]. To begin, fix a primitive positive definite quadratic form f of discriminant $-D$, and let $A \in I(\mathfrak{q})/H_0$ be the corresponding ideal class as in Lemma 3.9. Assume GRH for all Hecke L-functions associated with characters $\chi \,(\mathrm{mod}\, H_0)$. Furthermore, take a fixed even and bandlimited Schwartz function $F : \mathbb{R} \to \mathbb{R}$ such that $F(0) > 0$ and $\mathrm{supp}\,(\widehat{F}) \subset [-N, N]$, for some $N \geqslant 1$. We can extend F to an entire function, and using the Phragmén-Lindelöf principle, the hypotheses of Lemma 3.10 are satisfied. Let $0 < \Delta \leqslant 1$ and $1 < \sigma$ be free parameters, to be chosen later, such that

$$
2\pi \Delta N \leqslant \log \sigma.
$$

We remark that we will send $\sigma \to \infty$ and $\Delta \to 0$. In this section, we will allow all implicit constants to depend on the fixed quadratic form f, its discriminant, and the fixed function F, but not on the free parameters σ and Δ.

3.6.1 Asymptotic analysis

The following computations are similar to those in [22] and [33], so we highlight the differences. Consider the function $G(z) := \Delta F(\Delta z)\sigma^{iz}$. We apply Lemma 3.10 to G, with our specific choices of $\mathfrak{q}$, H_0 and A. This gives

$$\begin{aligned}
\sum_{\chi \,(\mathrm{mod}\, H_0)} \overline{\chi(A)} \sum_{\gamma_\chi} G(\gamma_\chi) = G\left(\frac{1}{2i}\right) + G\left(-\frac{1}{2i}\right) \\
+ \frac{h(-D)\kappa_{H_0}(A)}{\pi} \int_{-\infty}^{\infty} G(u) \left\{ \operatorname{Re} \frac{\Gamma'_{\mathbb{R}}}{\Gamma_{\mathbb{R}}}\left(\tfrac{1}{2}+iu\right) + \operatorname{Re} \frac{\Gamma'_{\mathbb{R}}}{\Gamma_{\mathbb{R}}}\left(\tfrac{3}{2}+iu\right) \right\} du \\
- \frac{h(-D)}{2\pi} \sum_{n=2}^{\infty} \frac{1}{\sqrt{n}} \widehat{G}\left(\frac{\log n}{2\pi}\right) \left\{ \sum_{\substack{\mathfrak{a} \in A \\ \mathrm{N}\mathfrak{a} = n}} \Lambda_K(\mathfrak{a}) \right\} \\
- \frac{1}{2\pi} \sum_{n=2}^{\infty} \frac{1}{\sqrt{n}} \widehat{G}\left(\frac{-\log n}{2\pi}\right) \left\{ \sum_{\chi \,(\mathrm{mod}\, H_0)} \overline{\chi(A)\Lambda_\chi(n)} \right\} + O(1),
\end{aligned} \tag{3.6.1}$$

where the inner sum on the left-hand side runs over the imaginary parts of the zeros of $L(s, \chi)$ on the line $\operatorname{Re} s = \frac{1}{2}$. The first, second, and fourth lines in the right-hand side of (3.6.1) can be estimated as in [22, pp. 553–554]. In this way, we obtain the following:

$$\begin{aligned}
\sum_{\chi \,(\mathrm{mod}\, H_0)} \overline{\chi(A)} \sum_{\gamma_\chi} G(\gamma_\chi) = \Delta F(0)\sqrt{\sigma} - \frac{h(-D)}{2\pi} \sum_{n=2}^{\infty} \frac{1}{\sqrt{n}} \widehat{G}\left(\frac{\log n}{2\pi}\right) \left\{ \sum_{\substack{\mathfrak{a} \in A \\ \mathrm{N}\mathfrak{a} = n}} \Lambda_K(\mathfrak{a}) \right\} \\
+ O\big(\Delta^2 \sqrt{\sigma}\big) + O(1).
\end{aligned}$$

Therefore,

$$\begin{aligned}
\Delta F(0)\sqrt{\sigma} \leqslant \sum_{\chi \,(\mathrm{mod}\, H_0)} \sum_{\gamma_\chi} \big|G(\gamma_\chi)\big| + \frac{h(-D)}{2\pi} \sum_{n=2}^{\infty} \frac{1}{\sqrt{n}} \widehat{G}\left(\frac{\log n}{2\pi}\right)_+ \left\{ \sum_{\substack{\mathfrak{a} \in A \\ \mathrm{N}\mathfrak{a} = n}} \Lambda_K(\mathfrak{a}) \right\} \\
+ O\big(\Delta^2 \sqrt{\sigma}\big) + O(1).
\end{aligned} \tag{3.6.2}$$

To analyze the first sum on the right-hand side of (3.6.2), we recall the formula [69, Theorem 5.8]

$$N(T, \chi) = \frac{T}{\pi} \log\left(\frac{D_\chi T^2}{(2\pi e)^2}\right) + O(\log T + \log D_\chi),$$

where $N(T, \chi)$ denotes the number of zeros of $L(s, \chi)$ in the rectangle $0 < \sigma < 1$ and $|\gamma| \leqslant T$. This holds for both primitive and non-primitive characters. Note that the term T^2 comes from the fact that K is an algebraic extension of $\mathbb{Q}$ of degree 2. For each $\chi \,(\mathrm{mod}\, H_0)$, integration by parts gives us (see [22, Eq. (5.4)]) that

$$\sum_{\gamma_\chi} |G(\gamma_\chi)| = \frac{\log(1/2\pi\Delta)}{\pi} \|F\|_1 + O(1).$$

Then,

$$\sum_{\chi \,(\mathrm{mod}\, H_0)} \sum_{\gamma_\chi} \big|G(\gamma_\chi)\big| = h(-D)\, \frac{\log(1/2\pi\Delta)}{\pi} \|F\|_1 + O(1). \tag{3.6.3}$$

3.6.2 From ideals to primes represented by f

We now consider the second sum on the right-hand side of (3.6.2). This sum is given by

$$\sum_{n=2}^{\infty} \frac{1}{\sqrt{n}}\, \widehat{G}\left(\frac{\log n}{2\pi}\right)_+ \left\{ \sum_{\substack{\mathfrak{a}\in A \\ \mathrm{N}\mathfrak{a}=n}} \Lambda_K(\mathfrak{a}) \right\} = \sum_{n=2}^{\infty} \frac{1}{\sqrt{n}}\, \widehat{F}\left(\frac{\log(n/\sigma)}{2\pi\Delta}\right)_+ \left\{ \sum_{\substack{\mathfrak{a}\in A \\ \mathrm{N}\mathfrak{a}=n}} \Lambda_K(\mathfrak{a}) \right\}. \tag{3.6.4}$$

We first make some reductions to the sum over n. Initially, since supp $(\widehat{F}) \subset [-N, N]$, the sum runs over $\sigma e^{-2\pi\Delta N} \leqslant n \leqslant \sigma e^{2\pi\Delta N}$. Note that the sum is supported over integers n that are (integer) prime powers, since Λ_K is supported on powers of prime ideals. Furthermore, by the relationship between ideals and forms (Lemma 3.9), the sum over n is actually supported over prime powers that are represented by f. Using (3.5.7), the contribution of the prime powers $n = p^k$, with $k \geqslant 2$, is $O(1)$. The sum (3.6.4) is therefore reduced, up to an error term $O(1)$, to a sum over primes p represented by f, such that $p \in [\sigma e^{-2\pi\Delta N}, \sigma e^{2\pi\Delta N}]$. Our version of the Brun-Titchmarsh theorem, Corollary 3.4, will be useful to estimate the contribution near the endpoints of this interval.

We continue by choosing the parameters Δ and σ, and bounding the corresponding contribution of the primes in the interval $(\sigma e^{-2\pi\Delta}, \sigma e^{2\pi\Delta}]$ to the sum (3.6.4). Fix $\alpha \geqslant 0$, and assume that $c > 0$ is a fixed constant such that

$$\liminf_{x\to\infty} \frac{\pi_f\big(x + c\sqrt{x}\log x\big) - \pi_f(x)}{\sqrt{x}} \leqslant \alpha.$$

Then, for any $\varepsilon > 0$, there exists a sequence of $x \to \infty$, such that there are at most $(\alpha+\varepsilon)\sqrt{x}$ primes represented by f in the interval $(x, x + c\sqrt{x}\log x]$. For each x in this sequence, we choose σ and Δ such that

$$\big[x, x + c\sqrt{x}\log x\big] = \Big[\sigma e^{-2\pi\Delta}, \sigma e^{2\pi\Delta}\Big].$$

This implies that (see [22, Eq. (5.7)-(5.8)])

$$4\pi\Delta = c\,\frac{\log x}{\sqrt{x}} + O\bigg(\frac{\log^2 x}{x}\bigg), \quad \text{and} \quad \sigma = x + O(\sqrt{x}\log x).$$

Note that $\delta_f = 1/2$ (defined in (3.1.3)) if and only if $A = \{\bar{\mathfrak{a}} : \mathfrak{a} \in A\}$. Using the factorization law of primes in imaginary quadratic fields [69, p. 57], we can plainly see that

$$\sum_{\substack{\mathfrak{a}\in A\\ \mathrm{N}\mathfrak{a}=p}} \Lambda_K(\mathfrak{a}) = \log p \sum_{\substack{\mathfrak{a}\in A\\ \mathrm{N}\mathfrak{a}=p}} 1 \leqslant \frac{\log p}{\delta_f}. \tag{3.6.5}$$

Using that $(\widehat{F}(t))_+ \leqslant \|F\|_1$ and (3.6.5), we bound the contribution in this interval by

$$\begin{aligned}\|F\|_1 \sum_{p\in(\sigma e^{-2\pi\Delta},\sigma e^{2\pi\Delta}]} \frac{1}{\sqrt{p}} \left\{\sum_{\substack{\mathfrak{a}\in A\\ \mathrm{N}\mathfrak{a}=p}} \Lambda_K(\mathfrak{a})\right\} &\leqslant \frac{\|F\|_1}{\delta_f} \sum_{p\in(\sigma e^{-2\pi\Delta},\sigma e^{2\pi\Delta}]} \frac{\log p}{\sqrt{p}} \\ &\leqslant \frac{\|F\|_1}{\delta_f}(\alpha+\varepsilon)\sqrt{x}\,\frac{\log x}{\sqrt{x}} = \frac{\|F\|_1}{\delta_f}(\alpha+\varepsilon)\log x.\end{aligned}$$

Finally, we estimate the contribution of the primes in the intervals $[\sigma e^{-2\pi\Delta N}, \sigma e^{-2\pi\Delta}]$ and $[\sigma e^{2\pi\Delta}, \sigma e^{2\pi\Delta N}]$. We will need the following estimate: for $g \in C^1([a,b])$ we have

$$0 \leqslant S(g_+, P) - \int_a^b (g(t))_+\, dt \leqslant \delta(b-a) \sup_{x\in[a,b]} |g'(x)|, \tag{3.6.6}$$

where P is a partition of $[a,b]$ of norm at most δ and $S(g_+, P)$ is the upper Riemann sum of the function g_+ and the partition P. We apply (3.6.6) with the function

$$g(t) = \widehat{F}\left(\frac{\log(t/\sigma)}{2\pi\Delta}\right),$$

and the partition $P = \{x_0 < \ldots < x_J\}$ that covers the interval $[\sigma e^{2\pi\Delta}, \sigma e^{2\pi\Delta N}] \subset \cup_{j=0}^{J-1}[x_j, x_{j+1}]$, with $x_0 = \sigma e^{2\pi\Delta}$, $x_{j+1} = x_j + \sqrt{x_j}$. Defining $M_j = \sup\{g^+(x) : x \in [x_j, x_{j+1}]\}$, by Corollary 3.4, (3.6.5), and (3.6.6) we bound the contribution in this interval as follows:[14]

$$\begin{aligned}&\sum_{1\leqslant \frac{\log p/\sigma}{2\pi\Delta}\leqslant N} \frac{1}{\sqrt{p}}\, \widehat{F}\left(\frac{\log(p/\sigma)}{2\pi\Delta}\right)_+ \left\{\sum_{\substack{\mathfrak{a}\in A\\ \mathrm{N}\mathfrak{a}=p}} \Lambda_K(\mathfrak{a})\right\} \\ &\quad\leqslant \frac{1}{\delta_f} \sum_{\substack{1\leqslant \frac{\log p/\sigma}{2\pi\Delta}\leqslant N\\ p \text{ represented by } f}} \widehat{F}\left(\frac{\log(p/\sigma)}{2\pi\Delta}\right)_+ \frac{\log p}{\sqrt{p}} \\ &\quad\leqslant \sum_{j=0}^{J-1}\left(\frac{\log x_j}{\sqrt{x_j}} M_j\right)\frac{(28+\varepsilon)\sqrt{x_j}}{h(-D)\log x_j} \leqslant \frac{(28+\varepsilon)\sqrt{\sigma}\,(2\pi\Delta)}{h(-D)} \int_1^N (\widehat{F}(t))_+\, \mathrm{d}t + O(1).\end{aligned}$$

[14] See [33, p. 7] for details in this computation.

We treat the other interval in a similar way. Combining the two intervals, we obtain

$$\sum_{1<\left|\frac{\log(p/\sigma)}{2\pi\Delta}\right|\leqslant N} \frac{1}{\sqrt{p}}\,(\widehat{F})_+\left(\frac{\log(p/\sigma)}{2\pi\Delta}\right)\left\{\sum_{\substack{\mathfrak{a}\in A\\ \mathrm{N}\mathfrak{a}=p}} \Lambda_K(\mathfrak{a})\right\} \leqslant \frac{(28+\varepsilon)\sqrt{\sigma}\,(2\pi\Delta)}{h(-D)}\int_{[-1,1]^c}(\widehat{F}(t))_+\,\mathrm{d}t + O(1).$$

Grouping the previous estimates, we conclude that

$$\sum_{n=2}^{\infty}\frac{1}{\sqrt{n}}\,(\widehat{G})_+\left(\frac{\log n}{2\pi}\right)\left\{\sum_{\substack{\mathfrak{a}\in A\\ \mathrm{N}\mathfrak{a}=n}} \Lambda_K(\mathfrak{a})\right\} \leqslant \frac{\|F\|_1}{\delta_f}(\alpha+\varepsilon)\log x + \frac{(28+\varepsilon)\sqrt{\sigma}\,(2\pi\Delta)}{h(-D)}\int_{[-1,1]^c}(\widehat{F}(t))_+\,\mathrm{d}t + O(1). \tag{3.6.7}$$

Then, inserting the estimates (3.6.3) and (3.6.7) in (3.6.2), and reordering the terms, we obtain

$$\sqrt{\sigma}\Delta\left(F(0)-(28+\varepsilon)\int_{[-1,1]^c}(\widehat{F}(t))_+\,\mathrm{d}t\right) \leqslant \frac{h(-D)\|F\|_1}{2\pi}\left[(\alpha+\varepsilon)\frac{\log x}{\delta_f}+2\log(1/2\pi\Delta)\right]+O(1).$$

Sending $x\to\infty$ along the sequence, and then sending $\varepsilon\to 0$, we obtain that

$$c \leqslant 2\frac{(\delta_f+\alpha)h(-D)}{\delta_f}\,\frac{\|F\|_1}{F(0)-28\int_{[-1,1]^c}(\widehat{F}(t))_+\,\mathrm{d}t}, \tag{3.6.8}$$

where we assume that the denominator is positive. By the approximation argument in [22, Section 4.1], equation (3.6.8) also holds for any even continuous function $F\in L^1(\mathbb{R})$, with the mentioned restriction on the denominator. Now we must find a suitable function F.

3.6.3 Construction of F

Inspired by Gorbachev's constructions in [63] for a related Fourier optimization problem (see also the remark in [22, p. 536]), we search numerically for optimal dilations of functions of the form

$$H(x)=\cos(2\pi x)\sum_{j=1}^{n}\frac{a_j}{(2j-1)^2-16x^2}. \tag{3.6.9}$$

Using a greedy algorithm, we found the function

$$F(x)=H\left(\frac{x}{0.98644}\right), \tag{3.6.10}$$

where

$$H(x) = \cos(2\pi x)\left(\frac{68}{1-16x^2} + \frac{5}{9-16x^2} + \frac{1}{25-16x^2}\right),$$

which, by numerical experiment,[15] gives

$$\frac{\|F\|_1}{F(0) - 28\int_{[-1,1]^c}(\widehat{F}(t))_+ \,\mathrm{d}t} < 0.91833. \tag{3.6.11}$$

Therefore, inserting it in (3.6.8) we conclude the desired result. □

3.7 Uncertainty and Fourier optimization

In this section, we discuss some qualitative aspects on the problem of choosing an optimal function F in (3.6.11). For $1 \leqslant A < \infty$, in [22] the authors introduced the functionals

$$J_A(F) := \frac{|F(0)| - A\int_{[-1,1]^c}|\widehat{F}(t)|\,\mathrm{d}t}{\|F\|_1}$$

and

$$J_A^+(F) := \frac{F(0) - A\int_{[-1,1]^c}(\widehat{F}(t))_+\,\mathrm{d}t}{\|F\|_1},$$

where F is a continuous function such that $F \in L^1(\mathbb{R})\backslash\{0\}$. They considered the following problems:

Extremal Problem 3.10.1. *Define $\mathcal{A}$ to be the class of continuous functions $F : \mathbb{R} \to \mathbb{C}$, with $F \in L^1(\mathbb{R})\backslash\{0\}$, and $\mathcal{E} = \{F \in \mathcal{A} : \operatorname{supp}\widehat{F} \subset [-1,1]\}$. Find*

$$\mathcal{C}(A) := \begin{cases} \sup\limits_{F\in\mathcal{A}} J_A(F), & \text{if } 1 \leqslant A < \infty; \\ \sup\limits_{F\in\mathcal{E}} \dfrac{|F(0)|}{\|F\|_1}, & \text{if } A = \infty. \end{cases}$$

Extremal Problem 3.10.2. *Define $\mathcal{A}^+$ to be the class of even and continuous functions $F : \mathbb{R} \to \mathbb{R}$, with $F \in L^1(\mathbb{R})\backslash\{0\}$, and $\mathcal{E}^+ = \{F \in \mathcal{A}^+ : \widehat{F}(t) \leqslant 0$ for $|t| \geqslant 1\}$. Find*

$$\mathcal{C}^+(A) := \begin{cases} \sup\limits_{F\in\mathcal{A}} J_A^+(F), & \text{if } 1 \leqslant A < \infty; \\ \sup\limits_{F\in\mathcal{E}^+} \dfrac{F(0)}{\|F\|_1}, & \text{if } A = \infty. \end{cases}$$

The authors show that, for all $1 \leqslant A \leqslant \infty$, we have $1 \leqslant \mathcal{C}(A) \leqslant \mathcal{C}^+(A) \leqslant 2$. The proof in Section 3.6 and an approximation argument ([22, Section 4.1]) show that, to optimize the value of the constant in Theorem 3.5, we must find $\mathcal{C}^+(28)$, where 28 is the constant in the Brun-Titchmarsh-type result given in Corollary 3.4.

[15] The bound 0.91833 in (3.6.11) was determined rigorously, using ball arithmetic with the ARB library.

One way to construct good functions for some Fourier optimization problems is to consider those of the form $F(x) = P(x)e^{-\pi x^2}$, where P is a polynomial. They were constructed in [33] via semidefinite programming. Note, however, that when $A = \infty$, these functions do not even belong to the family $\mathcal{E}$, as they are never bandlimited. Similarly, when $A \to \infty$, optimizing $J_A(F)$ requires an increasing concentration of the mass of $\widehat{F}$ in the interval $[-1, 1]$. For the same reason, by the uncertainty principle, we might expect that functions of the form $P(x)e^{-\pi x^2}$, when P has bounded degree, become inadequate as A grows, while bandlimited functions of the form (3.6.9), which give the best known bounds when $A = \infty$ (see [63]), become better. This qualitative observation can be formalized in the following way:

Proposition 3.11. *Let $n \geqslant 1$ be an integer. Let $\mathcal{F}_n$ be the class of functions of the form $P(x)e^{-\pi x^2}$, where $P \in \mathbb{R}[x]$ is a polynomial of degree at most n (not identically 0). Then, there exists $A_n > 1$, such that, for all $A \geqslant A_n$, we have*

$$\sup_{F \in \mathcal{F}_n} J_A(F) \leqslant 0.$$

In particular, for large A, polynomials of bounded degree times a gaussian are always far from the (positive) supremum.

Proof. Note that $\mathcal{F}_n \cup \{0\}$ is a vector space of dimension $n + 1$, and it is invariant under the Fourier transform. Clearly, for any interval $I \subset \mathbb{R}$, the function

$$(a_0, a_1, \ldots, a_n) \mapsto \int_I \left| \sum_{j=0}^{n} a_j x^j \right| e^{-\pi x^2} \, \mathrm{d}x$$

is a continuous function from $\mathbb{R}^{n+1}$ to $\mathbb{R}$, and homogeneous of degree 1. Therefore, by a compactness argument, there exists a function $F_0 \in \mathcal{F}_n$ that maximizes the quantity

$$D_n := \max_{F \in \mathcal{F}_n} \frac{\int_{-1}^{1} |F(x)| \, \mathrm{d}x}{\int_{\mathbb{R}} |F(x)| \, \mathrm{d}x} = \max_{F \in \mathcal{F}_n} \frac{\int_{-1}^{1} |\widehat{F}(t)| \, \mathrm{d}t}{\int_{\mathbb{R}} |\widehat{F}(t)| \, \mathrm{d}t}.$$

Since F_0 is not bandlimited, we have $0 < D_n < 1$. Additionally, note that, for $F \in \mathcal{F}_n$, we have

$$|F(0)| \leqslant \int_{\mathbb{R}} |\widehat{F}(t)| \, \mathrm{d}t \leqslant \frac{1}{1 - D_n} \int_{[-1,1]^c} |\widehat{F}(t)| \, \mathrm{d}t.$$

Therefore, for $A > \frac{1}{1-D_n}$, and $F \in \mathcal{F}_n$, we have $J_A(F) < 0$, and this implies the desired result. ☐

We conjecture that a similar behavior holds for the problem $\mathcal{C}^+(A)$, as $A \to \infty$. For instance, functions constructed by David de Laat[16] via semidefinite programming (applying the methods used in [33]), with polynomials of degree at most 122, imply the estimate

[16] Personal communication.

$\mathcal{C}^+(28) \geqslant 1.0865$. Meanwhile, the bandlimited function defined in (3.6.10) gives $\mathcal{C}^+(28) \geqslant 1.0889$.

In general, for some values[17] of A, Table 1 compares the lower bounds for $\mathcal{C}^+(A)$ that are obtained via semidefinite programming, with those obtained using bandlimited functions. The functions constructed via semidefinite programming (following [33, Section 4], and communicated by David de Laat) have the form $P(x)e^{-\pi x^2}$, where P is a polynomial of degree at most 82 or 122 (that is, functions in $\mathcal{F}_{82}$ or $\mathcal{F}_{122}$). On the other hand, the aforementioned bandlimited functions F are constructed as in (3.6.10) (that is, $F \in \mathcal{PW}$).[18] Table 2 gives the necessary parameters to define these functions. They have the form

$$F(x) = H\left(\frac{x}{\lambda}\right), \tag{3.7.1}$$

where

$$H(x) = \cos(2\pi x)\left(\frac{a_1}{1-16x^2} + \frac{a_2}{9-16x^2} + \frac{a_3}{25-16x^2}\right), \tag{3.7.2}$$

with $a_1, a_2, a_3 \in \mathbb{R}$. This gives strong evidence for the following conjecture:

Conjecture 3.12. *There exists an absolute $\varepsilon > 0$, such that the following holds: for $n \geqslant 1$ an integer, there exists $A_n^+ > 1$, such that, for $A \geqslant A_n^+$, we have*

$$\sup_{F \in \mathcal{F}_n} J_A^+(F) \leqslant \mathcal{C}^+(A) - \varepsilon.$$

However, proving it seems more subtle, and is related to the concentration of positive mass of a function, instead of total mass, similar to the sign uncertainty principles described in Chapter 2. In particular, a similar conjecture for the functions $P(x)e^{-\pi x^2}$ of bounded degree was stated in [35, Conjecture 3.2].

[17] From [22, Theorem 1.2], it is known that $\mathcal{C}^+(1)=2$, and we include our bounds for the sake of comparison. For the other values of A, our bounds in Table 1 slightly improve the general lower bounds obtained in [22, Theorem 1.2 and 1.3].

[18] The notation $\mathcal{PW}$ comes from the Paley-Wiener space.

A	$\mathcal{F}_{82}$	$\mathcal{F}_{122}$	$\mathcal{PW}$	A	$\mathcal{F}_{82}$	$\mathcal{F}_{122}$	$\mathcal{PW}$
1.0	1.9016	1.9307	1.9602	18.0	1.0893	1.0944	1.0931
1.5	1.4070	1.4089	1.3430	18.5	1.0887	1.0938	1.0928
2.0	1.2900	1.2933	1.2417	19.0	1.0881	1.0933	1.0925
2.5	1.2346	1.2378	1.1972	19.5	1.0875	1.0928	1.0922
3.0	1.2025	1.2049	1.1719	20.0	1.0870	1.0923	1.0919
3.5	1.1807	1.1830	1.1555	20.5	1.0865	1.0918	1.0917
4.0	1.1653	1.1673	1.1439	21.0	1.0860	1.0914	1.0914
4.5	1.1538	1.1555	1.1355	21.5	1.0856	1.0909	1.0912
5.0	1.1448	1.1467	1.1290	22.0	1.0852	1.0905	1.0909
5.5	1.1378	1.1396	1.1239	22.5	1.0848	1.0901	1.0907
6.0	1.1320	1.1339	1.1198	23.0	1.0845	1.0897	1.0905
6.5	1.1271	1.1294	1.1164	23.5	1.0841	1.0893	1.0903
7.0	1.1228	1.1255	1.1136	24.0	1.0838	1.0890	1.0901
7.5	1.1191	1.1222	1.1112	24.5	1.0835	1.0886	1.0900
8.0	1.1159	1.1192	1.1091	25.0	1.0832	1.0883	1.0898
8.5	1.1131	1.1166	1.1073	25.5	1.0830	1.0880	1.0896
9.0	1.1107	1.1142	1.1058	26.0	1.0827	1.0876	1.0895
9.5	1.1086	1.1121	1.1044	26.5	1.0825	1.0873	1.0893
10.0	1.1067	1.1101	1.1031	27.0	1.0823	1.0871	1.0892
10.5	1.1049	1.1084	1.1020	27.5	1.0820	1.0868	1.0890
11.0	1.1033	1.1068	1.1010	28.0	1.0818	1.0865	1.0889
11.5	1.1019	1.1054	1.1001	28.5	1.0816	1.0863	1.0888
12.0	1.1005	1.1041	1.0993	29.0	1.0814	1.0860	1.0886
12.5	1.0992	1.1030	1.0985	29.5	1.0812	1.0858	1.0885
13.0	1.0980	1.1019	1.0978	30.0	1.0810	1.0856	1.0884
13.5	1.0969	1.1009	1.0972	30.5	1.0809	1.0854	1.0883
14.0	1.0959	1.1000	1.0966	31.0	1.0807	1.0852	1.0882
14.5	1.0949	1.0992	1.0960	31.5	1.0805	1.0850	1.0881
15.0	1.0940	1.0984	1.0955	32.0	1.0804	1.0848	1.0880
15.5	1.0931	1.0976	1.0951	32.5	1.0802	1.0847	1.0879
16.0	1.0922	1.0969	1.0946	33.0	1.0800	1.0845	1.0878
16.5	1.0915	1.0962	1.0942	33.5	1.0799	1.0844	1.0877
17.0	1.0907	1.0956	1.0938	34.0	1.0797	1.0842	1.0876
17.5	1.0900	1.0950	1.0935	34.5	1.0796	1.0841	1.0875

Table 3.1: Table of lower bounds for $\mathcal{C}^+(A)$ via semidefinite programming and bandlimited functions.

A	$\mathcal{C}^+(A)$	$\{a_1, a_2, a_3\}$	λ	A	$\mathcal{C}^+(A)$	$\{a_1, a_2, a_3\}$	λ
1.0	1.9602	{81, -69, 0}	0.100000	18.0	1.0931	{297, 18, 1}	0.977220
1.5	1.3430	{189, -63, -20}	0.660234	18.5	1.0928	{297, 18, 1}	0.977843
2.0	1.2417	{243, -57, -20}	0.765530	19.0	1.0925	{270, 18, 1}	0.978433
2.5	1.1972	{216, -39, -20}	0.819517	19.5	1.0922	{270, 18, 1}	0.978992
3.0	1.1719	{216, -27, -20}	0.852929	20.0	1.0919	{270, 18, 1}	0.979523
3.5	1.1555	{216, -18, -20}	0.875775	20.5	1.0917	{270, 18, 2}	0.980027
4.0	1.1439	{243, -15, -20}	0.892422	21.0	1.0914	{270, 18, 2}	0.980508
4.5	1.1355	{270, -9, -20}	0.905109	21.5	1.0912	{270, 18, 2}	0.980966
5.0	1.1290	{297, -6, -20}	0.915104	22.0	1.0909	{270, 18, 2}	0.981402
5.5	1.1239	{324, -3, -20}	0.923186	22.5	1.0907	{270, 18, 2}	0.981820
6.0	1.1198	{378, 0, -20}	0.929858	23.0	1.0905	{270, 18, 2}	0.982219
6.5	1.1164	{405, 3, -20}	0.935461	23.5	1.0903	{270, 18, 2}	0.982600
7.0	1.1136	{243, 3, -10}	0.940232	24.0	1.0901	{270, 18, 3}	0.982966
7.5	1.1112	{297, 6, -12}	0.944345	24.5	1.0900	{243, 18, 2}	0.983317
8.0	1.1091	{270, 6, -9}	0.947928	25.0	1.0898	{243, 18, 3}	0.983653
8.5	1.1073	{216, 6, -7}	0.951076	25.5	1.0896	{243, 18, 3}	0.983976
9.0	1.1058	{297, 9, -8}	0.953865	26.0	1.0895	{243, 18, 3}	0.984287
9.5	1.1044	{270, 9, -7}	0.956353	26.5	1.0893	{297, 21, 4}	0.984586
10.0	1.1031	{243, 9, -5}	0.958586	27.0	1.0892	{297, 21, 4}	0.984874
10.5	1.1020	{297, 12, -6}	0.960601	27.5	1.0890	{297, 21, 4}	0.985151
11.0	1.1010	{270, 12, -5}	0.962429	28.0	1.0889	{68, 5, 1}	0.986440
11.5	1.1001	{270, 12, -4}	0.964095	28.5	1.0888	{297, 21, 4}	0.985676
12.0	1.0993	{243, 12, -3}	0.965619	29.0	1.0886	{297, 21, 4}	0.985924
12.5	1.0985	{243, 12, -3}	0.967019	29.5	1.0885	{297, 21, 4}	0.986165
13.0	1.0978	{297, 15, -3}	0.968309	30.0	1.0884	{270, 21, 4}	0.986397
13.5	1.0972	{297, 15, -2}	0.969502	30.5	1.0883	{270, 21, 4}	0.986622
14.0	1.0966	{270, 15, -2}	0.970609	31.0	1.0882	{270, 21, 4}	0.986839
14.5	1.0960	{270, 15, -1}	0.971638	31.5	1.0881	{270, 21, 4}	0.987049
15.0	1.0955	{270, 15, -1}	0.972597	32.0	1.0880	{270, 21, 4}	0.987253
15.5	1.0951	{270, 15, -1}	0.973494	32.5	1.0879	{270, 21 ,4}	0.987450
16.0	1.0946	{243, 15, 0}	0.974334	33.0	1.0878	{270, 21, 4}	0.987642
16.5	1.0942	{243, 15, 0}	0.975122	33.5	1.0877	{270, 21, 4}	0.987827
17.0	1.0938	{243, 15, 0}	0.975863	34.0	1.0876	{270, 21, 4}	0.988007
17.5	1.0935	{297, 18, 0}	0.976561	34.5	1.0875	{270, 21, 4}	0.988182

Table 3.2: Table of lower bounds for $\mathcal{C}^+(A)$ via bandlimited functions, with the corresponding parameters as defined in (3.7.1) and (3.7.2).

Chapter 4

The Riemann zeta-function: the antiderivatives of its argument

This chapter is comprised of the paper [A3]. Our goal, as explained in Section 1.3.5, is to obtain an asymptotic expression for the second moment of the antiderivatives of $S(t)$, up to the second-order term.

4.1 Introduction

Recall that $N(t)$ was defined in Section 1.3.1, and the Riemann von-Mangoldt formula in (1.3.2) states that

$$N(t) = \frac{t}{2\pi}\log\frac{t}{2\pi} - \frac{t}{2\pi} + \frac{7}{8} + S(t) + O\left(\frac{1}{t}\right).$$

To understand the distribution of the zeros of $\zeta(s)$, the formula (1.3.2) has led to studying the oscillatory character of $S(t)$. J. E. Littlewood [76, 77] and A. Selberg [93, 94] investigated the behavior and the power of the cancellation in $S(t)$ using its antiderivatives $S_n(t)$. Setting $S_0(t) = S(t)$ we define, for $n \geqslant 1$ an integer and $t > 0$,

$$S_n(t) = \int_0^t S_{n-1}(\tau)\,\mathrm{d}\tau\, + \delta_n\,,$$

where δ_n is a specific constant depending on n. These are given by

$$\delta_{2k-1} = \frac{(-1)^{k-1}}{\pi}\int_{1/2}^{\infty}\int_{\sigma_{2k-2}}^{\infty}\cdots\int_{\sigma_2}^{\infty}\int_{\sigma_1}^{\infty}\log|\zeta(\sigma_0)|\,\mathrm{d}\sigma_0\,\mathrm{d}\sigma_1\,\ldots\,\mathrm{d}\sigma_{2k-2}$$

for $n = 2k-1$, with $k \geqslant 1$, and

$$\delta_{2k} = (-1)^{k-1}\int_{1/2}^{1}\int_{\sigma_{2k-1}}^{1}\cdots\int_{\sigma_2}^{1}\int_{\sigma_1}^{1}\mathrm{d}\sigma_0\,\mathrm{d}\sigma_1\,\ldots\,\mathrm{d}\sigma_{2k-1} = \frac{(-1)^{k-1}}{(2k)!\cdot 2^{2k}}$$

for $n = 2k$, with $k \geqslant 1$.

Let us recall some estimates for $S_n(t)$. In 1924, assuming the RH, Littlewood [76, Theorem 11] established the bounds

$$S_n(t) = O_n\left(\frac{\log t}{(\log\log t)^{n+1}}\right), \tag{4.1.1}$$

for $n \geqslant 0$. The order of magnitude in (4.1.1) has never been improved, and efforts have thus been concentrated in optimizing the values of the implicit constants. The best known versions of these results are due to Carneiro, Chandee and Milinovich [18] for $n = 0$ and $n = 1$, and Carneiro and Chirre [19] for $n \geqslant 2$ (see also [20, Theorem 2] for a refinement in the error term). In the other direction, Selberg [93] and Littlewood [77] first studied the largest positive and negative values of $S_n(t)$. These have also been the subject of recent research, with improvements for $S(t)$ and $S_1(t)$ in the work of Bondarenko and Seip [11]. Further refinements for $S_n(t)$ were obtained by Chirre and Mahatab [32] (see also [29] and [31]).

4.1.1 The second moment of $S_n(t)$

The next step to understand the behavior of the function $S_n(t)$ is to obtain an asymptotic formula for its moments. In this chapter we will concentrate on the second moment.

In 1925, assuming RH, Littlewood [77, Theorem 9] proved for $n \geqslant 1$ that

$$\int_0^T |S_n(t)|^2 \,\mathrm{d}t = O(T). \tag{4.1.2}$$

A few years later, in 1928, Titchmarsh [101, Theorem II] gave the first explicit version of the above result, for $n = 1$, establishing that

$$\int_0^T |S_1(t)|^2 \,\mathrm{d}t \sim \frac{C_1}{2\pi^2}\,T,$$

where

$$C_1 = \sum_{m=2}^{\infty} \frac{\Lambda^2(m)}{m\,(\log m)^4}.$$

Here, $\Lambda(m)$ is the von-Mangoldt function, which is defined to be $\log p$ if $m = p^k$ (for some prime number p and integer $k \geqslant 1$), and zero otherwise. Unconditionally, in 1946 Selberg [94, Theorems 6 and 7] established that

$$\int_0^T |S(t)|^2 \,\mathrm{d}t = \frac{T}{2\pi^2}\,\log\log T + O(T\sqrt{\log\log T}), \tag{4.1.3}$$

and[1]

$$\int_0^T |S_1(t)|^2 \, \mathrm{d}t = \frac{C_1}{2\pi^2}\, T + O\left(\frac{T}{\log T}\right). \tag{4.1.4}$$

Assuming RH, Selberg [93] had proved (4.1.3) with the error term $O(T)$. Going even further, he computed all even moments for $S(t)$ and $S_1(t)$. Using these even moments for $S(t)$, Ghosh [51, 52] obtained the asymptotic behavior for all moments of $|S(t)|^\lambda$, with $\lambda > -1$. Furthermore, Fujii [49] established, assuming RH,

$$\int_0^T |S_n(t)|^2 \, \mathrm{d}t = \frac{C_n}{2\pi^2}\, T + O\left(\frac{T}{\log T}\right), \tag{4.1.5}$$

for $n \geqslant 2$, where C_n is defined in (4.1.6).

Our main result in this section is an explicit version of (4.1.2) up to the second-order term, extending the result of Goldston (1.3.10) for the cases $n \geqslant 1$. In particular, we obtain refinements of (4.1.4) and (4.1.5), under RH. Note that our second-order term improves the error terms in (4.1.4) and (4.1.5). Our main result is Theorem 1.3, which we restate here for the reader's convenience:

Theorem 4.1. *Let $n \geqslant 1$ be an integer. Assume the Riemann hypothesis. Then*

$$\int_0^T |S_n(t)|^2 \, \mathrm{d}t = \frac{C_n}{2\pi^2}\, T + \frac{T}{2\pi^2\,(\log T)^{2n}}\left[\int_1^\infty \frac{F(\alpha)}{\alpha^{2n+2}}\,\mathrm{d}\alpha - \frac{1}{2n}\right] + O\left(\frac{T\sqrt{\log\log T}}{(\log T)^{2n+1/2}}\right),$$

as $T \to \infty$, where

$$C_n = \sum_{m=2}^{\infty} \frac{\Lambda^2(m)}{m\,(\log m)^{2n+2}}. \tag{4.1.6}$$

Let us analyze the constants that appear on Theorem 4.1. We highlight that $C_n \to \infty$ when $n \to \infty$. In fact, the growth of these constants is exponential (see Section 4.5), of order

$$C_n \sim \frac{1}{2(\log 2)^{2n}}.$$

Table 1 puts in perspective the constant that appears in front of the first-order term, in the small cases $1 \leqslant n \leqslant 10$. For the second-order term, by following Goldston's argument using [53, Lemma A], it is straightforward to obtain upper and lower bounds for the integral in the second-order term of Theorem 4.1. For any $n \geqslant 1$ we get[2]

$$\frac{2}{3^{2n+3}} - \varepsilon \leqslant \int_1^\infty \frac{F(\alpha)}{\alpha^{2n+2}}\,\mathrm{d}\alpha \leqslant \frac{8}{3}\,\zeta(2n+2) + \varepsilon, \tag{4.1.7}$$

[1] In [94], Selberg actually calculated the second moment for the function $S_1(t) - \delta_1$. His formula can be used to deduce (4.1.4), by using the unconditional estimate for $S_2(t)$ given by Fujii [48, Theorem 2].

[2] The constants in (4.1.7) may be slightly improved. However, this is far from the expected behavior suggested by the strong pair correlation conjecture [81], and it seems difficult to obtain anything qualitatively closer.

n	$C_n/2\pi^2$	n	$C_n/2\pi^2$
1	0.079290...	6	2.064933...
2	0.124743...	7	4.290884...
3	0.239241...	8	8.925169...
4	0.483838...	9	18.571837...
5	0.996243...	10	38.650937...

Table 4.1: Values for $1 \leqslant n \leqslant 10$.

for any $\varepsilon > 0$ and T sufficiently large. This implies that the second-order term in Theorem 4.1 has the growth $T/(\log T)^{2n}$. We highlight that this term has a decreasing order of magnitude as n grows. Furthermore, assuming the pair correlation conjecture in the form (1.3.13), and using integration by parts, we find, as $T \to \infty$

$$\int_1^{\infty} \frac{F(\alpha)}{\alpha^{2n+2}}\,\mathrm{d}\alpha = \frac{1}{2n+1} + o(1).$$

Corollary 4.2. *Let $n \geqslant 1$ be an integer. Assume the Riemann hypothesis and the pair correlation conjecture* (1.3.13)*. Then*

$$\int_0^T |S_n(t)|^2\,\mathrm{d}t = \frac{C_n}{2\pi^2}\,T - \frac{T}{4n(2n+1)\pi^2\,(\log T)^{2n}} + o\bigg(\frac{T}{(\log T)^{2n}}\bigg),$$

as $T \to \infty$, where C_n was defined in (4.1.6)*.*

4.1.2 Outline of the proof

Our proof follows the ideas developed by Goldston in [53], and involves additional technical challenges. In Section 4.2, we start by obtaining a new representation formula for $S_n(t)$, for $n \geqslant 1$, associated with a suitable real-valued function f_n. For each $n \geqslant 1$ define the function $f_n : (0,2) \to \mathbb{R}$ as follows:

$$f_n(x) = \frac{x^{n+1}}{n!} \int_0^{\infty} y^n \frac{2\sinh\big(y(1-x)\big)}{\big(e^y + (-1)^{n+1}e^{-y}\big)}\,\mathrm{d}y. \tag{4.1.8}$$

To get the desired formula for $S_n(t)$, we combine an explicit formula due to Montgomery [81] with an expression for $S_n(t)$ implicit in the work of Fujii [48] (see also [19, Lemma 2]) that depends on the logarithmic derivative of $\zeta(s)$. Our formula relates $S_n(t)$ to a Dirichlet polynomial over primes involved with the function f_n, a sum over the zeros of the Riemann zeta-function, and a few extra terms that depend on the parity of n. By squaring and integrating, we obtain an expression for the second moment of $S_n(t)$. Using the asymptotic behavior of each term in this expression, we obtain Theorem 4.1. These asymptotic formulas will be obtained in the following sections. We highlight that some of the additional technical difficulties come from controlling both the imaginary and real parts of the logarithm of $\zeta(s)$, which will have repercussions throughout this chapter.

In Section 4.3, we analyze the second moment of the sum over the zeros of the Riemann zeta-function. Following Goldston, we use the ideas developed by Montgomery [81] to express sums over pairs of zeros of $\zeta(s)$ in terms of the function $F(\alpha)$ defined in (1.3.5). In Section 4.4, we analyze the terms associated with the sum over primes. Here, we use an argument of Titchmarsh [101] in the estimate of certain integrals involving $S_n(t)$ with oscillatory functions, which have some peculiarities when $n \geqslant 1$. Combining the terms in an appropriate way and using properties of f_n, we can take advantage of a surprising cancellation in our analysis. Finally, in Section 4.5, we analyze the constants C_n numerically using some estimates of sums with prime numbers that could be of independent interest.

4.2 The representation for the second moment of $S_n(t)$

4.2.1 Representation lemma for $S_n(t)$

We start by obtaining a new representation for the functions $S_n(t)$ for $n \geqslant 1$. This representation connects $S_n(t)$ with the zeros of the Riemann zeta-function and the prime numbers.

Lemma 4.3. *For each fixed $n \geqslant 1$ let $f_n : \mathbb{R} \to \mathbb{R}$ be defined as in* (4.1.8). *Assume the Riemann hypothesis. Then, for $t \geqslant 1$ and $x \geqslant 4$, we have:*

$$\begin{aligned} S_n(t) = &\frac{1}{\pi n!\,(\log x)^n} \sum_{\gamma} \operatorname{Im}\{i^{n+2} e^{i(\gamma-t)\log x}\} \int_0^\infty \frac{y^{n+1}}{y^2 + ((\gamma-t)\log x)^2} \frac{2}{e^y + (-1)^{n+1}e^{-y}}\,\mathrm{d}y \\ &+ \frac{1}{\pi} \sum_{2\leqslant m\leqslant x} \operatorname{Im}\{i^n m^{-it}\} \frac{\Lambda(m)}{\sqrt{m}(\log m)^{n+1}}\, f_n\!\left(\frac{\log m}{\log x}\right) \\ &+ \mu_n\, \frac{\operatorname{Im}\{i^n\}}{\pi(\log x)^{n+1}} \log\frac{t}{2\pi} + O\!\left(\frac{\sqrt{x}}{t\,(\log x)^{n+2}}\right), \end{aligned} \tag{4.2.1}$$

where the first sum runs over the ordinates of the non-trivial zeros of $\zeta(s)$, and $\mu_n = 2^{-n-1}(1-2^{-n})\zeta(n+1)$ when n is odd, and zero otherwise.

Proof. Assuming RH, by [19, Lemma 2], we have for $n \geqslant 1$ that

$$S_n(t) = -\frac{1}{\pi} \operatorname{Im}\left\{ \frac{i^n}{n!} \int_{1/2}^\infty (\sigma - 1/2)^n \, \frac{\zeta'}{\zeta}(\sigma + it)\,\mathrm{d}\sigma \right\}. \tag{4.2.2}$$

Let us analyze the integrand in the above expression. By an explicit formula of Montgomery (see [53, Eq. (2.1) and p. 155]), for $x \geqslant 4$ and $s = \sigma + it$ with $\sigma > \frac{1}{2}$ and $t \geqslant 1$, it follows that

$$x^{\sigma-1/2}\frac{\zeta'}{\zeta}(\sigma+it)-x^{1/2-\sigma}\frac{\zeta'}{\zeta}(1-\sigma+it)$$
$$=(2\sigma-1)\sum_{\gamma}\frac{x^{i(\gamma-t)}}{(\sigma-1/2)^2+(\gamma-t)^2}-\sum_{m\leqslant x}\frac{\Lambda(m)}{m^{it}}\left(\frac{x^{\sigma-1/2}}{m^{\sigma}}-\frac{x^{1/2-\sigma}}{m^{1-\sigma}}\right)$$
$$+x^{1/2-it}\left(\frac{2\sigma-1}{(\sigma-it)(1-\sigma-it)}\right)+O\left(\frac{x^{-5/2}(\sigma-1/2)}{t}\right). \tag{4.2.3}$$

First, we need a relationship between $\frac{\zeta'}{\zeta}(\sigma+it)$ and $\frac{\zeta'}{\zeta}(1-\sigma+it)$ in the above formula. Using the functional equation of $\zeta(s)$ in the form $\zeta(1-s)=\pi^{-s}2^{1-s}\cos(\pi s/2)\,\Gamma(s)\zeta(s)$, the reflection principle, Stirling's formula and the bound $|\mathrm{Re}\,\{\tan s\}|\ll e^{-2\,\mathrm{Im}\,s}$ for $|\mathrm{Im}\,s|\geqslant 1$, we obtain for $t\geqslant 1$ and $\sigma>\frac{1}{2}$:

$$\mathrm{Re}\,\frac{\zeta'}{\zeta}(1-\sigma+it)=-\mathrm{Re}\,\frac{\zeta'}{\zeta}(\sigma+it)-\log\frac{t}{2\pi}+O\left(\frac{\sigma^2}{t}\right). \tag{4.2.4}$$

By [53, Eq. (2.3)] we also get

$$\mathrm{Im}\,\frac{\zeta'}{\zeta}(1-\sigma+it)=\mathrm{Im}\,\frac{\zeta'}{\zeta}(\sigma+it)+O\left(\frac{\sigma-1/2}{t}\right). \tag{4.2.5}$$

Then, combining (4.2.4) and (4.2.5), we obtain

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

Inserting it into (4.2.3) and ordering conveniently, one can see that

$$\left(x^{\sigma-1/2}+(-1)^{n+1}x^{1/2-\sigma}\right)\frac{\zeta'}{\zeta}(\sigma+it)$$
$$=-x^{1/2-\sigma}\left((-1)^n\frac{\zeta'}{\zeta}(\sigma+it)+\overline{\frac{\zeta'}{\zeta}(\sigma+it)}\right)$$
$$+(2\sigma-1)\sum_{\gamma}\frac{x^{i(\gamma-t)}}{(\sigma-1/2)^2+(\gamma-t)^2}-\sum_{m\leqslant x}\frac{\Lambda(m)}{m^{it}}\left(\frac{x^{\sigma-1/2}}{m^{\sigma}}-\frac{x^{1/2-\sigma}}{m^{1-\sigma}}\right)$$
$$-x^{1/2-\sigma}\log\frac{t}{2\pi}+x^{1/2-it}\left(\frac{2\sigma-1}{(\sigma-it)(1-\sigma-it)}\right)+O\left(\frac{\sigma^2}{t}\left(x^{-5/2}+x^{1/2-\sigma}\right)\right). \tag{4.2.6}$$

Dividing the above expression by $C_n(\sigma):=x^{\sigma-1/2}+(-1)^{n+1}x^{1/2-\sigma}$ and inserting it into (4.2.2), we get

$$S_n(t)=\frac{1}{\pi n!}\int_{1/2}^{\infty}\frac{(\sigma-1/2)^n}{C_n(\sigma)}\,\mathrm{Im}\left\{i^n\left((-1)^n\frac{\zeta'}{\zeta}(\sigma+it)+\overline{\frac{\zeta'}{\zeta}(\sigma+it)}\right)x^{1/2-\sigma}\right\}\mathrm{d}\sigma$$

$$
\begin{aligned}
&- \frac{1}{\pi n!}\int_{1/2}^{\infty} \frac{(\sigma-1/2)^n}{C_n(\sigma)} \operatorname{Im}\left\{ i^n\,(2\sigma-1)\sum_{\gamma} \frac{x^{i(\gamma-t)}}{(\sigma-1/2)^2+(\gamma-t)^2} \right\} \mathrm{d}\sigma \\
&+ \frac{1}{\pi n!}\int_{1/2}^{\infty} \frac{(\sigma-1/2)^n}{C_n(\sigma)} \operatorname{Im}\left\{ i^n \sum_{m\leqslant x} \frac{\Lambda(m)}{m^{it}} \left(\frac{x^{\sigma-1/2}}{m^{\sigma}} - \frac{x^{1/2-\sigma}}{m^{1-\sigma}} \right) \right\} \mathrm{d}\sigma \\
&+ \frac{1}{\pi n!}\int_{1/2}^{\infty} \frac{(\sigma-1/2)^n}{C_n(\sigma)} \operatorname{Im}\left\{ i^n\, x^{1/2-\sigma} \log\frac{t}{2\pi} \right\} \mathrm{d}\sigma \\
&- \frac{1}{\pi n!}\int_{1/2}^{\infty} \frac{(\sigma-1/2)^n}{C_n(\sigma)} \operatorname{Im}\left\{ i^n\, x^{1/2-it} \left(\frac{2\sigma-1}{(\sigma-it)(1-\sigma-it)} \right) \right\} \mathrm{d}\sigma \\
&+ O\left(\int_{1/2}^{\infty} \frac{(\sigma-1/2)^n}{C_n(\sigma)}\, \frac{\sigma^2}{t}\left(x^{-5/2}+x^{1/2-\sigma}\right)\, \mathrm{d}\sigma \right) \\
&= I_{1,n}(x,t) + I_{2,n}(x,t) + I_{3,n}(x,t) + I_{4,n}(x,t) + I_{5,n}(x,t) + O\big(I_{6,n}(x,t)\big).
\end{aligned}
$$

We analyze each term in the above expression.

1. *First term*: Using the fact that $\operatorname{Im}\{i^n((-1)^n z + \overline{z})\} = 0$, for $z \in \mathbb{C}$ and $n \geqslant 1$ we get that $I_{1,n}(x,t) = 0$.

2. *Second term*: Using Fubini's theorem[3] and the change of variables $y = (\sigma - 1/2)\log x$, it follows that

$$
\begin{aligned}
I_{2,n}(x,t) &= -\frac{2}{\pi n!}\sum_{\gamma} \operatorname{Im}\{i^n x^{i(\gamma-t)}\} \int_{1/2}^{\infty} \frac{(\sigma-1/2)^{n+1}}{(\sigma-1/2)^2+(\gamma-t)^2}\, \frac{1}{x^{\sigma-1/2}+(-1)^{n+1}x^{1/2-\sigma}}\, \mathrm{d}\sigma \\
&= \frac{1}{\pi n!(\log x)^n}\sum_{\gamma} \operatorname{Im}\{i^{n+2} e^{i(\gamma-t)\log x}\} \int_{0}^{\infty} \frac{y^{n+1}}{y^2+((\gamma-t)\log x)^2}\, \frac{2}{e^{y}+(-1)^{n+1}e^{-y}}\, \mathrm{d}y.
\end{aligned}
$$

3. *Third term*: Recalling that $f_n(x)$ is defined in (4.1.8), similar computations give us

$$
I_{3,n}(x,t) = \frac{1}{\pi}\sum_{m\leqslant x} \operatorname{Im}\{i^n m^{-it}\}\, \frac{\Lambda(m)}{\sqrt{m}(\log m)^{n+1}}\, f_n\!\left(\frac{\log m}{\log x}\right).
$$

4. *Fourth term*: Note that when n is even, we obtain that $I_{4,n}(x,t) = 0$. Let us suppose that n is odd. Then $C_n(\sigma) = 2\cosh((\sigma-1/2)\log x)$. By a change of variables and [64, Eq. 3.552-3] we get that

$$
\begin{aligned}
I_{4,n}(x,t) &= \frac{\operatorname{Im}\{i^n\}}{2\pi n!}\log\frac{t}{2\pi}\int_{1/2}^{\infty} \frac{(\sigma-1/2)^n\, x^{1/2-\sigma}}{\cosh((\sigma-1/2)\log x)}\, \mathrm{d}\sigma \\
&= \frac{\operatorname{Im}\{i^n\}}{\pi\,(\log x)^{n+1}}\, 2^{-n-1}(1-2^{-n})\zeta(n+1)\log\frac{t}{2\pi}.
\end{aligned}
$$

5. *Fifth term*: Using the same change of variables,

$$
|I_{5,n}(x,t)| \ll \sqrt{x}\int_{1/2}^{\infty} \frac{(\sigma-1/2)^{n+1}}{|(\sigma-it)(1-\sigma-it)|}\, \frac{1}{x^{\sigma-1/2}+(-1)^{n+1}x^{1/2-\sigma}}\, \mathrm{d}\sigma
$$

[3]It is justified by the fact that the number of zeros on the interval $[t, t+1]$ is $O(\log t)$.

$$
\begin{aligned}
&= \frac{\sqrt{x}}{(\log x)^n} \int_0^\infty \frac{y^{n+1}}{|((1/2 - it)\log x)^2 - y^2|} \frac{1}{e^y + (-1)^{n+1}e^{-y}} \, \mathrm{d}y \\
&\ll \frac{\sqrt{x}}{t\,(\log x)^{n+2}} \int_0^\infty \frac{y^{n+1}}{e^y + (-1)^{n+1}e^{-y}} \, \mathrm{d}y \ll \frac{\sqrt{x}}{t\,(\log x)^{n+2}}.
\end{aligned}
$$

6. *Sixth term*: As in the previous term, we have

$$
|I_{6,n}(x,t)| \ll \frac{1}{t\,(\log x)^{n+1}}.
$$

Combining all the terms, we obtain the desired result. □

Note that in the above lemma we establish the connection between $S_n(t)$ and the function f_n. The following lemma summarizes useful information related to the function f_n and a new auxiliary function g_n.

Lemma 4.4. *Let $n \geqslant 1$ be an integer and $f_n : (0,2) \to \mathbb{R}$ be the real valued function defined in (4.1.8). Then, the function $g_n : (0,2) \to \mathbb{R}$ given by*

$$
g_n(x) = \frac{1 - f_n(x)}{x^{n+1}} \tag{4.2.7}
$$

satisfies the following properties:

(I) g_n can be extended to the interval $(-2,2)$, such that $g_n \in C^\infty\big((-2,2)\big)$, and g_n^2 is an even function.

(II) For $x \in (-2,2)$, the function g_n has the representation

$$
g_n(x) = \frac{1}{n!} \int_0^\infty e^{-y} y^n \left(\frac{e^{xy} + (-1)^{n+1}e^{-xy}}{e^y + (-1)^{n+1}e^{-y}} \right) \mathrm{d}y. \tag{4.2.8}
$$

(III) In particular, $g_n(0) = 2^{-n}(1 - 2^{-n})\zeta(n+1)$ when n is odd, and zero otherwise.

Proof. Using the definition of f_n, it follows that for $x \in (0,2)$,

$$
\begin{aligned}
\frac{f_n(x)}{x^{n+1}} + \frac{1}{n!} \int_0^\infty e^{-y} y^n \left(\frac{e^{xy} + (-1)^{n+1}e^{-xy}}{e^y + (-1)^{n+1}e^{-y}} \right) \mathrm{d}y &= \frac{1}{n!} \int_0^\infty y^n \left(\frac{e^{(1-x)y} + (-1)^{n+1}e^{-(x+1)y}}{e^y + (-1)^{n+1}e^{-y}} \right) \mathrm{d}y \\
&= \frac{1}{n!} \int_0^\infty y^n e^{-xy} \, \mathrm{d}y = \frac{1}{x^{n+1}},
\end{aligned}
$$

where in the last equality we have used [64, Eq. 3.351-3]. This implies that

$$
g_n(x) = \frac{1}{n!} \int_0^\infty e^{-y} y^n \left(\frac{e^{xy} + (-1)^{n+1}e^{-xy}}{e^y + (-1)^{n+1}e^{-y}} \right) \mathrm{d}y, \tag{4.2.9}
$$

for $x \in (0,2)$. Using dominated convergence one can see that the right-hand side of (4.2.9) defines a function in $C^\infty\big((-2,2)\big)$. Then, this representation allows us to extend the function g_n to $(-2,2)$. On the other hand, $g_n(-x) = (-1)^{n+1} g_n(x)$, and this implies that g_n^2 is an even function. When n is even, g_n is an odd function and therefore $g_n(0) = 0$. When n is odd, using [64, Eq. 3.552-3] we get

$$g_n(0) = \frac{1}{n!}\int_0^\infty \frac{e^{-y}y^n}{\cosh y}\,\mathrm{d}y = 2^{-n}(1-2^{-n})\,\zeta(n+1).$$

$\square$

4.2.2 Proof of Theorem 4.1

Lemma 4.3 allows us to obtain the second moment of $S_n(t)$ in terms of certain integrals depending of each summand involved in (4.2.1). Let $n \geqslant 1$ be a fixed integer. Using Lemma 4.3, we have for $t \geqslant 1$ and $x \geqslant 4$ that

$$S_n(t) - I_{3,n}(x,t) - I_{4,n}(x,t) = I_{2,n}(x,t) + O\left(\frac{\sqrt{x}}{t\,(\log x)^{n+2}}\right),$$

where

$$I_{2,n}(x,t) = \frac{1}{\pi n!(\log x)^n}\sum_{\gamma}\mathrm{Im}\left\{i^{n+2}e^{i(\gamma-t)\log x}\right\}\int_0^\infty \frac{y^{n+1}}{y^2+((\gamma-t)\log x)^2}\,\frac{2}{e^y+(-1)^{n+1}e^{-y}}\,\mathrm{d}y,$$

$$I_{3,n}(x,t) = \frac{1}{\pi}\sum_{m\leqslant x}\mathrm{Im}\left\{i^n m^{-it}\right\}\frac{\Lambda(m)}{\sqrt{m}(\log m)^{n+1}}\,f_n\!\left(\frac{\log m}{\log x}\right),$$

and

$$I_{4,n}(x,t) = \mu_n\frac{\mathrm{Im}\left\{i^n\right\}}{\pi(\log x)^{n+1}}\log\frac{t}{2\pi}.$$

Then, for $T \geqslant 3$, squaring the above expression and integrating from 1 to T we obtain

$$\begin{aligned}\int_1^T |S_n(t)|^2\,\mathrm{d}t = &\int_1^T |I_{2,n}(x,t)|^2\,\mathrm{d}t + 2\int_1^T S_n(t)\,I_{3,n}(x,t)\,\mathrm{d}t - \int_1^T |I_{3,n}(x,t)|^2\,\mathrm{d}t\\ &- \int_1^T |I_{4,n}(x,t)|^2\,\mathrm{d}t + 2\int_1^T S_n(t)\,I_{4,n}(x,t)\,\mathrm{d}t - 2\int_1^T I_{3,n}(x,t)\,I_{4,n}(x,t)\,\mathrm{d}t\\ &+ O\left(\frac{\sqrt{x}}{(\log x)^{n+2}}\int_1^T\frac{|I_{2,n}(x,t)|}{t}\,\mathrm{d}t\right) + O\left(\frac{x}{(\log x)^{2n+4}}\right).\end{aligned} \tag{4.2.10}$$

Using the continuity of $S_n(t)$, we get

$$\int_1^T |S_n(t)|^2\,\mathrm{d}t = \int_0^T |S_n(t)|^2\,\mathrm{d}t + O(1). \tag{4.2.11}$$

Now, let us analyze the right-hand side of (4.2.10). Note that $\mu_n = 0$ when n is even. Then, we have that

$$\begin{aligned}\int_1^T |I_{4,n}(x,t)|^2 \,\mathrm{d}t &= \mu_n^2 \frac{(\operatorname{Im}\{i^n\})^2}{\pi^2(\log x)^{2n+2}} \int_1^T \log^2 \frac{t}{2\pi}\,\mathrm{d}t \\ &= \frac{\mu_n^2}{\pi^2(\log x)^{2n+2}}\, T\log^2 T + O\bigg(\frac{T\log T}{(\log x)^{2n+2}}\bigg).\end{aligned} \tag{4.2.12}$$

Furthermore, using the relation $S'_{n+1}(t) = S_n(t)$, the bound $S_n(t) = O(\log t)$ (see (4.1.1)), and integration by parts, we obtain

$$2\int_1^T S_n(t)\, I_{4,n}(x,t)\ \mathrm{d}t = \mu_n \frac{2\operatorname{Im}\{i^n\}}{\pi(\log x)^{n+1}} \int_1^T S'_{n+1}(t) \log\frac{t}{2\pi}\,\mathrm{d}t = O\bigg(\frac{\log^2 T}{(\log x)^{n+1}}\bigg). \tag{4.2.13}$$

Observe that by (I) from Lemma 4.4, it is clear that $|f_n(y)| \ll 1$ for $y \in (0,1]$. Then, using the estimate $\Lambda(m) \leqslant \log m$ and integration by parts, we have

$$\begin{aligned}\bigg|2\int_1^T I_{3,n}(x,t)\, I_{4,n}(x,t)\ \mathrm{d}t\bigg| &\ll \frac{1}{(\log x)^{n+1}} \sum_{m\leqslant x} \frac{\Lambda(m)}{\sqrt{m}(\log m)^{n+1}} \bigg|\int_1^T \operatorname{Im}\{i^n m^{-it}\}\log\frac{t}{2\pi}\,\mathrm{d}t\bigg| \\ &\ll \frac{\log T}{(\log x)^{n+1}} \sum_{m\leqslant x}\frac{1}{\sqrt{m}} \ll \frac{\sqrt{x}\log T}{(\log x)^{n+1}}.\end{aligned} \tag{4.2.14}$$

We estimate the first error term in (4.2.10) using Cauchy-Schwarz to get

$$\frac{\sqrt{x}}{(\log x)^{n+1}} \int_1^T \frac{|I_{2,n}(x,t)|}{t}\,\mathrm{d}t \leqslant \frac{\sqrt{x}}{(\log x)^{n+1}} \bigg(\int_1^T |I_{2,n}(x,t)|^2\,\mathrm{d}t\bigg)^{1/2}. \tag{4.2.15}$$

Let us define the following integrals:

$$R_n(x,T) = \int_1^T |I_{2,n}(x,t)|^2\,\mathrm{d}t, \qquad H_n(x,T) = 2\int_1^T S_n(t)\, I_{3,n}(x,t)\ \mathrm{d}t,$$

and

$$G_n(x,T) = \int_1^T |I_{3,n}(x,t)|^2\,\mathrm{d}t.$$

Plugging (4.2.11), (4.2.12), (4.2.13), (4.2.14) and (4.2.15) into (4.2.10) gives us

$$\begin{aligned}\int_0^T |S_n(t)|^2\ \mathrm{d}t &= R_n(x,T) + H_n(x,T) - G_n(x,T) - \frac{\mu_n^2}{\pi^2(\log x)^{2n+2}}\, T\log^2 T \\ &\quad + O\bigg(\frac{T\log T}{(\log x)^{2n+2}}\bigg) + O\bigg(\frac{\sqrt{xR_n(x,T)}}{(\log x)^{n+1}}\bigg) + O\bigg(\frac{x\log^2 T}{(\log x)^{2n+4}}\bigg).\end{aligned} \tag{4.2.16}$$

Choosing $x = T^\beta$, for a fixed $0 < \beta < \frac{1}{2}$, we get that

$$\int_0^T |S_n(t)|^2\ \mathrm{d}t = R_n(T^\beta,T) + H_n(T^\beta,T) - G_n(T^\beta,T)$$

$$-\frac{\mu_n^2}{\pi^2\beta^{2n+2}}\frac{T}{(\log T)^{2n}}+O\left(\frac{T}{(\log T)^{2n+1}}\right)+O\biggl(\frac{T^{\beta/2}\sqrt{R_n(T^\beta,T)}}{(\log T)^{n+1}}\biggr).$$

We conclude our desired result by using the formulas for $R_n(T^\beta,T)$ and $H_n(T^\beta,T)-G_n(T^\beta,T)$ given by Propositions 4.6 and 4.9, respectively. We remark that by Proposition 4.6 and (4.1.7), we can use the bound $R_n(T^\beta,T)=O(T)$ to estimate the error term. □

In the following sections, we will concentrate on obtaining the asymptotic formulas for $R_n(x,T), H_n(x,T)$ and $G_n(x,T)$. Throughout these sections, we will assume that $n\geqslant 1$ is a given fixed integer.

4.3 Asymptotic formula for $R_n(x,T)$: The sum over the zeros of $\zeta(s)$

Our objective is to evaluate the mean square of the sum over the zeros of the Riemann zeta-function that appears in (4.2.16). We recall that for $T\geqslant 3$ and $x\geqslant 4$,

$$\begin{aligned}R_n(x,T)=&\frac{1}{\pi^2(n!)^2(\log x)^{2n}}\\ &\times\int_1^T\left|\sum_\gamma \operatorname{Im}\{i^{n+2}e^{i(\gamma-t)\log x}\}\int_0^\infty\frac{y^{n+1}}{y^2+((\gamma-t)\log x)^2}\frac{2}{(e^y+(-1)^{n+1}e^{-y})}\,\mathrm{d}y\right|^2\mathrm{d}t.\end{aligned}$$

Lemma 4.5. *Let g_n be the function defined in* (4.2.7). *Assume the Riemann hypothesis. Then, for $T\geqslant 3$ and $x\geqslant 4$ we have*

$$R_n(x,T)=\frac{1}{(\log x)^{2n+1}}\sum_{0<\gamma,\gamma'\leqslant T}\widehat{k_n}((\gamma-\gamma')\log x)+O\biggl(\frac{\log^3 T}{(\log x)^{2n}}\biggr),\tag{4.3.1}$$

where the function $k_n:\mathbb{R}\to\mathbb{R}$ is given by

$$k_n(\xi)=\begin{cases} g_n^2(2\pi\xi), & \text{if } |\xi|\leqslant\frac{1}{2\pi}\\ \dfrac{1}{(2\pi\xi)^{2n+2}}, & \text{if } |\xi|\geqslant\frac{1}{2\pi}.\end{cases}\tag{4.3.2}$$

Moreover, we have that

$$|\widehat{k_n}(y)|\ll\min\left\{1,\frac{1}{|y|^2}\right\}.\tag{4.3.3}$$

Proof. Define the function

$$h_n(u)=\operatorname{Im}\{i^{n+2}e^{iu}\}\int_0^\infty\frac{y^{n+1}}{y^2+u^2}\frac{2}{(e^y+(-1)^{n+1}e^{-y})}\,\mathrm{d}y.$$

Since $|h_n(u)| \ll \min\{1, 1/u^2\} \ll 1/(1+u^2)$, using Fubini's theorem we have

$$R_n(x,T) = \frac{1}{\pi^2(n!)^2(\log x)^{2n}} \sum_{\gamma,\gamma} \int_1^T h_n((\gamma - t)\log x)\, h_n((\gamma' - t)\log x)\ \mathrm{d}t.$$

Note that h_n is an even function when n is odd and h_n is an odd function when n is even. Using an argument of Montgomery [81, p. 187] (see also [53, p. 158]) one can see that

$$\begin{aligned} R_n(x,T) &= \frac{1}{\pi^2(n!)^2(\log x)^{2n}} \sum_{0<\gamma,\gamma'\leqslant T} \int_{-\infty}^{\infty} h_n((\gamma - t)\log x)\, h_n((\gamma' - t)\log x)\ \mathrm{d}t + O\left(\frac{\log^3 T}{(\log x)^{2n}}\right) \\ &= \frac{(-1)^{n+1}}{\pi^2(n!)^2(\log x)^{2n+1}} \sum_{0<\gamma,\gamma'\leqslant T} h_n * h_n((\gamma - \gamma')\log x) + O\left(\frac{\log^3 T}{(\log x)^{2n}}\right). \end{aligned} \tag{4.3.4}$$

Let us calculate the Fourier transform of h_n. Using Fubini's theorem, it follows that for $\xi > 0$

$$\begin{aligned} \widehat{h_n}(\xi) &= \int_{-\infty}^{\infty} \left(\mathrm{Im}\,\{i^{n+2} e^{iu}\} \int_0^{\infty} \frac{y^{n+1}}{y^2+u^2} \frac{2}{(e^y + (-1)^{n+1}e^{-y})}\ \mathrm{d}y \right) (\cos(2\pi\xi u) - i\sin(2\pi\xi u))\ \mathrm{d}u \\ &= \mathrm{Im}\,\{i^{n+2}\} \int_0^{\infty} \left(\int_0^{\infty} \frac{\cos(2\pi\xi u)\cos(u)}{y^2+u^2}\ \mathrm{d}u \right) \frac{4\,y^{n+1}}{(e^y + (-1)^{n+1}e^{-y})}\ \mathrm{d}y \\ &\quad - i\,\mathrm{Im}\,\{i^{n+3}\} \int_0^{\infty} \left(\int_0^{\infty} \frac{\sin(2\pi\xi u)\sin(u)}{y^2+u^2}\ \mathrm{d}u \right) \frac{4\,y^{n+1}}{(e^y + (-1)^{n+1}e^{-y})}\ \mathrm{d}y, \end{aligned}$$

where we have used the parity of the involved functions. Then, using the formulas [64, Eq. 3.742-1 and 3.742-3] we write

$$\begin{aligned} \widehat{h_n}(\xi) &= \pi\,\mathrm{Im}\,\{i^{n+2}\} \int_0^{\infty} \left(e^{-|2\pi\xi - 1|y} + e^{-(2\pi\xi+1)y}\right) \frac{y^n}{(e^y + (-1)^{n+1}e^{-y})}\ \mathrm{d}y \\ &\quad - i\pi\,\mathrm{Im}\,\{i^{n+3}\} \int_0^{\infty} \left(e^{-|2\pi\xi - 1|y} - e^{-(2\pi\xi+1)y}\right) \frac{y^n}{(e^y + (-1)^{n+1}e^{-y})}\ \mathrm{d}y. \end{aligned}$$

For $2\pi\xi \geqslant 1$, making a separate computation of the n odd and n even cases, using [64, Eq. 3.351-3], we obtain

$$\widehat{h_n}(\xi) = \left(\mathrm{Im}\,\{i^{n+2}\} - i\,\mathrm{Im}\,\{i^{n+3}\}\right) \frac{n!}{2^{n+1}\pi^n \xi^{n+1}}.$$

On the other hand, for $0 < 2\pi\xi < 1$ we obtain that

$$\begin{aligned} \widehat{h_n}(\xi) =& \pi\,\mathrm{Im}\,\{i^{n+2}\} \int_0^{\infty} e^{-y} y^n \frac{2\cosh(2\pi\xi y)}{(e^y + (-1)^{n+1}e^{-y})}\ \mathrm{d}y \\ & - i\pi\,\mathrm{Im}\,\{i^{n+3}\} \int_0^{\infty} e^{-y} y^n \frac{2\sinh(2\pi\xi y)}{(e^y + (-1)^{n+1}e^{-y})}\ \mathrm{d}y. \end{aligned}$$

Defining the even real-valued function

$$k_n(\xi) = \frac{(-1)^{n+1}}{\pi^2(n!)^2}(\widehat{h_n}(\xi))^2,$$

we have

$$\widehat{k_n}(y) = \frac{(-1)^{n+1}}{\pi^2(n!)^2}\big(h_n * h_n\big)(y),$$

and this implies in (4.3.4) that

$$R_n(x,T) = \frac{1}{(\log x)^{2n+1}} \sum_{0<\gamma,\gamma'\leqslant T} \widehat{k_n}((\gamma-\gamma')\log x) + O\bigg(\frac{\log^3 T}{(\log x)^{2n}}\bigg).$$

Finally, we calculate k_n. For $2\pi\xi \geqslant 1$ we obtain

$$k_n(\xi) = \frac{(-1)^{n+1}}{\pi^2(n!)^2}\bigg(\big(\mathrm{Im}\,\{i^{n+2}\} - i\,\mathrm{Im}\,\{i^{n+3}\}\big)\frac{n!}{2^{n+1}\pi^n\xi^{n+1}}\bigg)^2 = \frac{1}{(2\pi\xi)^{2n+2}},$$

and using the parity of the involved functions, we get that the above expression holds for $|2\pi\xi| \geqslant 1$. On the other hand, for $0 < 2\pi\xi < 1$, we have that

$$\begin{aligned} k_n(\xi) = \frac{(-1)^{n+1}}{\pi^2(n!)^2}\Bigg(&\pi\,\mathrm{Im}\,\{i^{n+2}\}\int_0^\infty e^{-y}y^n\frac{2\cosh(2\pi\xi y)}{(e^y+(-1)^{n+1}e^{-y})}\,\mathrm{d}y \\ &- i\pi\,\mathrm{Im}\,\{i^{n+3}\}\int_0^\infty e^{-y}y^n\frac{2\sinh(2\pi\xi y)}{(e^y+(-1)^{n+1}e^{-y})}\,\mathrm{d}y\Bigg)^2 \\ = g_n^2(2\pi\xi),& \end{aligned}$$

where in the last line we have treated separately the cases n odd and n even, and used (4.2.8). Using (I) from Lemma 4.4, it follows that the above expression holds for $|\xi| \leqslant \frac{1}{2\pi}$. To prove the estimate (4.3.3) (see [53, p. 161]), we use that $k_n \in L^1(\mathbb{R})$ implies $|\widehat{k_n}(\xi)| \ll 1$, and that integration by parts twice[4] implies $|\widehat{k_n}(y)| \ll \frac{1}{|y|^2}$. □

Finally, the following proposition establishes the relation between $R_n(x,T)$ and the function $F(\alpha,T)$.

Proposition 4.6. *Let $0 < \beta \leqslant 1$ be a fixed number. Assume the Riemann hypothesis. Then,*

$$\begin{aligned} R_n(T^\beta,T) =& \frac{T}{2\pi^2(\log T)^{2n}}\Bigg[\bigg(A_n + \frac{1}{2n}\bigg)\frac{1}{\beta^{2n}} + \bigg(\int_1^\infty \frac{F(\alpha)}{\alpha^{2n+2}}\,\mathrm{d}\alpha - \frac{1}{2n}\bigg) + \frac{2\,\mu_n^2}{\beta^{2n+2}}\Bigg] \\ &+ O\bigg(\frac{T\sqrt{\log\log T}}{(\log T)^{2n+1/2}}\bigg), \end{aligned}$$

[4] The function k_n is absolutely continuous and has bounded derivatives on $\mathbb{R} - \{\pm\frac{1}{2\pi}\}$.

as $T \to \infty$, where

$$A_n = \int_0^1 \alpha\, g_n^2(\alpha)\, \mathrm{d}\alpha, \tag{4.3.5}$$

and μ_n is defined as in Lemma 4.3.

Proof. Let us analyze the main term in (4.3.1). The estimate (4.3.3) and a classical argument [53, p. 161] imply that

$$\sum_{0<\gamma,\gamma'\leqslant T} \widehat{k_n}((\gamma-\gamma')\log x) = \sum_{0<\gamma,\gamma'\leqslant T} \widehat{k_n}((\gamma-\gamma')\log x)\, w(\gamma-\gamma') + O(T), \tag{4.3.6}$$

where $w(u) = 4/(4+u^2)$. Letting $x = T^\beta$, from (1.3.5) one can see that

$$\sum_{0<\gamma,\gamma'\leqslant T} \widehat{k_n}((\gamma-\gamma')\log x)\, w(\gamma-\gamma') = \frac{T\log T}{(2\pi)^2\beta}\int_{-\infty}^{\infty} F(\alpha)\, k_n\left(\frac{\alpha}{2\pi\beta}\right) \mathrm{d}\alpha. \tag{4.3.7}$$

To evaluate the integral on the right-hand side of (4.3.7), we use the fact that $F(\alpha)$ is even and we split this integral into the intervals $[0,\beta]$, $[\beta,1]$ and $[1,\infty)$. Moreover, we calculate these integrals using the asymptotic formula ADD REF for $F(\alpha)$: As $T \to \infty$, we have

$$F(\alpha) = \left(\alpha + T^{-2\alpha}\log T\right)(1+o(1)), \tag{4.3.8}$$

uniformly for $0 \leqslant \alpha \leqslant 1$, where $o(1) = O\left(\sqrt{\frac{\log\log T}{\log T}}\right)$.

1. *On the interval* $[0,\beta]$: Note that, using (I) from Lemma 4.4, we have that $g_n^2(\alpha) = g_n^2(0) + O(\alpha^2)$ for $\alpha \in [0,1]$. Then, using (4.3.2), (4.3.8) and the fact that $\beta\int_0^1 T^{-2\beta\alpha}\log T\, \mathrm{d}\alpha = \frac{1}{2} + O\left(\frac{1}{\log^2 T}\right)$, we get

$$\int_0^\beta F(\alpha) k_n\left(\frac{\alpha}{2\pi\beta}\right) \mathrm{d}\alpha = \left(\beta^2\int_0^1 \alpha\, g_n^2(\alpha)\, \mathrm{d}\alpha + \frac{g_n^2(0)}{2} + O\left(\frac{1}{\log^2 T}\right)\right)(1+o(1)).$$

We remark, by (III) from Lemma 4.4, that $g_n^2(0) = 4\mu_n^2$.

2. *On the interval* $[\beta,1]$: Here, by (4.3.8), $F(\alpha) = \alpha + o(1)$. Then, we handle this integral using (4.3.2) to get

$$\int_\beta^1 F(\alpha)\, k_n\left(\frac{\alpha}{2\pi\beta}\right) \mathrm{d}\alpha = \int_\beta^1 (\alpha + o(1))\left(\frac{\beta}{\alpha}\right)^{2n+2} \mathrm{d}\alpha = \frac{1}{2n}\beta^2 - \frac{1}{2n}\beta^{2n+2} + o(1).$$

3. *On the interval* $[1,\infty)$: In this case we write

$$\int_1^\infty F(\alpha)\, k_n\left(\frac{\alpha}{2\pi\beta}\right) \mathrm{d}\alpha = \int_1^\infty F(\alpha)\left(\frac{\beta}{\alpha}\right)^{2n+2} \mathrm{d}\alpha = \beta^{2n+2}\int_1^\infty \frac{F(\alpha)}{\alpha^{2n+2}}\, \mathrm{d}\alpha.$$

Finally, inserting the above estimates in (4.3.7) and combining with (4.3.6) and Lemma 4.5, we conclude the desired result. □

4.4 Asymptotic formulas for $G_n(x,T)$ and $H_n(x,T)$: The sum over the prime numbers

4.4.1 The terms $G_n(x,T)$ and $H_n(x,T)$

We recall that, for $T \geqslant 3$ and $x \geqslant 4$, we have defined

$$G_n(x,T) = \frac{1}{\pi^2}\int_1^T \left| \sum_{m\leqslant x} \operatorname{Im}\{i^n m^{-it}\} \frac{\Lambda(m)}{\sqrt{m}(\log m)^{n+1}}\, f_n\!\left(\frac{\log m}{\log x}\right)\right|^2 \mathrm{d}t$$

and

$$H_n(x,T) = \frac{2}{\pi}\sum_{m\leqslant x}\left(\int_1^T S_n(t)\operatorname{Im}\{i^n m^{-it}\}\ \mathrm{d}t\right)\frac{\Lambda(m)}{\sqrt{m}(\log m)^{n+1}}\, f_n\!\left(\frac{\log m}{\log x}\right). \tag{4.4.1}$$

We can get the following expression for $G_n(x,T)$ using similar computations as Goldston.

Lemma 4.7. *For $T \geqslant 3$ and $x \geqslant 4$, we have that*

$$G_n(x,T) = \frac{T}{2\pi^2}\sum_{m\leqslant x}\frac{\Lambda^2(m)}{m(\log m)^{2n+2}}\, f_n^2\!\left(\frac{\log m}{\log x}\right) + O(x^2).$$

Proof. See [53, pp. 164-165]. □

The expression for $H_n(x,T)$ is more subtle, since it requires some modification to the computations of Titchmarsh [101] that arises when $n \geqslant 1$.

Lemma 4.8. *Assume the Riemann hypothesis. Then, for $T \geqslant 3$ and $x \geqslant 4$, we have*

$$H_n(x,T) = \frac{T}{\pi^2}\sum_{m\leqslant x}\frac{\Lambda^2(m)}{m(\log m)^{2n+2}}\, f_n\!\left(\frac{\log m}{\log x}\right) + O(x^2\log T).$$

Proof. First, let us calculate the integral inside of (4.4.1). Using integration by parts in (4.2.2), it follows that, for $t > 0$,

$$S_n(t) = \frac{1}{\pi}\operatorname{Im}\left\{\frac{i^n}{(n-1)!}\int_{1/2}^{\infty}(\sigma-1/2)^{n-1}\,\log\zeta(\sigma+it)\ \mathrm{d}\sigma\right\}.$$

Then, using the identity

$$\operatorname{Im}\{i^n m^{-it}\} = \frac{(-1)^n i^{n+1}}{2}(m^{it} + (-1)^{n+1}m^{-it}),$$

and Fubini's theorem, we get

$$\begin{aligned}\int_1^T & S_n(t)\,\mathrm{Im}\,\{i^n m^{-it}\}\ \mathrm{d}t \\ &= \frac{1}{2\pi(n-1)!}\int_{1/2}^{\infty}(\sigma-1/2)^{n-1}\,\mathrm{Re}\left\{\int_0^T \log\zeta(\sigma+it)(m^{it}+(-1)^{n+1}m^{-it})\ \mathrm{d}t\right\}\ \mathrm{d}\sigma+O(1).\end{aligned} \tag{4.4.2}$$

Now, we compute the integral from 0 to T, following the idea in [101, Lemma γ]. Let $m \geqslant 2$ be a natural number and $\frac{1}{2} < \sigma < 2$. Consider the integral

$$\int_{\partial R} \log\zeta(s)\, m^s\,\mathrm{d}s,$$

where R is the rectangle with vertices σ, 2, $2+iT$ and $\sigma+iT$ with suitable indentations to exclude the point $s=1$. The function $\log\zeta(s)$ is analytic inside the contour R, and the radii of $s=1$ may be made to tend to zero. Then, using Cauchy's theorem we have that

$$\begin{aligned} i\int_0^T & \log\zeta(\sigma+it)\, m^{\sigma+it}\,\mathrm{d}t \\ &= \int_\sigma^2 \log\zeta(\alpha)\, m^{\alpha}\ \mathrm{d}\alpha + i\int_0^T \log\zeta(2+it)\, m^{2+it}\,\mathrm{d}t - \int_\sigma^2 \log\zeta(\alpha+iT)\, m^{\alpha+iT}\,\mathrm{d}\alpha.\end{aligned}$$

Note that $\int_\sigma^2 \log\zeta(\alpha)\, m^{\alpha}\ \mathrm{d}\alpha = O(m^2)$. Then, by [101, Lemmas α and β] we get that

$$\int_0^T \log\zeta(\sigma+it)m^{it}\,\mathrm{d}t = \frac{\Lambda(m)}{m^\sigma \log m}T + O(m^{2-\sigma}\log T). \tag{4.4.3}$$

Similarly, using the integral

$$\int_{\partial R} \log\zeta(s)\, m^{-s}\,\mathrm{d}s,$$

around the same contour, it follows that

$$\int_0^T \log\zeta(\sigma+it)m^{-it}\,\mathrm{d}t = O(\log T). \tag{4.4.4}$$

Therefore, combining (4.4.3) and (4.4.4), we get for $\frac{1}{2} < \sigma < 2$ that

$$\int_0^T \log\zeta(\sigma+it)\big(m^{it}+(-1)^{n+1}m^{-it}\big)\,\mathrm{d}t = \frac{\Lambda(m)}{m^\sigma \log m}T + O(m^{2-\sigma}\log T). \tag{4.4.5}$$

On the other hand, using the expansion of the logarithm of $\zeta(s)$ and Fubini's theorem, we have for $\sigma \geqslant 2$ that

$$\begin{aligned}\int_0^T \log\zeta(\sigma+it)\big(m^{it}+(-1)^{n+1}m^{-it}\big)\,\mathrm{d}t &= \sum_{k\geqslant 2}\frac{\Lambda(k)}{k^\sigma\log k}\int_0^T \frac{m^{it}+(-1)^{n+1}m^{-it}}{k^{it}}\,\mathrm{d}t \\ &= \frac{\Lambda(m)}{m^\sigma\log m}\int_0^T \big(1+(-1)^{n+1}m^{-2it}\big)\,\mathrm{d}t \\ &\quad+\sum_{\substack{k\geqslant 2\\ k\neq m}}\frac{\Lambda(k)}{k^\sigma\log k}\int_0^T\left(\left(\frac{m}{k}\right)^{it}+(-1)^{n+1}(mk)^{-it}\right)\mathrm{d}t \\ &= \frac{\Lambda(m)}{m^\sigma\log m}T+O\left(\sum_{k\geqslant 2}\frac{1}{k^\sigma}\right)+O\left(\sum_{\substack{k\geqslant 2\\ k\neq m}}\frac{1}{k^\sigma|\log(m/k)|}\right) \\ &= \frac{\Lambda(m)}{m^\sigma\log m}T+O\left(\frac{1}{2^\sigma}\right),\end{aligned} \tag{4.4.6}$$

where in the last sum we have used that $\sum_{\substack{k\geqslant 2\\ k\neq m}}\frac{1}{k^2|\log(m/k)|}$ is bounded (see [101, p. 451]). Therefore, inserting (4.4.5) and (4.4.6) in (4.4.2) and using [64, Eq. 3.351-3] we have

$$\int_1^T S_n(t)\,\mathrm{Im}\,\{i^n m^{-it}\}\,\mathrm{d}t = \frac{\Lambda(m)\,T}{2\pi\sqrt{m}(\log m)^{n+1}}+O(m^{3/2}\log T).$$

Inserting it in (4.4.1) we get

$$H_n(x,T)=\frac{T}{\pi^2}\sum_{m\leqslant x}\frac{\Lambda^2(m)}{m\,(\log m)^{2n+2}}f_n\left(\frac{\log m}{\log x}\right)+O\left(\sum_{m\leqslant x}\frac{m\,\Lambda(m)}{(\log m)^{n+1}}\left|f_n\left(\frac{\log m}{\log x}\right)\right|\log T\right).$$

Finally, using the bound $|f_n(y)|\ll 1$ for $y\in(0,1]$ in the error term, we get

$$\left|\sum_{m\leqslant x}\frac{m\,\Lambda(m)}{(\log m)^{n+1}}f_n\left(\frac{\log m}{\log x}\right)\right|\ll\sum_{m\leqslant x}m\ll x^2.$$

□

4.4.2 The power of cancelation in $H_n(x,T)-G_n(x,T)$

Here, we will obtain the asymptotic behavior for the difference $H_n(T^\beta,T)-G_n(T^\beta,T)$, as $T\to\infty$. It is possible to obtain asymptotic formulas for $H_n(T^\beta,T)$ and $G_n(T^\beta,T)$ independently, as we did in Proposition 4.6 for $R_n(T^\beta,T)$. However, the expressions are much more complicated, so we will take advantage of a surprising cancellation in their difference.

Proposition 4.9. *Let $0<\beta<\frac{1}{2}$ be a fixed number. Assume the Riemann hypothesis.*

Then,

$$H_n(T^\beta,T)-G_n(T^\beta,T)=\frac{T}{2\pi^2}\sum_{m=2}^{\infty}\frac{\Lambda^2(m)}{m(\log m)^{2n+2}}-\frac{T}{2\pi^2\beta^{2n}(\log T)^{2n}}\left[A_n+\frac{1}{2n}\right]$$
$$+O\left(\frac{T}{(\log T)^{2n+1}}\right),$$

as $T\to\infty$, where A_n is defined as in (4.3.5).

Proof. Using Lemmas 4.7 and 4.8, and completing the square, we get for $x=T^\beta$,

$$\begin{aligned}
&H_n(T^\beta,T)-G_n(T^\beta,T)\\
&\quad=\frac{T}{2\pi^2}\sum_{m\leqslant x}\frac{\Lambda^2(m)}{m(\log m)^{2n+2}}\left[2f_n\left(\frac{\log m}{\log x}\right)-f_n^2\left(\frac{\log m}{\log x}\right)\right]+O\big(T^{2\beta}\log T\big)\\
&\quad=\frac{T}{2\pi^2}\sum_{m\leqslant x}\frac{\Lambda^2(m)}{m(\log m)^{2n+2}}-\frac{T}{2\pi^2}\sum_{m\leqslant x}\frac{\Lambda^2(m)}{m(\log m)^{2n+2}}\left[1-f_n\left(\frac{\log m}{\log x}\right)\right]^2+O\big(T^{2\beta}\log T\big)\\
&\quad=\frac{T}{2\pi^2}\sum_{m\leqslant x}\frac{\Lambda^2(m)}{m(\log m)^{2n+2}}-\frac{T}{2\pi^2(\log x)^{2n+2}}\sum_{m\leqslant x}\frac{\Lambda^2(m)}{m}\,g_n^2\left(\frac{\log m}{\log x}\right)+O\big(T^{2\beta}\log T\big).
\end{aligned}\tag{4.4.7}$$

Using Lemma 4.10 and partial summation, it is clear that

$$\sum_{m\leqslant x}\frac{\Lambda^2(m)}{m(\log m)^{2n+2}}=\sum_{m=2}^{\infty}\frac{\Lambda^2(m)}{m(\log m)^{2n+2}}-\frac{1}{2n(\log x)^{2n}}+O\left(\frac{1}{\sqrt{x}(\log x)^{2n-1}}\right).\tag{4.4.8}$$

Let us analyze the second term in (4.4.7). By the estimate $|g_n(y)|\ll 1$ for $y\in[0,1]$, we get

$$\sum_{m\leqslant x}\frac{\Lambda^2(m)}{m}\,g_n^2\left(\frac{\log m}{\log x}\right)=\sum_{p\leqslant x}\frac{\log^2 p}{p}\,g_n^2\left(\frac{\log p}{\log x}\right)+O(1).\tag{4.4.9}$$

To analyze the sum over primes on the right-hand side of (4.4.9), we use[5]

$$P(y)=\sum_{p\leqslant y}\frac{\log^2 p}{p}=\frac{\log^2 y}{2}+O(\log y),$$

for $y\geqslant 2$. Then, using integration by parts and the bound $|g_n(y)\,g_n'(y)|\ll 1$ for $y\in[0,1]$ we get

$$\sum_{p\leqslant x}\frac{\log^2 p}{p}\,g_n^2\left(\frac{\log p}{\log x}\right)=\int_{2^-}^{x^+}g_n^2\left(\frac{\log u}{\log x}\right)\,\mathrm{d}P(u)=\left(\int_0^1\alpha\,g_n^2(\alpha)\,\mathrm{d}\alpha\right)\log^2 x+O(\log x).\tag{4.4.10}$$

Therefore, combining (4.4.8), (4.4.9) and (4.4.10) in (4.4.7), we conclude the proof of the proposition. □

[5]This can be obtained using integration by parts in [84, Theorem 2.7 (b)].

4.5 Computing C_n numerically

In this section we study the series that appears in the main term. For each $n \geqslant 1$, let C_n be the series defined in (4.1.6), i.e.

$$C_n = \sum_{m=2}^{\infty} \frac{\Lambda^2(m)}{m\,(\log m)^{2n+2}}.$$

Then, Theorem 4.1 implies that

$$\int_0^T |S_n(t)|^2\, \mathrm{d}t \sim \frac{C_n}{2\pi^2} T.$$

Clearly, C_n satisfies the estimates

$$\frac{1}{2(\log 2)^{2n}} \leqslant C_n \leqslant \frac{1}{2(\log 2)^{2n}} + \frac{A}{(\log 3)^{2n}},$$

for some universal constant $A > 0$. Since $\log 2 < 1$, then $C_n \to \infty$ as $n \to \infty$, with

$$C_n \sim \frac{1}{2(\log 2)^{2n}}.$$

Let us obtain numerical bounds for C_n. To do this, we calculate numerically the first x_n terms of the series and obtain explicit bounds for the tail

$$V_n(x) = \sum_{m>x} \frac{\Lambda^2(m)}{m\,(\log m)^{2n+2}}.$$

Lemma 4.10. *Assume the Riemann hypothesis. Define*

$$M(x) := \sum_{m\leqslant x} \Lambda^2(m).$$

Then, for all $x \geqslant 10^5$,

$$-0.047\sqrt{x}(\log x)^3 \leqslant M(x) - (x\log x - x) \leqslant 0.057\sqrt{x}(\log x)^3, \tag{4.5.1}$$

and

$$-\frac{0.017n + 0.167}{\sqrt{x}(\log x)^{2n-1}} \leqslant V_n(x) - \frac{1}{2n(\log x)^{2n}} \leqslant \frac{0.020n + 0.181}{\sqrt{x}(\log x)^{2n-1}}. \tag{4.5.2}$$

Proof. We recall an explicit version of the Prime Number Theorem error term under RH (see [92, Theorem 10]): letting $\theta(x) = \sum_{p\leqslant x} \log p$, for all $x \geqslant 600$ we have

$$\theta(x) = x + O^*\left(\frac{\sqrt{x}\log^2 x}{8\pi}\right).$$

We start by obtaining explicit bounds for $N(x) := \sum_{p\leqslant x} \log^2 p$. Using integration by parts we have, for $x \geqslant 10^5$,

$$N(x) = N(600) + \int_{600^+}^{x^+} \log y \, \mathrm{d}\theta(y) = x\log x - x + c_0 \\ + O^*\left(\frac{\sqrt{x}\log^3 x}{8\pi}\right) + O^*\left(\frac{1}{8\pi}\int_{600}^{x} \frac{\log^2 y}{\sqrt{y}}\,\mathrm{d}y\right),$$

where $c_0 := N(600) - \theta(600)\log 600 + 600 = 62.9734...$ The above integral is bounded by

$$0 \leqslant \frac{1}{8\pi}\int_{600}^{x} \frac{\log^2 y}{\sqrt{y}}\,\mathrm{d}y \leqslant \frac{\log^2 x}{8\pi}\int_{0}^{x} \frac{\mathrm{d}y}{\sqrt{y}} \leqslant \frac{\sqrt{x}\log^2 x}{4\pi} \leqslant 0.00692\sqrt{x}\log^3 x.$$

This gives

$$N(x) = x\log x - x + c_0 + O^*\big(0.04671\sqrt{x}\log^3 x\big). \tag{4.5.3}$$

In particular, we obtain for $x \geqslant 10^5$ that $N(x) \leqslant x\log x$. This inequality is also true for $45 \leqslant x < 10^5$ by numerical experiment. Now, using these estimates for $N(x)$, we obtain bounds for $M(x)$ as follows:

$$\begin{aligned} \sum_{p\leqslant x} \log^2 p \leqslant \sum_{m\leqslant x} \Lambda^2(m) & \\ &= \sum_{p\leqslant x} \log^2 p + \sum_{p^2\leqslant x} \log^2 p + \sum_{k=3}^{\lfloor \frac{\log x}{\log 2}\rfloor} \sum_{p^k\leqslant x} \log^2 p \\ &\leqslant N(x) + N(\sqrt{x}) + \frac{\log x}{\log 2} N(\sqrt[3]{x}) \\ &\leqslant x\log x - x + c_0 + 0.04671\sqrt{x}\log^3 x + 0.5\sqrt{x}\log x + 0.4809\sqrt[3]{x}\log^2 x \\ &\leqslant x\log x - x + 0.0568\sqrt{x}\log^3 x, \end{aligned}$$

for $x \geqslant 10^5$. The lower bound follows from (4.5.3) and the fact that $c_0 > 0$. This proves (4.5.1). Finally, let us prove (4.5.2). We write $M(x) = x\log x - x + E(x)$. Then, integration by parts gives us

$$V_n(x) = \int_{x^+}^{\infty} \frac{\mathrm{d}M(y)}{y(\log y)^{2n+2}} = \frac{1}{2n(\log x)^{2n}} - \frac{E(x)}{x(\log x)^{2n+2}} + \int_{x}^{\infty} \frac{E(y)\,(2n+2+\log y)}{y^2(\log y)^{2n+3}}\,\mathrm{d}y. \tag{4.5.4}$$

Using the upper bound for $E(x)$ obtained in (4.5.1), we have for $x \geqslant 10^5$,

$$\begin{aligned} \int_{x}^{\infty} \frac{E(y)\,(2n+2+\log y)}{y^2(\log y)^{2n+3}}\,\mathrm{d}y &\leqslant 0.057\int_{x}^{\infty} \frac{(2n+2+\log y)}{y^{3/2}(\log y)^{2n}}\,\mathrm{d}y \\ &\leqslant \frac{0.057}{(\log x)^{2n}}\int_{x}^{\infty} \frac{(2n+2)}{y^{3/2}}\,\mathrm{d}y + \frac{0.057}{(\log x)^{2n-1}}\int_{x}^{\infty} \frac{1}{y^{3/2}}\,\mathrm{d}y \\ &\leqslant \frac{0.020\,n + 0.134}{\sqrt{x}(\log x)^{2n-1}}. \end{aligned}$$

n	x_n	Lower bound for C_n	Upper bound for C_n
1	10^8	1.5651238	1.5651260
2	10^7	2.46232872	2.46232876
3	$5 \cdot 10^5$	4.72243168	4.72243169
4	10^5	9.55058572	9.55058573
5	10^5	19.6650658	19.6650659
6	10^5	40.7601579	40.7601580
7	10^5	84.6986707	84.6986708
8	10^5	176.175788	176.175789
9	10^5	366.593383	366.593384
10	10^5	762.938920	762.938921

Table 4.2: Upper and lower bounds for C_n, for $1 \leqslant n \leqslant 10$.

Similarly, for the same integral we obtain the lower bound $(-0.017\,n - 0.110)/\sqrt{x}(\log x)^{2n-1}$. Finally, combining these estimates with (4.5.1) in (4.5.4) we conclude (4.5.2). $\square$

Table 2 gives the bounds for C_n, applying (4.5.2) for a specific value x_n, in the small cases $1 \leqslant n \leqslant 10$. For $n \geqslant 11$, it can be verified that C_n is essentially given by its exponentially-growing first term $\frac{1}{2(\log 2)^{2n}}$, up to an error of at most 0.1.

Chapter 5

The Riemann zeta-function: the number variance of its zeros

This chapter is comprised of the paper [A4]. As described in Section 1.3.6, our main goal is to obtain a precise formula for the number variance of zeta zeros that holds simultaneously in short and long intervals.

5.1 Introduction

Consider the quantity

$$\int_0^T \Big[S\Big(t + \tfrac{2\pi\delta}{\log T}\Big) - S(t) \Big]^2 \, \mathrm{d}t.$$

As mentioned in Section 1.3.6, Berry [5] (see also [6]) has given a precise conjecture for the asymptotic behavior for this integral (see Section 5.1.3) for details. In the *universal regime* of his model, when $\delta = o(\log T)$, Berry conjectured an asymptotic formula that matches exactly the variance of eigenvalues of GUE random matrices. However, when $\delta \gg \log T$, in the so-called *non-universal regime* of his model, his prediction is no longer described by the predictions from GUE and incorporates additional input from the primes.

Building upon ideas of Selberg [93] and Goldston [53], Gallagher and Mueller [50] and Fujii [46] have given a conditional proof of Berry's conjecture in the universal regime assuming both RH and versions of Montgomery's pair correlation conjecture. In this section, we introduce new ideas to prove novel results on the number variance of zeta zeros in the non-universal regime when $\delta \gg \log T$. In particular, we show that new input from both the zeros and primes is needed in this regime, requiring information on the zeros beyond pair correlation (since we no longer expect GUE behavior in this range). In Section 5.1.2, we give three different formulations of these results, stated as Theorems 5.2 – 5.4. In Section 5.1.3, we show how our results give a conditional proof of Berry's conjecture in the non-universal regime assuming RH and a conjecture of Chan [23] for the pair correlation of zeta zeros in longer ranges (which examines how often gaps between zeros can be close to a fixed nonzero value). Roughly, pair correlation studies the distribution of gap sizes localized near zero with respect to the average spacing, whereas our new results require information about the distribution of gap sizes localized near other points.

Before stating our new results on the number variance of zeta zeros, we first revisit the work of Selberg [93, 94] and Goldston [53] on the moments of $S(t)$ and $\log|\zeta(\frac{1}{2}+it)|$ and the connection to the pair correlation of zeta zeros, which we described in Section 1.3.4. Analogous to Goldston's result (1.3.10) for $S(t)$, our Theorem 5.1 gives lower-order terms for the second moment of $\log|\zeta(\frac{1}{2}+it)|$ assuming RH, in terms of the pair correlation of zeta zeros. Assuming Montgomery's pair correlation conjecture, Theorem 5.1 establishes a special case of a conjecture of Keating and Snaith [72].

5.1.1 The variance in Selberg's central limit theorem

Our first theorem of this chapter is an analogue of Goldston's more precise result for the second moment of $\log|\zeta(\frac{1}{2}+it)|$, refining the case $k=1$ of the Selberg/Tsang result in (1.3.9).

Theorem 5.1. *Assume RH and let $F(\alpha)$ be defined by* (1.3.5)*. Then, as $T\to\infty$,*

$$\int_0^T \log^2|\zeta(\tfrac{1}{2}+it)|\,\mathrm{d}t = \frac{T}{2}\log\log T + aT + o(T),$$

where the constant a is given by (1.3.11)*.*

Assuming Montgomery's strong pair correlation conjecture, we see that

$$a = \frac{1}{2}\left(1+\gamma_0+\sum_{m=2}^{\infty}\sum_p\left(\frac{1}{m^2}-\frac{1}{m}\right)\frac{1}{p^m}\right),$$

and Theorem 5.1 establishes a special case of a conjecture of Keating and Snaith [72, eq. (97)]. We note that Keating and Snaith also made analogous conjectures for families of L-functions in [71].

Though the statement of our first result is very similar to Goldston's theorem, the proofs are considerably different. One reason for this is easy to explain. From the formula for $N(t)$ in (1.3.2), we see that the function $S(t)$ is bounded near the zeros of $\zeta(\frac{1}{2}+it)$, with a jump discontinuity at each zero. On the other hand, $\log|\zeta(\frac{1}{2}+it)|$ is not bounded near the zeros, and can be arbitrarily large in the negative direction. These logarithmic singularities do not substantially change the end result, but they do cause technical difficulties within the proof. Another major difference from Goldston's work is that our proof relies on a delicate cancellation of main terms, which we accomplish by introducing the function $g(x)$ in Section 5.2. Though an analogous cancellation of main terms was not present in Goldston's work, it is present in the work described in Chapter 4, where we introduced related functions to obtain similar cancellations in the study of the second moment of the iterated antiderivatives of $S(t)$ (see Lemma 4.4). However, as we shall see, when considering $\log|\zeta(\frac{1}{2}+it)|$ there are important new technical differences in the properties of our functions due to the unbounded discontinuities.

Remark. The error term in Theorem 5.1 could be improved using additional assumptions such as a quantitative form of the twin prime conjecture (see [25]), or a more precise conjectural formula for pair correlation by Bogomolny and Keating [9] or Conrey and Snaith [38]. For details, see the work of Chan [24].

5.1.2 Number variance of zeta zeros

In a series of papers, Fujii [45, 46, 47] considered the $2k$th moments of the difference of $S(t+\Delta) - S(t)$. Using Selberg's methods, for T sufficiently large, Fujii [45] showed unconditionally that

$$\int_0^T [S(t+\Delta) - S(t)]^{2k} \, \mathrm{d}t = \frac{(2k)!}{(2\pi)^{2k} k!} T (2\log(2+\Delta\log T))^k + O\Big(T\,(\log(2+\Delta\log T))^{k-1/2}\Big) \tag{5.1.1}$$

when $0 < \Delta \ll 1$ and, assuming RH, Fujii [47] showed that

$$\int_0^T [S(t+\Delta) - S(t)]^{2k} \, \mathrm{d}t = \frac{(2k)!2^k}{(2\pi)^{2k} k!} T\big(\log\log T - \log|\zeta(1+i\Delta)|\big)^k + O\Big(T\big(\log\log T\big)^{k-1}\Big) \tag{5.1.2}$$

when $1 \leqslant \Delta \leqslant T$. Fujii's result in (5.1.1) gives an asymptotic formula when $\Delta \log T$ goes to infinity with T (sufficiently slowly). If $\Delta \log T \ll 1$, then the main term and error term in this result are the same order of magnitude and this result does not give an asymptotic formula. Fujii's result in (5.1.2) has an error term of the same order of magnitude as Selberg's conditional result in (1.3.7). In particular, when $k = 1$, the error term in (5.1.2) is $O(T)$. In this case, similarly to Goldston's result for the second moment of $S(t)$, the contribution from the zeros of $\zeta(s)$ give a leading-order term of size T, whereas Selberg's method only treats the contribution from the primes as the main term. Realizing this, Fujii [46] applies Goldston's methods [53] to his own work and, assuming RH, he shows that for $0 < \Delta = o(1)$ we have

$$\begin{aligned}\int_0^T [S(t+\Delta) - S(t)]^2 \, \mathrm{d}t = &\frac{T}{\pi^2}\left\{\int_0^1 \frac{1-\cos(\alpha\Delta\log T)}{\alpha}\,\mathrm{d}\alpha + \int_1^\infty \frac{F(\alpha)\,[1-\cos(\alpha\Delta\log T)]}{\alpha^2}\,\mathrm{d}\alpha\right\}\\ &+ o(T),\end{aligned} \tag{5.1.3}$$

as $T \to \infty$. Gallagher and Mueller [50] had previously given a similar estimate in the limited range $\Delta \simeq \frac{1}{\log T}$ assuming both RH and Montgomery's pair correlation conjecture. A calculation related to (5.1.3) can also be found in recent work of Heap [68, Proposition 9]. Notice that the expression of the main term in (5.1.3) is stated using information from the zeros, in the form of $F(\alpha)$. As we shall see, more information about the distribution of the zeros of $\zeta(s)$ is required in order to accurately describe the situation when $\Delta \gg 1$.

Our next results refine Fujii's calculation in (5.1.3) by giving an asymptotic formula of similar precision but with a much larger range of Δ. This requires expressing the main term in a different manner, giving a better understanding of the behavior of the number variance for zeta zeros for different sizes of Δ. To achieve this, we must overcome significant technical challenges, as new main terms arise and a more careful consideration of the error terms is required. Our result relies on finer information from both the primes and the zeros of $\zeta(s)$. In particular, we require a variation of Montgomery's function $F(\alpha)$ introduced by Chan [23] in his study of the pair correlation of zeros in *longer ranges*. We define[1]

$$F_\Delta(\alpha) = F_\Delta(\alpha, T) := \frac{2\pi}{T\log T} \sum_{0<\gamma,\,\gamma'\leqslant T} T^{i\alpha(\gamma-\gamma'-\Delta)}\, w\big(\gamma-\gamma'-\Delta\big)\,, \tag{5.1.4}$$

and we prove the following theorem.

Theorem 5.2. *Assume RH and let* $0<\Delta = o(\log^2 T)$. *Then, as* $T\to\infty$,

$$\int_0^T [S(t+\Delta)-S(t)]^2\,\mathrm{d}t = \frac{T}{\pi^2}\left\{\frac{1}{2i}\int_0^\Delta \left(\frac{\zeta'}{\zeta}(1+it) - \frac{\zeta'}{\zeta}(1-it) - \frac{2i\cos(t\log T)}{t}\right)\mathrm{d}t + \widetilde{C}(\Delta) \right.$$
$$\left. + \frac{1}{2}\int_1^\infty \frac{2F(\alpha)-F_\Delta(\alpha)-F_{-\Delta}(\alpha)}{\alpha^2}\,\mathrm{d}\alpha\right\} + o(T)$$

and

$$\int_0^T \big[\log\big|\zeta\big(\tfrac12+it+i\Delta\big)\big| - \log\big|\zeta\big(\tfrac12+it\big)\big|\big]^2\,\mathrm{d}t$$
$$= T\left\{\frac{1}{2i}\int_0^\Delta\left(\frac{\zeta'}{\zeta}(1+it)-\frac{\zeta'}{\zeta}(1-it)-\frac{2i\cos(t\log T)}{t}\right)\mathrm{d}t\right.$$
$$\left. + \widetilde{C}(\Delta) + \frac{1}{2}\int_1^\infty \frac{2F(\alpha)-F_\Delta(\alpha)-F_{-\Delta}(\alpha)}{\alpha^2}\,\mathrm{d}\alpha\right\} + o(T),$$

where

$$\widetilde{C}(\Delta) = \sum_{m\geqslant 2}\sum_p \left(\frac{1}{m^2}-\frac{1}{m}\right)\frac{1}{p^m}\Big(1-\cos\left(\Delta m\log p\right)\Big). \tag{5.1.5}$$

[1]Chan works only with the real part of F_Δ.

We highlight that there is new input from the zeros contained in the function F_Δ, and new input from the primes codified in the integral of the logarithmic derivatives of $\zeta(s)$ on the line $\operatorname{Re} s = 1$. The integral involving F_Δ is convergent and remains bounded as $T \to \infty$ (see the remark after Proposition 5.23). Conceivably, Theorem 5.2 continues to hold in a much longer range of Δ. We give two alternative formulations of this theorem. Our first reformulation better illustrates the connection to Fujii's previous result in (5.1.3).

Theorem 5.3. *Assume RH and let $0 < \Delta = o(\log^2 T)$. For $y \geqslant 1$, define*

$$E(y) = \sum_{n \leqslant y} \Lambda(n)^2 - y \log y + y. \tag{5.1.6}$$

Then, as $T \to \infty$,

$$\int_0^T [S(t+\Delta) - S(t)]^2 \, \mathrm{d}t = \frac{T}{\pi^2} \left\{ \int_0^1 \frac{1 - \cos(\Delta\alpha \log T)}{\alpha} \, \mathrm{d}\alpha \right.$$
$$\left. + \frac{1}{2} \int_1^\infty \frac{2F(\alpha) - F_\Delta(\alpha) - F_{-\Delta}(\alpha)}{\alpha^2} \, \mathrm{d}\alpha + c(\Delta) \right\} + o(T)$$

and

$$\int_0^T \left[\log\left|\zeta\left(\tfrac{1}{2} + it + i\Delta\right)\right| - \log\left|\zeta\left(\tfrac{1}{2} + it\right)\right| \right]^2 \mathrm{d}t$$
$$= T \left\{ \int_0^1 \frac{1 - \cos(\Delta\alpha \log T)}{\alpha} \, \mathrm{d}\alpha + \frac{1}{2} \int_1^\infty \frac{2F(\alpha) - F_\Delta(\alpha) - F_{-\Delta}(\alpha)}{\alpha^2} \, \mathrm{d}\alpha \right\}$$
$$+ T\, c(\Delta) + o(T),$$

where

$$c(v) := \int_1^\infty \frac{E(y)}{y^2 \log^3 y} \left[-v \log y \, \sin(v \log y) + \sin^2\!\left(\frac{v \log y}{2}\right) (\log y + 2) \right] \mathrm{d}y - \frac{v^2}{2}. \tag{5.1.7}$$

Using Theorem 5.2, the function $c(v)$ can also be written in terms of the Taylor series expansion of

$$\frac{\zeta'}{\zeta}(1+it) - \frac{\zeta'}{\zeta}(1-it) + \frac{2}{it}$$

about $t = 0$. Note that, for $1 \leqslant y < 2$, we have $E(y) = -y \log y + y$, and the prime number theorem (unconditionally) implies that $E(y) = O(y/\log y)$, as $y \to \infty$. These two facts, together with the inequality $|\sin x| \leqslant |x|$, imply that $c(v)$ is well-defined and that $c(v) \ll v^2$, for all $v \geqslant 0$. In particular, if $\Delta = o(1)$, as in Fujii's case in (5.1.3), then the term $T\, c(\Delta) = o(T)$ and can be absorbed into the error term. Moreover, when $\Delta = o(1)$, we show that this integral reduces to the analogous term in (5.1.3) involving $F(\alpha)$ (see Section 5.6), recovering Fujii's result in this range. This reduction, while based on simple ideas, is quite subtle, and requires another technical but straightforward modification of Montgomery's theorem for $F(\alpha)$ to control some of the error terms.

As explained above for Theorem 5.1, the proofs for the imaginary and real parts of $\log\zeta(\frac{1}{2}+it)$ are similar, but the proof for the real part is significantly more difficult. For this reason, we give the details only for the latter. Although we present the main steps of the proofs of Theorem 5.1 and Theorem 5.3 in parallel, it is important to note that the proof of Theorem 5.1 is independent of the proof of Theorem 5.3. Additionally, we will use Theorem 5.1 to control some of the error terms in some steps for Theorem 5.3 (see Lemma 5.20 below).

Our second reformulation of Theorem 5.2 illustrates the input from the primes and the zeros in a simpler way. As we shall see in the next section, this has the advantage of allowing for a simple comparison with a conjecture of Berry [5].

Theorem 5.4. *Assume RH and let $0 < \Delta = o(\log^2 T)$. Then, as $T \to \infty$,*

$$\int_0^T [S(t+\Delta) - S(t)]^2 \,\mathrm{d}t = \frac{T}{\pi^2}\left\{ \sum_{n\leqslant T} \frac{\Lambda^2(n)}{n\log^2 n}(1-\cos(\Delta\log n)) + \frac{1}{2}\int_1^\infty \frac{2F(\alpha)-F_\Delta(\alpha)-F_{-\Delta}(\alpha)}{\alpha^2}\,\mathrm{d}\alpha\right\} + o(T)$$

and

$$\int_0^T \left[\log\left|\zeta\left(\tfrac{1}{2}+it+i\Delta\right)\right| - \log\left|\zeta\left(\tfrac{1}{2}+it\right)\right|\right]^2 \mathrm{d}t$$

$$= T\left\{ \sum_{n\leqslant T} \frac{\Lambda^2(n)}{n\log^2 n}(1-\cos(\Delta\log n)) + \frac{1}{2}\int_1^\infty \frac{2F(\alpha)-F_\Delta(\alpha)-F_{-\Delta}(\alpha)}{\alpha^2}\,\mathrm{d}\alpha\right\} + o(T).$$

The proofs of all of our theorems rely on knowledge of $F(\alpha)$ and $F_\Delta(\alpha)$ for $|\alpha| \leqslant 1$. It is known that $F(\alpha)$ is real-valued, positive, and even. Moreover, refining Montgomery's original work [81], Goldston and Montgomery [58] showed that

$$F(\alpha) = \left(T^{-2\alpha}\log T + \alpha\right)(1+o(1)), \tag{5.1.8}$$

uniformly for $0 \leqslant \alpha \leqslant 1$. Here, the term of $o(1)$ is of size $O\left(\sqrt{\frac{\log\log T}{\log T}}\right)$. In contrast, the function $F_\Delta(\alpha)$ is no longer positive, nor real, nor even; however, it satisfies the symmetry relations

$$\overline{F_\Delta(\alpha)} = F_\Delta(-\alpha) = F_{-\Delta}(\alpha). \tag{5.1.9}$$

Combining the methods of Chan [23, Theorem 1.1] with Goldston-Montgomery [58], it can be shown that

$$F_\Delta(\alpha) = T^{-2\alpha}\log T + \alpha\, w(\Delta)\, T^{-i\alpha\Delta} + O\left(\frac{1}{\sqrt{\log T}}\right) + O(T^{-2\alpha}) + O_\varepsilon\left(\frac{(\Delta+1)\, T^{-\alpha\left(\frac{1}{2}-\varepsilon\right)}}{\log T}\right), \tag{5.1.10}$$

uniformly for $0 \leqslant \alpha \leqslant 1$ and small $\varepsilon > 0$.

5.1.3 A conjecture of Berry

The Hilbert-Pólya conjecture states that the imaginary parts of the zeros of $\zeta(s)$ correspond to the eigenvalues of some self-adjoint operator, and this would imply RH. In 1973, as a consequence of his work on the pair correlation of zeros, Montgomery [81] was led to conjecture that the zeros of $\zeta(s)$ are distributed as the eigenvalues of a random matrix from the Gaussian unitary ensemble (GUE), giving support to a spectral interpretation of the zeta zeros. Montgomery's conjecture is supported by numerical evidence of Odlyzko [88], which suggests that the GUE model holds for short-range statistics between zeros, such as the distribution of the gap between consecutive zeros. However, Odlyzko's evidence shows that the GUE model fails for long-range statistics, such as the correlation between zeros that are very far apart. In this case, Berry [5] suggested that these long-range statistics are better described in terms of primes, instead of GUE statistics.

Berry [5] proposed a conjectural model for the zeros of $\zeta(s)$, as the eigenvalues of a quantum Hamiltonian operator. His model is expected to conform to the behavior of both short-range and long-range statistics of zeros, as described above. In 1988, Berry used his model to conjecture an asymptotic formula (in terms of our notation) for

$$\int_0^T \left[S\left(t + \tfrac{2\pi\delta}{\log T}\right) - S(t)\right]^2 \mathrm{d}t. \tag{5.1.11}$$

As described above, the universal regime of his model is when $\delta = o(\log T)$, while the non-universal regime corresponds to $\delta \gg \log T$.

We first briefly describe Berry's conjecture following his notation. For $E > 0$, define

$$\mathcal{N}(E) := \frac{E}{2\pi}\left(\log\frac{E}{2\pi} - 1\right) + \frac{7}{8},$$

so that, by (1.3.2), we have $N(E) = \mathcal{N}(E) + S(E) + O\left(\frac{1}{E}\right)$. For $m \geqslant 1$, let $x_m = \mathcal{N}(\gamma_m)$ be the renormalized zeros of $\zeta(s)$, so that the sequence x_m has average spacing 1. In what follows, we let E, x and Δx be three large parameters, which we think of as going to infinity, satisfying the relations $\Delta x = o(x)$ and $x = \mathcal{N}(E) \sim \frac{E}{2\pi}\log E$. For $L < x$, let $n(L; x)$ be the number of renormalized zeros x_m in the interval $\left[x - \frac{L}{2}, x + \frac{L}{2}\right]$. In particular, note that

$$n(L;x) = L + S\left(\mathcal{N}^{-1}\left(x + \frac{L}{2}\right)\right) - S\left(\mathcal{N}^{-1}\left(x - \frac{L}{2}\right)\right) + O\left(\frac{\log x}{x}\right).$$

We define the variance as

$$V(L;x) = \left\langle [n(L;x) - L]^2 \right\rangle := \frac{1}{\Delta x} \int_{x-\frac{\Delta x}{2}}^{x+\frac{\Delta x}{2}} [n(L;y) - L]^2 \, \mathrm{d}y.$$

Finally, we let τ^* be another parameter, such that $\tau^* = \frac{\Phi(E)}{\log(E/2\pi)}$ for some function $\Phi(E)$ that goes to infinity as $E \to \infty$. Berry's conjectural formula [5, Eq. (19)] states that

$$\begin{aligned} V(L;x) \sim & \frac{1}{\pi^2} \left[\log(2\pi L) - \mathrm{Ci}(2\pi L) - 2\pi L \, \mathrm{Si}(2\pi L) + \pi^2 L - \cos(2\pi L) + 1 + \gamma_0 \right] \\ & + \frac{1}{\pi^2} \left[2 \sum_{r=1}^{\infty} \sum_{p}^{p^r < (E/2\pi)^{\tau^*}} \frac{\sin^2(\pi L r \log p / \log(E/2\pi))}{r^2 p^r} + \mathrm{Ci}(2\pi L \tau^*) - \log(2\pi L \tau^*) - \gamma_0 \right], \end{aligned}$$

as $E \to \infty$, where γ_0 is Euler's constant,

$$\mathrm{Si}(x) := \int_0^x \frac{\sin u}{u} \, \mathrm{d}u, \quad \text{and} \quad \mathrm{Ci}(x) := -\int_x^{\infty} \frac{\cos u}{u} \, \mathrm{d}u. \tag{5.1.12}$$

The right-hand side does not depend on the choice of τ^*, as $E \to \infty$. The universal regime is when $L = o(1/\tau^*)$, where the term in the first set of brackets is the dominant (leading order) term. See also [5, Eqs. (20) and (21)] for simplifications in different ranges of L. Translating to our normalization and our notation, Berry made the following conjecture.

Conjecture 5.5 (Berry, 1988)**.** *Let $\delta > 0$. Then, as $T \to \infty$, the following asymptotic formulae hold.*
(a): *If $\delta = o(\log T)$, then*

$$\int_0^T \left[S\left(t + \tfrac{2\pi\delta}{\log T}\right) - S(t) \right]^2 \mathrm{d}t \sim \frac{T}{\pi^2} \left[\log(2\pi\delta) - \mathrm{Ci}(2\pi\delta) - 2\pi\delta \, \mathrm{Si}(2\pi\delta) + \pi^2\delta - \cos(2\pi\delta) + 1 + \gamma_0 \right]$$

(b): *If $\delta \gg \log T$, then*

$$\int_0^T \left[S\left(t + \tfrac{2\pi\delta}{\log T}\right) - S(t) \right]^2 \mathrm{d}t \sim \frac{T}{\pi^2} \left[\sum_{n \leqslant T} \frac{\Lambda^2(n)}{n \log^2 n} \left(1 - \cos\left(\frac{2\pi\delta \, \log n}{\log T} \right) \right) + 1 \right]$$

In 1990, Fujii [46] proved an asymptotic formula for (5.1.11), assuming RH, in the universal regime where $\delta = o(\log T)$. In particular, assuming RH and Montgomery's strong pair correlation conjecture, Fujii proves Berry's conjecture in the universal regime (part (a) of the above conjecture). However, Fujii's proof relies on the fact that $\frac{\delta}{\log T} \to 0$ as $T \to \infty$ in numerous places, and it is not obvious that his proof can be modified to establish part (b) up to an error of size $o(T)$.

Assuming RH and a version of the strong pair correlation conjecture (in longer ranges) due to Chan, we show that our formulae in Theorems 5.2 – 5.4 imply Berry's conjecture in both the universal and the non-universal regimes. Although Berry never conjectures the range of δ for which part (b) of Conjecture 5.5 holds, we verify his conjecture holds in the range $\delta = o(\log^{\frac{4}{3}} T)$. Conceivably part (b) continues to hold for δ in a much longer range. We require the following generalization of the strong form of Montgomery's pair correlation conjecture due to Chan [23, Conjecture 1.1].

Conjecture 5.6 (Chan, 2004)**.** *For $|\alpha| \geqslant 1$ and $\Delta = o\Big(\log^{\frac{1}{3}} T\Big)$, we have*

$$F_\Delta(\alpha) = T^{-i\alpha\Delta}\, w(\Delta)\, \big(1 + o(1)\big),$$

uniformly for α in compact intervals as $T \to \infty$.

Corollary 5.7. *Assume RH and Conjecture 5.6. Then, Conjecture 5.5 holds for all $\delta = o\Big(\log^{\frac{4}{3}} T\Big)$.*

The restriction on δ in the above corollary comes from Conjecture 5.6. As we shall see, the restriction $\Delta = o(\log^2 T)$ in Theorems 5.2 – 5.4, corresponding to $\delta = o(\log^3 T)$, arises naturally in two different places. It first arises from the last error term in the formula (5.1.10) for $F_\Delta(\alpha)$ from [23, Theorem 1.1] (see Lemma 5.16), and it again arises from estimating a sum over primes in Lemma 5.21 below. In the following sections, we attempt to state each lemma in the largest possible range of Δ to clarify where these restrictions appear.

5.2 A representation formula for $\log|\zeta(1/2 + it)|$

5.2.1 Some auxiliary functions

Following the ideas developed by Goldston [53], we must obtain a representation formula for $\log|\zeta(1/2+it)|$ in terms of a Dirichlet polynomial supported over prime powers and a sum over the zeros of $\zeta(s)$. This is based on an explicit formula of Montgomery [81] and, in our case, requires introducing three auxiliary, real-valued functions, whose technical properties play important roles in our proof. For $u \in (0, 2)$, define

$$f(u) := u \int_0^\infty \frac{\sinh[y(1-u)]}{\cosh y}\, \mathrm{d}y; \tag{5.2.1}$$

for $u \in (-2, 2)$, define

$$g(u) := \int_0^\infty \frac{e^{-y}\cosh(uy)}{\cosh y}\, \mathrm{d}y; \tag{5.2.2}$$

and for $u \in \mathbb{R}\backslash\{0\}$, define

$$h(u) := \cos u \int_0^\infty \frac{y}{\cosh y} \frac{\mathrm{d}y}{y^2 + u^2}. \tag{5.2.3}$$

Before stating our representation formula, we collect relevant properties of f, h and g in the following lemma. This is similar to the ideas and functions used in Lemmas 4.4 and 4.5, and they will be used to obtain a delicate cancellation of main terms.

Lemma 5.8. *Let f, h, and g be defined in* (5.2.1), (5.2.3), *and* (5.2.2), *respectively. Then*

(*a*) *we have $g \in C^{\infty}(-2, 2)$ and g is even;*

(*b*) *for $u \in (0, 2)$, we have*

$$g(u) = \frac{1 - f(u)}{u};$$

(*c*) *we have $h \in L^1(\mathbb{R}) \cap L^2(\mathbb{R})$, h is even, and*

$$\widehat{h}(a) = \pi \begin{cases} g(2\pi a), & \text{if } 2\pi|a| \leqslant 1, \\ \dfrac{1}{2\pi|a|}, & \text{if } 2\pi|a| > 1. \end{cases}$$

Remark. We highlight that h has an unbounded but integrable singularity at the origin, which is different from the situation in both [53] and in Chapter 4. We also note that f, g, and their derivatives are uniformly bounded on the interval $[0, 1]$.

Proof. First we consider $g(u)$ as defined in (5.2.2). By the Dominated Convergence Theorem we have that $g \in C^{\infty}(-2, 2)$. The fact that g is even follows from the fact that $\cosh(y)$ is even. Now let $u \in (0, 2)$. Then for all $u > 0$, we know

$$\frac{1}{u} = \int_0^{\infty} e^{-uy} \, \mathrm{d}\, y.$$

Using this representation for $\frac{1}{u}$, it follows that

$$\frac{1 - f(u)}{u} = \int_0^{\infty} \frac{e^{-y}\left(e^{uy} + e^{-uy}\right)}{e^{y} + e^{-y}} \, \mathrm{d}\, y = \int_0^{\infty} \frac{e^{-y}\cosh(uy)}{\cosh y} \, \mathrm{d}\, y = g(u),$$

as claimed. Next we consider $h(u)$ defined in (5.2.3). First, observe that $h(u)$ is even by construction. Next, we will show that $h \in L^1(\mathbb{R})$. By the definition of h, observe that

$$\int_{-\infty}^{\infty} |h(v)| \, \mathrm{d}v \leqslant 2 \int_0^{\infty} \frac{1}{\cosh u} \int_0^{\infty} \frac{u}{u^2 + v^2} \, \mathrm{d}v \, \mathrm{d}u = \pi \int_0^{\infty} \frac{\mathrm{d}u}{\cosh u} = \pi^2,$$

which implies $h \in L^1(\mathbb{R})$. Next, we calculate the Fourier transform of $h(v)$ using the well known Fourier pair

$$\varphi(y) = e^{-2\pi|y|} \quad \text{and} \quad \widehat{\varphi}(\xi) = \frac{1}{\pi}\frac{1}{1 + \xi^2}. \tag{5.2.4}$$

Let $a \in \mathbb{R}$. Since h is even, we may assume $a \geqslant 0$. Using the variable change $w = \frac{v}{u}$ and (5.2.4), it follows that

$$\begin{aligned}
\widehat{h}(a) &= \int_{-\infty}^{\infty} h(v)\, e^{-2\pi i a v}\ \mathrm{d}v \\
&= \int_0^{\infty} \frac{u}{\cosh u} \int_{-\infty}^{\infty} \frac{\cos v}{u^2+v^2}\ e^{-2\pi i a v}\ \mathrm{d}v\ \mathrm{d}u \\
&= \frac{1}{2}\int_0^{\infty} \frac{1}{\cosh u} \int_{-\infty}^{\infty} \frac{\left(e^{u(\frac{1}{2\pi}-a)2\pi i w} + e^{u(-\frac{1}{2\pi}-a)2\pi i w}\right)}{1+w^2}\ \mathrm{d}w\ \mathrm{d}u \\
&= \frac{\pi}{2}\int_0^{\infty} \frac{1}{\cosh u}\left(e^{-u|1-2\pi a|} + e^{-u|1+2\pi a|}\right)\ \mathrm{d}u \\
&= \begin{cases} \pi\ g(2\pi a), & 0 \leqslant 2\pi a \leqslant 1, \\ \dfrac{1}{2a}, & 2\pi a > 1. \end{cases}
\end{aligned}$$

Clearly, $\widehat{h} \in L^2(\mathbb{R})$, and therefore $h \in L^2(\mathbb{R})$. This completes the proof. $\square$

5.2.2 Representation formula

We now state our formula for $\log|\zeta(\frac{1}{2}+it)|$.

Lemma 5.9. *Assume RH. For $x \geqslant 4$, $t \geqslant 1$, and $t \neq \gamma$, we have*

$$\log|\zeta(\tfrac{1}{2}+it)| = -\sum_{\gamma} h[(\gamma - t)\log x] + \sum_{n \leqslant x} \frac{\Lambda(n)\cos(t\log n)}{n^{1/2}\log n} f\left(\frac{\log n}{\log x}\right) + \frac{\log 2\ \log\frac{t}{2\pi}}{2\log x} + O\left(\frac{x^{1/2}}{t\log^2 x}\right).$$

Proof. We begin with the fact that, for $t \neq \gamma$, we have

$$\log|\zeta(\tfrac{1}{2}+it)| = -\int_{1/2}^{\infty} \operatorname{Re}\frac{\zeta'}{\zeta}(\sigma+it)\,\mathrm{d}\sigma.$$

Now we use the slightly modified version of Montgomery's explicit formula [81] obtained in (4.2.6). For $\rho = \frac{1}{2}+i\gamma$, $x \geqslant 4$, $s = \sigma + it$ with $\sigma > \frac{1}{2}$ and $t \geqslant 1$, we have

$$\begin{aligned}
(x^{\sigma-\frac{1}{2}} + x^{\frac{1}{2}-\sigma})\operatorname{Re}\frac{\zeta'}{\zeta}(\sigma+it) &= \sum_{\gamma}\cos((t-\gamma)\log x)\frac{2(\sigma-\frac{1}{2})}{(\sigma-\frac{1}{2})^2+(t-\gamma)^2} \\
&\quad - \sum_{n\leqslant x}\Lambda(n)\cos(t\log n)\left(\frac{x^{\sigma-\frac{1}{2}}}{n^{\sigma}} - \frac{x^{\frac{1}{2}-\sigma}}{n^{1-\sigma}}\right)
\end{aligned}$$

$$
\begin{aligned}
&- x^{\frac{1}{2}}\mathrm{Re}\left(\frac{x^{-it}(1-2\sigma)}{(\sigma-it)(1-\sigma-it)}\right) - x^{\frac{1}{2}-\sigma}\log\left(\frac{t}{2\pi}\right) \\
&+ O\bigg(\frac{\sigma^2}{t}\left(x^{-5/2}+x^{1/2-\sigma}\right)\bigg). \qquad (5.2.5)
\end{aligned}
$$

This immediately follows from (4.2.6) by letting $n = 1$ therein and taking real parts. Dividing by $(x^{\sigma-\frac{1}{2}} + x^{\frac{1}{2}-\sigma}) = 2\cosh((\sigma-\frac{1}{2})\log x)$ and integrating (5.2.5) from $\frac{1}{2}$ to infinity, for $x \geqslant 4$, $t \geqslant 1$, and $t \neq \gamma$ we have

$$
\begin{aligned}
\log|\zeta(\tfrac{1}{2}+it)| = &-\sum_{\gamma}\cos((t-\gamma)\log x)\int\limits_{1/2}^{\infty}\frac{(\sigma-\frac{1}{2})}{(\sigma-\frac{1}{2})^2+(t-\gamma)^2}\frac{\mathrm{d}\sigma}{\cosh((\sigma-\frac{1}{2})\log x)} \\
&+\sum_{n\leqslant x}\Lambda(n)\cos(t\log n)\int\limits_{1/2}^{\infty}\left(\frac{x^{\sigma-\frac{1}{2}}}{n^{\sigma}}-\frac{x^{\frac{1}{2}-\sigma}}{n^{1-\sigma}}\right)\frac{\mathrm{d}\sigma}{2\cosh((\sigma-\frac{1}{2})\log x)} \\
&+x^{1/2}\mathrm{Re}\left(x^{-it}\int\limits_{1/2}^{\infty}\frac{(\frac{1}{2}-\sigma)}{(\sigma-it)(1-\sigma-it)}\frac{\mathrm{d}\sigma}{\cosh((\sigma-\frac{1}{2})\log x)}\right) \\
&+\frac{1}{2}\log\frac{t}{2\pi}\int\limits_{1/2}^{\infty}\frac{x^{\frac{1}{2}-\sigma}}{\cosh((\sigma-\frac{1}{2})\log x)}\,\mathrm{d}\sigma + O\left(\frac{1}{t}\int\limits_{1/2}^{\infty}\frac{\sigma^2\left(x^{-5/2}+x^{1/2-\sigma}\right)}{\cosh((\sigma-\frac{1}{2})\log x)}\,\mathrm{d}\sigma\right).
\end{aligned}
\qquad (5.2.6)
$$

By using the substitution, $u = (\sigma-\frac{1}{2})\log x$, the integral in the second main term of (5.2.6) yields

$$
\int\limits_{1/2}^{\infty}\left(\frac{x^{\sigma-\frac{1}{2}}}{n^{\sigma}}-\frac{x^{\frac{1}{2}-\sigma}}{n^{1-\sigma}}\right)\frac{\mathrm{d}\sigma}{2\cosh((\sigma-\frac{1}{2})\log x)} = \frac{1}{n^{1/2}\log n}f\left(\frac{\log n}{\log x}\right),
$$

where f is defined in (5.2.1). Again, by the same substitution, for the first main term of (5.2.6), we have

$$
-\sum_{\gamma}\cos((t-\gamma)\log x)\int\limits_{1/2}^{\infty}\frac{(\sigma-\frac{1}{2})}{(\sigma-\frac{1}{2})^2+(t-\gamma)^2}\frac{\mathrm{d}\sigma}{\cosh((\sigma-\frac{1}{2})\log x)} = -\sum_{\gamma}h[(t-\gamma')\log x],
$$

where h is defined in (5.2.3). Finally, the fourth term of (5.2.6) equals

$$
\frac{\log\frac{t}{2\pi}}{2}\int\limits_{1/2}^{\infty}\frac{x^{\frac{1}{2}-\sigma}}{\cosh((\sigma-\frac{1}{2})\log x)}\,\mathrm{d}\sigma = \frac{\log 2\log\frac{t}{2\pi}}{2\log x}.
$$

The other terms are error terms and can be treated similarly to the proof of [53, Lemma 1]. Combining all the terms of (5.2.6) completes the proof. $\square$

Note that we have the extra main term $\frac{\log 2 \log t/2\pi}{\log x}$ when compared to Goldston's formula for $S(t)$ in [53, Lemma 1]. This comes from Stirling's formula when analyzing the real part of $\frac{\zeta'}{\zeta}(s)$, and it does not appear when taking the imaginary part. We use Lemma 5.9 to obtain an expression for the quantities we want to compute in Theorems 5.1 and 5.3. We now adopt some notation for the expressions we will consider. Henceforth, let $T \geqslant 4$ and $\Delta = \Delta(T)$ be a function of T such that $0 < \Delta \ll T^b$, for some fixed $0 < b < 1$. For $t \geqslant 1$, denote

$$A(t) := \sum_{n \leqslant x} \frac{\Lambda(n)\cos(t\log n)}{n^{1/2}\log n} f\left(\frac{\log n}{\log x}\right) \quad \text{and} \quad B(t) := -\sum_{\gamma} h[(\gamma - t)\log x], \tag{5.2.7}$$

so that $A(t)$ contains the information on primes and $B(t)$ contains the information on zeros in our expression for $\log|\zeta(1/2+it)|$. Additionally, denote

$$\begin{aligned}
G_1 &:= -\int_1^T |A(t)|^2 \, \mathrm{d}t, \qquad G_2 := -\int_1^T |A(t+\Delta) - A(t)|^2 \, \mathrm{d}t,\\
H_1 &:= 2\int_1^T A(t) \log|\zeta(\tfrac12 + it)| \, \mathrm{d}t,\\
H_2 &:= 2\int_1^T [A(t+\Delta) - A(t)]\left[\log\left|\zeta\left(\tfrac12 + it + i\Delta\right)\right| - \log\left|\zeta\left(\tfrac12 + it\right)\right|\right] \, \mathrm{d}t,\\
R_1 &:= \int_1^T |B(t)|^2 \, \mathrm{d}t, \qquad R_2 := \int_1^T |B(t+\Delta) - B(t)|^2 \, \mathrm{d}t.
\end{aligned} \tag{5.2.8}$$

In the next result, we use Lemma 5.9 to write the objects in Theorems 5.1 and 5.3 in terms of the above expressions G_i, H_i, and R_i.

Lemma 5.10. *Assume RH. Let $4 \leqslant x \leqslant T$ and let $0 < \Delta \ll T^b$, where $b < \frac12$. Then, as $T \to \infty$, we have*

(a) $$\int_1^T \log^2|\zeta(\tfrac12 + it)| \, \mathrm{d}t = G_1 + H_1 + R_1 - T\log^2 T \frac{\log^2 2}{4\log^2 x} + O\left(\frac{T\log T}{\log^2 x}\right) + O\left(\frac{\sqrt{xR_1}}{\log^2 x}\right);$$

(b) $$\int_1^T \left[\log\left|\zeta\left(\tfrac12 + it + i\Delta\right)\right| - \log\left|\zeta\left(\tfrac12 + it\right)\right|\right]^2 \mathrm{d}t = G_2 + H_2 + R_2 + O\left(\frac{T}{\log^4 x}\right) + O\left(\frac{\sqrt{TR_2}}{\log^2 x}\right).$$

Proof. Let $4 \leqslant x \leqslant T$ and let $0 < \Delta \ll T^b$, where $b < \frac12$. By rearranging the terms in Lemma 5.9, we have

$$B(t) + O\left(\frac{x^{1/2}}{t\log^2 x}\right) = \log|\zeta(\tfrac12 + it)| - A(t) - \frac{\log 2 \log \frac{t}{2\pi}}{2\log x}.$$

Squaring the above expression and then integrating from 1 to T yields

$$\begin{aligned} R_1 &+ O\left(\frac{\sqrt{x R_1}}{\log^2 x}\right) + O\left(\frac{x}{\log^4 x}\right) \\ &= \int_1^T \log^2 |\zeta(\tfrac{1}{2}+it)| \, \mathrm{d}t - H_1 - G_1 + \frac{\log^2 2}{4} \frac{T \log^2 T}{\log^2 x} + O\left(\frac{T \log T}{\log^2 x}\right) \\ &\quad + O\left(\frac{1}{\log x}\left|\int_1^T A(t) \log t \, \mathrm{d}t\right|\right) + O\left(\frac{1}{\log x}\left|\int_1^T \log|\zeta(\tfrac{1}{2}+it)| \log t \, \mathrm{d}t\right|\right), \end{aligned} \tag{5.2.9}$$

where we used the Cauchy-Schwarz inequality to bound the first error term on the left-hand side. For the second error term on the right-hand side of (5.2.9), since $f(v)$ is uniformly bounded for all $v \in [0,1]$, $|\cos(v)| \leqslant 1$ for all $v \in \mathbb{R}$, and $\int_1^T n^{it} \log t \, \mathrm{d}t \ll \log T$ for $n \geqslant 2$, we see that

$$\int_1^T A(t) \frac{\log t}{\log x} \, \mathrm{d}t \ll \frac{\log T}{\log x} \sum_{n \leqslant x} \frac{\Lambda(n)}{n^{1/2} \log n} \ll \frac{\sqrt{x}}{\log x} \log T.$$

To control the last error term on the right-hand side of (5.2.9), consider the antiderivative of $\log|\zeta(\frac{1}{2}+it)|$. Assuming RH, it is known that

$$\int_1^T \log|\zeta(\tfrac{1}{2}+it)| \, \mathrm{d}t \ll \log T.$$

(See [15, Lemma 2.2] for a slightly stronger estimate.) Thus, using integration by parts, we obtain

$$\frac{1}{\log x} \int_1^T \log|\zeta(\tfrac{1}{2}+it)| \log t \, \mathrm{d}t \ll \frac{\log^2 T}{\log x}.$$

By combining and rearranging all the calculations for the terms in (5.2.9), we complete the proof of part (a).

For the proof of part (b), since $\Delta \ll T^b$, we observe that for $t > 1$, $x \geqslant 4$, and $\varepsilon > 0$ the Mean Value Theorem implies that

$$\frac{\log 2 \left[\log\left(\frac{t+\Delta}{2\pi}\right) - \log \frac{t}{2\pi}\right]}{2 \log x} \ll_{\varepsilon} \frac{T^{\frac{1}{2}-\varepsilon}}{t \log x},$$

so that this term is absorbed into the error bound. The rest of the proof of part (b) is analogous to the proof of part (a). Consequently, the proof is complete. □

In order to conclude the proofs of Theorems 5.1 and 5.3, the following sections are devoted to estimating the quantities G_i, H_i and R_i.

5.3 Contributions from the zeros

5.3.1 Auxilliary lemmas

Before we compute R_i, we remark that the constant a as defined in (1.3.11) actually has a mild dependence on T, since it is defined in terms of $F(\alpha, T)$. In this subsection, we collect several useful technical estimates regarding the zeros and the function $F_\Delta(\alpha, T)$, and we show that this dependence on T can be controlled in the proofs of our main theorems.

Lemma 5.11. *Assume RH. Let $T \geqslant 4$ and $\Delta = O(\log^2 T)$. Then, for $\beta > 0$, we have*

$$\int_0^\beta 2F(\alpha) - F_\Delta(\alpha) - F_{-\Delta}(\alpha) \, \mathrm{d}\alpha \ll (1+\beta)\left(1 + \frac{|\Delta|}{\log^2 T}\right) \quad \textit{and}$$

$$\int_1^\infty \frac{2F(\alpha) - F_\Delta(\alpha) - F_{-\Delta}(\alpha)}{\alpha^2} \, \mathrm{d}\alpha \ll 1 + \frac{|\Delta|}{\log^2 T},$$

where the implied constants are universal.

Proof. Consider the identity

$$\begin{aligned} 2F(\alpha) - F_\Delta(\alpha) - F_{-\Delta}(\alpha) &= \\ \frac{8\pi^2}{T \log T} \int_{-\infty}^{\infty} e^{-4\pi|u|} &\left[1 - \cos(\Delta\alpha \log T + 2\pi\Delta u)\right] \left| \sum_{0<\gamma\leqslant T} T^{i\alpha\gamma} e^{2\pi i u\gamma} \right|^2 \mathrm{d}u. \end{aligned} \tag{5.3.1}$$

In particular, $2F(\alpha) - F_\Delta(\alpha) - F_{-\Delta}(\alpha) \geqslant 0$. Lemma 5.11 follows by modifying an argument of Goldston [53, Lemma A] in a straightforward manner and applying Chan's theorem for $F_\Delta(\alpha)$ in the form given in (5.1.10). $\square$

Lemma 5.12. *Let $T \geqslant 4$, $0 \leqslant |\Delta| \leqslant T$, $0 < H \leqslant T$, and $w(u) = \frac{4}{4+u^2}$. Then,*

(a) $\displaystyle\sum_{0<\gamma,\gamma'\leqslant T} |\gamma - \gamma' - \Delta| w(\gamma - \gamma' - \Delta) \ll T \log^3 T;$

(b) $\displaystyle\sum_{T-|\Delta|-1\leqslant\gamma,\gamma'\leqslant T+H} w(\gamma - \gamma' - \Delta) \ll (H + |\Delta| + 1) \log^2 T;$

(c) $\displaystyle\sum_{\substack{0<\gamma<T-|\Delta|-1 \\ T\leqslant\gamma'\leqslant T+H}} w(\gamma - \gamma' - \Delta) \ll \log^3 T;$

where the implied constants are universal.

Proof. By interchanging γ and γ', we may assume that $\Delta \geqslant 0$. We have

$$\begin{aligned}\sum_{0<\gamma,\gamma'\leqslant T} |\gamma-\gamma'-\Delta| w(\gamma-\gamma'-\Delta) = & \sum_{\substack{0<\gamma,\gamma'\leqslant T \\ \gamma-\gamma'-\Delta<0}} (\Delta+\gamma'-\gamma) w(\gamma-\gamma'-\Delta) \\ & + \sum_{\substack{0<\gamma,\gamma'\leqslant T \\ \gamma-\gamma'-\Delta>0}} (\gamma-\gamma'-\Delta) w(\gamma-\gamma'-\Delta) \\ & = Z_1 + Z_2,\end{aligned}$$

say. We use the inequality

$$\frac{4|u|}{4+u^2} \leqslant \min\left(1, \frac{4}{|u|}\right)$$

and the fact that there are $O(\log T)$ zeros in the interval $[T-\Delta-2, T-\Delta]$ to estimate Z_1 as follows:

$$\begin{aligned}Z_1 &\leqslant \sum_{0<\gamma\leqslant T} \sum_{\gamma-\Delta<\gamma'<\gamma-\Delta+2} 1 + \sum_{0<\gamma\leqslant T} \sum_{\gamma-\Delta+2<\gamma'\leqslant T} \frac{4}{\Delta+\gamma'-\gamma} \\ &\ll \sum_{0<\gamma\leqslant T} \log T + \sum_{0<\gamma\leqslant T} \sum_{\gamma+2<n\leqslant T+\Delta} \frac{\log n}{n-\gamma} \\ &\ll T\log^2 T + \sum_{0<\gamma\leqslant T} \log^2(\Delta+T) \\ &\ll T\log^3 T,\end{aligned}$$

since $\Delta \leqslant T$. The bound $Z_2 \ll T\log^3 T$ is similar. This proves part (a).

For part (b), since $0 < H \leqslant T$, we use that there are $O(\log T)$ zeros in the interval $(n, n+1)$ (for $0 \leqslant n \leqslant T+H$) to obtain:

$$\begin{aligned}&\sum_{T-|\Delta|-1\leqslant\gamma,\gamma'\leqslant T+H} w(\gamma-\gamma'-\Delta) \\ &\ll \log T \sum_{T-|\Delta|-1\leqslant\gamma\leqslant T+H} \sum_{0\leqslant n\leqslant H+|\Delta|+1} \frac{1}{1+(\gamma-T+|\Delta|+1-n-\Delta)^2} \\ &\ll \log T \sum_{T-|\Delta|-1\leqslant\gamma\leqslant T+H} 1 \ll (H+|\Delta|+1)\log^2 T.\end{aligned}$$

In the last line, we used that, since the summand is positive, we may bound the sum over n by a sum over all integers, and the function

$$\sum_{n\in\mathbb{Z}} \frac{1}{1+(x+n)^2}$$

converges to a continuous periodic function of $x \in \mathbb{R}$. In particular, it is uniformly bounded.

For part (c), note that, for $0 < \gamma < T - |\Delta| - 1$ and $T \leqslant \gamma' \leqslant T + H$, we have

$|\gamma-\gamma'-\Delta| \geqslant T+\Delta-\gamma \geqslant 1$. Then, using that $w(u) \leqslant \frac{4}{u^2}$, we have

$$\begin{aligned}\sum_{\substack{0<\gamma<T-|\Delta|-1 \\ T\leqslant\gamma'\leqslant T+H}} w(\gamma-\gamma'-\Delta) &\ll \log T \sum_{0<\gamma<T-|\Delta|-1}\ \sum_{0\leqslant n\leqslant H+1} \frac{1}{(T+n+\Delta-\gamma)^2} \\ &\ll \log T \sum_{0<\gamma<T-|\Delta|-1} \frac{1}{T+\Delta-\gamma} \\ &\ll \log^2 T \sum_{1\leqslant n\leqslant T+|\Delta|} \frac{1}{n} \ll \log^3 T,\end{aligned}$$

since $|\Delta| \leqslant T$.

$\square$

Lemma 5.13. *Assume RH. For $T \geqslant 4$, let $|\Delta| \leqslant \log^2 T$, and let $0 < H \leqslant T$. We have*

(a) $$\int_1^\infty \frac{F(\alpha,T+H)}{\alpha^2}\,d\alpha = \int_1^\infty \frac{F(\alpha,T)}{\alpha^2}\,d\alpha + O\Big(\frac{(H+1)}{T}\log^3 T\Big);$$

(b) $$\int_1^\infty \frac{2F(\alpha,T+H)-F_\Delta(\alpha,T+H)-F_{-\Delta}(\alpha,T+H)}{\alpha^2}\,d\alpha$$
$$= \int_1^\infty \frac{2F(\alpha,T)-F_\Delta(\alpha,T)-F_{-\Delta}(\alpha,T)}{\alpha^2}\,d\alpha + O\Big(\frac{(H+|\Delta|+1)}{T}\log^3 T\Big).$$

Here, the implied constants are universal.

Proof. First, we prove a pointwise estimate for $F_\Delta(\alpha, T+H)$ that holds in the larger range $|\Delta| \leqslant T$ and is useful for both parts (a) and (b). By the mean-value theorem, for $\theta \in \mathbb{R}$, we have

$$|(T+H)^{i\theta} - T^{i\theta}| \ll \frac{H|\theta|}{T} \quad \text{and} \quad \frac{1}{(T+H)\log(T+H)} = \frac{1}{T\log T}\left(1+O\left(\frac{H}{T}\right)\right).$$

Therefore, for $\Delta \in \mathbb{R}$ with $|\Delta| \leqslant T$, we have

$$F_\Delta(\alpha,T+H) = \frac{2\pi}{T\log T}\sum_{0<\gamma,\gamma'\leqslant T+H}(T+H)^{i\alpha(\gamma-\gamma'-\Delta)}w(\gamma-\gamma'-\Delta)+O\left(\frac{H}{T}F_\Delta(0,T+H)\right).$$

To bound the last error term, one can see that $|F_\Delta(\alpha,T)| \leqslant F_\Delta(0,T) \ll \log T$ (uniformly for $0 \leqslant |\Delta| \leqslant T$), analogously to the classical bound for $\Delta = 0$. Now, to estimate the difference $|F_\Delta(\alpha,T+H)-F_\Delta(\alpha,T)|$, we separate the double sum over zeros in $F_\Delta(\alpha,T+H)$ depending on whether the zeros lie in the interval $(0,T]$ or $(T,T+H]$. Using the triangle inequality, we obtain

$$\begin{aligned}|F_\Delta(\alpha,T+H)-F_\Delta(\alpha,T)| \leqslant{}& \frac{2\pi}{T\log T}\sum_{0<\gamma,\gamma'\leqslant T}\big|(T+H)^{i\alpha(\gamma-\gamma'-\Delta)} - T^{i\alpha(\gamma-\gamma'-\Delta)}\big|w(\gamma-\gamma'-\Delta) \\ &+ \frac{2\pi}{T\log T}\sum_{T<\gamma,\gamma'\leqslant T+H} w(\gamma-\gamma'-\Delta)\end{aligned}$$

$$
\begin{aligned}
&+ \frac{2\pi}{T\log T} \sum_{\substack{0<\gamma\leqslant T\\ T<\gamma'\leqslant T+H}} w(\gamma-\gamma'-\Delta)\\
&+ \frac{2\pi}{T\log T} \sum_{\substack{0<\gamma'\leqslant T\\ T<\gamma\leqslant T+H}} w(\gamma-\gamma'-\Delta) + O\left(\frac{H}{T}\log T\right)\\
&= Y_1+Y_2+Y_3+Y_4+O\left(\frac{H}{T}\log T\right),
\end{aligned}
$$

say. By the mean-value theorem and part (a) of Lemma 5.12, we find that $Y_1 \ll \frac{H}{T}|\alpha|\log^2 T$. Since $w(u)\geqslant 0$, we may extend the sum in Y_2 to apply part (b) of Lemma 5.12. Therefore, $Y_2 \ll \frac{1}{T}(H+|\Delta|+1)\log T$. We estimate Y_3 by further dividing the sum into two parts:

$$
\begin{aligned}
\sum_{\substack{0<\gamma\leqslant T\\ T<\gamma'\leqslant T+H}} w(\gamma-\gamma'-\Delta) &= \sum_{\substack{T-|\Delta|-1\leqslant\gamma\leqslant T\\ T<\gamma'\leqslant T+H}} w(\gamma-\gamma'-\Delta) + \sum_{\substack{0<\gamma<T-|\Delta|-1\\ T<\gamma'\leqslant T+H}} w(\gamma-\gamma'-\Delta)\\
&\ll (H+|\Delta|+1)\log^2 T + \log^3 T,
\end{aligned}
$$

where we used that $w(u)\geqslant 0$ to extend the first sum and applied parts (b) and (c) of Lemma 5.12, respectively. This yields $Y_3 \ll \frac{1}{T}(H+|\Delta|+1)\log^2 T$. Y_4 can be treated similarly to Y_3, since we may interchange γ and γ', use that $w(u)$ is even, and replace Δ with $-\Delta$. Combining the above estimates, we obtain that

$$
F_\Delta(\alpha, T+H) = F_\Delta(\alpha,T) + O\left(\frac{(|\alpha|+1)(H+|\Delta|+1)\log^2 T}{T}\right), \tag{5.3.2}
$$

uniformly for $\alpha\in\mathbb{R}$, $T\geqslant 4$, $0<H\leqslant T$, and $\Delta\in\mathbb{R}$ with $0\leqslant|\Delta|\leqslant T$.

We now use the pointwise estimate (5.3.2) to prove part (a) as follows. It is known that

$$
\int_0^\beta F(\alpha,T)\,\mathrm{d}\alpha \ll 1+\beta, \tag{5.3.3}
$$

uniformly for $\beta\geqslant 0$ and $T\geqslant 4$ (see [53, Lemma A]). Integrating by parts, for $\beta\geqslant 1$ this implies that

$$
\int_\beta^\infty \frac{F(\alpha,T)}{\alpha^2}\,\mathrm{d}\alpha \ll \frac{1}{\beta}.
$$

Therefore, by the case $\Delta=0$ of the estimate (5.3.2), we obtain

$$
\begin{aligned}
\int_1^\infty \frac{F(\alpha,T+H)}{\alpha^2}\,\mathrm{d}\alpha &= \int_1^T \frac{F(\alpha,T+H)}{\alpha^2}\,\mathrm{d}\alpha + O\left(\frac{1}{T}\right)\\
&= \int_1^T \frac{F(\alpha,T)}{\alpha^2}\,\mathrm{d}\alpha + O\left(\frac{(H+1)\log^3 T}{T}\right)\\
&= \int_1^\infty \frac{F(\alpha,T)}{\alpha^2}\,\mathrm{d}\alpha + O\left(\frac{(H+1)\log^3 T}{T}\right).
\end{aligned}
$$

This proves part (a). Part (b) is similar, using that $|\Delta|\leqslant\log^2 T$ and Lemma 5.11 in place of (5.3.3). $\square$

5.3.2 Unbounded discontinuities

In this section, our goal is to express R_i as a sum over pairs of zeros of $\zeta(s)$ in order to apply Montgomery's pair correlation method to estimate R_i. The arguments of Montgomery and Goldston consist of localizing the sum to zeros in the interval $[0,\, T]$ and then extending the integral in the definition of R_i in (5.2.8) to infinity, up to small errors. However, due to the unbounded discontinuity of our weight function h at the origin, their arguments do not apply directly. This leads to difficulties, and we must use a different and delicate approach to control the error terms in this case. The first part of this approach lies in the introduction of a sequence of T_n's for which the following lemmas will hold. The idea of using such a sequence is classical (for instance, see [41, Ch.17]). Since $N(T+1) - N(T) \ll \log T$, by the pigeonhole principle, for every $n \in \mathbb{N}$ we can find a sequence $\{T_n\}$ satisfying

$$n \leqslant T < n+1 \quad \text{and} \quad |\gamma - T_n| \gg \frac{1}{\log n}. \tag{5.3.4}$$

In this way, we obtain similar results to Goldston on a sequence of points tending to infinity, despite the unbounded discontinuity of our function h. Now, we define

$$k(\xi) := \frac{1}{\pi^2} \widehat{h}(\xi)^2, \tag{5.3.5}$$

and we consider the following lemma.

Lemma 5.14. *Assume RH. Let $T \in \{T_n\}$, where T_n satisfies* (5.3.4)*. Define k as in* (5.3.5) *and R_i as in* (5.2.8)*. For $4 \leqslant x \leqslant T$ and $0 < \Delta \ll T^b$, with $0 < b < \frac{1}{2}$, we have*

(a) $R_1 = \dfrac{\pi^2}{\log x} \displaystyle\sum_{0<\gamma,\, \gamma' \leqslant T} \widehat{k}[(\gamma-\gamma')\log x] + O\Big(\sqrt{T}\log^2 T\Big)$;

(b) $R_2 = \dfrac{2\pi^2}{\log x} \displaystyle\sum_{0<\gamma, \gamma' \leqslant T} \Big\{\widehat{k}[(\gamma-\gamma')\log x] - \widehat{k}\left[(\gamma-\gamma'-\Delta)\log x\right]\Big\} + O\left(T\sqrt{\dfrac{\log\log T}{\log T}}\right)$.

Proof of part (a). First note that for $\gamma \neq t$, using an argument of Goldston [53, p. 158], we find that

$$\sum_{\gamma} h[(t-\gamma)\log x] \;=\; \sum_{|t-\gamma| \leqslant \frac{1}{\log x}} h[(t-\gamma)\log x] + O(\log \tau), \tag{5.3.6}$$

since $h(v) \ll \frac{1}{v^2}$ for $|v| > 1$. Here, $\tau = |t| + 2$. Similarly, modifying an argument of Montgomery [81, p. 187], we deduce that for $t \in [0, T]$ we have

$$\sum_{\substack{\gamma \\ \gamma \notin [0,T]}} h[(t-\gamma)\log x] = \sum_{\gamma \in I} h[(t-\gamma)\log x] + O\Big(\Big[\tfrac{1}{T-t+1} + \tfrac{1}{t+1}\Big]\log T\Big), \tag{5.3.7}$$

where $I = \{\gamma : T < \gamma \leqslant T + \frac{1}{\log x}\}$. We now show that the terms in the sum for which $\gamma \notin [0, T]$ contribute an amount of size $o(T)$ to R_1. Using (5.3.6) and (5.3.7), we restrict the interval of zeros within the sum in R_1 to $\gamma, \gamma' \in [0, T]$. Then by expanding the integral, we rewrite R_1 as

$$\begin{aligned}
R_1 = &\sum_{0<\gamma,\gamma'\leqslant T} \int_1^T h[(t-\gamma)\log x]\, h[(t-\gamma')\log x]\; \mathrm{d}t \\
&+ O\Bigg(\int_1^T \sum_{\gamma\in I} \big|h[(t-\gamma)\log x]\big| \sum_{|t-\gamma'|\leqslant \frac{1}{\log x}} \big|h[(t-\gamma')\log x]\big|\; \mathrm{d}t \Bigg) \\
&+ O\Bigg(\int_1^T \sum_{\gamma\in I} \big|h[(t-\gamma)\log x]\big| \log\tau\; \mathrm{d}t \Bigg) + O\Bigg(\log T \int_1^T \Big[\tfrac{1}{T-t+1} + \tfrac{1}{t+1}\Big] \log\tau\; \mathrm{d}t \Bigg) \\
&+ O\Bigg(\log T \int_1^T \Big[\tfrac{1}{T-t+1} + \tfrac{1}{t+1}\Big] \sum_{|t-\gamma'|\leqslant \frac{1}{\log x}} \big|h[(t-\gamma')\log x]\big|\; \mathrm{d}t \Bigg),
\end{aligned} \tag{5.3.8}$$

where $I = \{\gamma : T < \gamma \leqslant T + \frac{1}{\log x}\}$. Integrating the third error term on the right-hand side of (5.3.8) gives

$$\log T \int_1^T \Big[\tfrac{1}{T-t+1} + \tfrac{1}{t+1}\Big] \log t\; \mathrm{d}t \ll \log^3 T.$$

Using the facts that $h \in L^1$ and $|I| < 1$, the second error term on the right-hand side of (5.3.8) reduces to

$$\int_1^T \sum_{\gamma\in I} \big|h[(t-\gamma)\log x]\big| \log t\; \mathrm{d}t \ll \log T \sum_{\gamma\in I} \int_{-\infty}^{\infty} \big|h[(t-\gamma)\log x]\big|\; \mathrm{d}t \ll \frac{\log^2 T}{\log x}.$$

Similarly, the fourth error term on the right-hand side of (5.3.8) yields

$$\begin{aligned}
\log T &\int_1^T \Big[\tfrac{1}{T-t+1} + \tfrac{1}{t+1}\Big] \sum_{|t-\gamma'|\leqslant \frac{1}{\log x}} \big|h[(t-\gamma')\log x]\big|\; \mathrm{d}t \\
&= \log T \int_1^T \tfrac{1}{T-t+1} \sum_{|t-\gamma'|\leqslant \frac{1}{\log x}} \big|h[(t-\gamma')\log x]\big|\; \mathrm{d}t + \log T \int_1^T \tfrac{1}{t+1} \sum_{|t-\gamma'|\leqslant \frac{1}{\log x}} \big|h[(t-\gamma')\log x]\big|\; \mathrm{d}t \\
&= S_1 + S_2.
\end{aligned}$$

We introduce a parameter $1 < H < T$ to split the range of integration for S_1, as follows:

$$S_1 = \log T \int_1^{T-H} \frac{1}{T-t+1} \sum_{|t-\gamma'| \leqslant \frac{1}{\log x}} \left|h[(t-\gamma')\log x]\right| \, \mathrm{d}t + \log T \int_{T-H}^{T} \frac{1}{T-t+1} \sum_{|t-\gamma'| \leqslant \frac{1}{\log x}} \left|h[(t-\gamma')\log x]\right| \, \mathrm{d}t$$
$$= S_{11} + S_{12}.$$

To estimate S_{11}, we note that $T - t + 1 \geqslant H + 1$, extend the sum over γ' and use that $h \in L^1$. We find that

$$\begin{aligned} S_{11} &\ll \frac{\log T}{H+1} \sum_{0 \leqslant \gamma' \leqslant T} \int_1^{T-H} \left|h[(t-\gamma')\log x]\right| \, \mathrm{d}t \\ &\ll \frac{T \log^2 T}{H+1}. \end{aligned}$$

For S_{12}, we use that $T - t + 1 \geqslant 1$ and extend the sum slightly to obtain

$$\begin{aligned} S_{12} &\ll \log T \sum_{(T-H-1) \leqslant \gamma' \leqslant (T+1)} \int_{T-H}^{T} \left|h[(t-\gamma')\log x]\right| \, \mathrm{d}t \\ &\ll H \log^2 T. \end{aligned}$$

To balance these two error terms, we choose $H = \sqrt{T}$. Therefore, we conclude that

$$S_1 \ll \sqrt{T} \log^2 T.$$

We estimate S_2 similarly, by splitting the range of integration from 1 to H and from H to T. We again find that

$$S_2 \ll \sqrt{T} \log^2 T.$$

By combining the estimates for S_1 and S_2, the fourth error term on the right-hand side of (5.3.8) can be estimated as

$$\log T \int_1^T \left[\tfrac{1}{T-t+1} + \tfrac{1}{t+1}\right] \sum_{|t-\gamma'| \leqslant \frac{1}{\log x}} \left|h[(t-\gamma')\log x]\right| \, \mathrm{d}t \ll \sqrt{T} \log^2 T. \tag{5.3.9}$$

For the first error term of (5.3.8), we again split the range of integration and find that

$$\int_1^T \sum_{\gamma \in I} \left|h[(t-\gamma)\log x]\right| \sum_{|t-\gamma'| \leqslant \frac{1}{\log x}} \left|h[(t-\gamma')\log x]\right| \, \mathrm{d}t$$

$$
\begin{aligned}
&= \int_{1}^{T-1} \sum_{\gamma\in I} \left|h[(t-\gamma)\log x]\right| \sum_{|t-\gamma'|\leqslant\frac{1}{\log x}} \left|h[(t-\gamma')\log x]\right| \,\mathrm{d}t \\
&\quad + \int_{T-1}^{T} \sum_{\gamma\in I} \left|h[(t-\gamma)\log x]\right| \sum_{|t-\gamma'|\leqslant\frac{1}{\log x}} \left|h[(t-\gamma')\log x]\right| \,\mathrm{d}t \\
&= \Sigma_1 + \Sigma_2.
\end{aligned}
$$

For $\gamma \in I$ and $t \in [1, T-1]$, we know $h[(t-\gamma)\log x] \ll \frac{1}{(t-\gamma)^2 \log^2 x}$. Since $h \in L^1$, by an argument similar to the proof of (5.3.7), we see

$$
\begin{aligned}
\Sigma_1 &\ll \int_{1}^{T-1} \sum_{\gamma\in I} \frac{1}{(t-\gamma)^2 \log^2 x} \sum_{|t-\gamma'|\leqslant\frac{1}{\log x}} \left|h[(t-\gamma')\log x]\right| \,\mathrm{d}t \\
&\ll \int_{1}^{T-1} \left[\frac{1}{T-t+1} + \frac{1}{t+1}\right] \log T \sum_{|t-\gamma'|\leqslant\frac{1}{\log x}} \left|h[(t-\gamma')\log x]\right| \,\mathrm{d}t \\
&\ll \sqrt{T}\log^2 T,
\end{aligned}
$$

where we used (5.3.9) in the last line. Since $T \in \{T_n\}$, we know that $|\gamma - T| \gg \frac{1}{\log T}$. Thus for $t \in I$, we have that $T-1 \leqslant t \leqslant T$ and $T < \gamma \leqslant T + \frac{1}{\log x}$ imply $|t-\gamma| \gg \frac{1}{\log T}$. Since $|I| < 1$ and $x \geqslant 4$, again using that $h(u) \ll u^2$ for all $u > 0$, we know that

$$
\sum_{\gamma\in I} \left|h[(t-\gamma)\log x]\right| \ll \sum_{\gamma\in I} \left|h\left(\tfrac{\log x}{\log T}\right)\right| \ll \log^2 T \sum_{\gamma\in I} 1 \ll \log^3 T.
$$

Hence, since γ' is contained in an interval of size less than 1, it follows that

$$
\begin{aligned}
\Sigma_2 &\ll \log^3 T \int_{T-1}^{T} \sum_{|t-\gamma'|\leqslant\frac{1}{\log x}} \left|h[(t-\gamma')\log x]\right| \,\mathrm{d}t \\
&\ll \frac{\log^3 T}{\log x} \sum_{|T-\gamma'|\leqslant 2} \int_{-\infty}^{\infty} |h(u)| \,\mathrm{d}u \\
&\ll \frac{\log^4 T}{\log x}
\end{aligned}
$$

for all $T \in \{T_n\}$. Hence combining our estimates for Σ_1 and Σ_2 gives

$$
\int_{1}^{T} \sum_{\gamma\in I} \left|h[(t-\gamma)\log x]\right| \sum_{|t-\gamma'|\leqslant\frac{1}{\log x}} \left|h[(t-\gamma')\log x]\right| \,\mathrm{d}t = \Sigma_1 + \Sigma_2 \ll \sqrt{T}\log^2 T.
$$

Therefore, R_1 is confined to $\gamma, \gamma' \in [0, T]$ with an added error of $O(\sqrt{T}\log^2 T)$. Similarly, we may extend the integral range of $[1,T]$ to $(-\infty,\infty)$ with the same error. Thus,

$$R_1 = \sum_{0<\gamma,\gamma'\leqslant T} \int_{-\infty}^{\infty} h[(t-\gamma)\log x]\ h[(t-\gamma')\log x]\,\mathrm{d}t + O(\sqrt{T}\log^2 T).$$

We now use the properties of $h(v)$ expressed in Lemma 5.8 to simplify our expression for R_1. Since $h \in L^1$ and it is even, we can use the substitution $u = (t-\gamma')\log x$ together with convolution to find that

$$\begin{aligned} R_1 &= \frac{1}{\log x} \sum_{0<\gamma,\gamma'\leqslant T} \int_{-\infty}^{\infty} h(a-u)\ h(u)\,\mathrm{d}u + O(\sqrt{T}\log^2 T) \\ &= \frac{1}{\log x} \sum_{0<\gamma,\gamma'\leqslant T} h * h(a) + O(\sqrt{T}\log^2 T), \end{aligned}$$

with $a = (\gamma-\gamma')\log x$. Since $h \in L^1$, we know that convolution is well-defined and $\widehat{h*h} = \hat{h}^2$. Furthermore, from Lemma 5.8, we know that $\widehat{h} \in L^2$, and therefore $k(\xi) = \frac{1}{\pi^2}\widehat{h}(\xi)^2 \in L^1$. Thus by Lemma 5.8, (5.3.5), and the properties of Fourier Transform, we have

$$R_1 = \frac{\pi^2}{\log x} \sum_{0<\gamma,\gamma'\leqslant T} \hat{k}[(\gamma-\gamma')\log x] + O(\sqrt{T}\log^2 T),$$

as claimed.

Proof of part (b). The proof here is similar, but we highlight some important differences. Recall that

$$R_2 = \int_0^T [B(t+\Delta) - B(t)]^2\ \mathrm{d}t,$$

where we defined $B(t)$ in (5.2.7). First, by Lemma 5.13 and part (a) of Lemma 5.16, since $\Delta \ll T^b$ with $b < \frac{1}{2}$, we have that

$$\int_{1+\Delta}^{T+\Delta} B(t)^2\ \mathrm{d}t = \int_1^T B(t)^2\ \mathrm{d}t + O\left(T\sqrt{\frac{\log\log T}{\log T}}\right).$$

Therefore, we find that

$$R_2 = 2R_1 - 2R_{22} + O\left(T\sqrt{\frac{\log\log T}{\log T}}\right),$$

where

$$R_{22} := \int_0^T \sum_{\gamma,\gamma'} h[(t+\Delta-\gamma)\log x]h[(t-\gamma')\log x]\ \mathrm{d}t. \tag{5.3.10}$$

As in part (a), we restrict the double sum in (5.3.10) to the interval $[0,T]$ and then extend the integral to $\mathbb{R}$, up to an error term $o(T)$. For this purpose, note that

$$\sum_{\substack{\gamma \\ \gamma\notin[0,T]}} h[(t+\Delta-\gamma)\log x] = \sum_{\gamma\in I_\Delta} h[(t+\Delta-\gamma)\log x] + O\Big(\Big[\tfrac{1}{T-t+1}+\tfrac{1}{t+1}\Big]\log T\Big),$$

where $I_\Delta = \{\gamma : T < \gamma \leqslant T+\Delta+\frac{1}{\log x}\}$. Note that $|I_\Delta| \ll (\Delta+1)\log T$. By computations similar to those of part (a), we find that

$$R_{22} = \sum_{0<\gamma,\gamma'\leqslant T} \int_1^T h[(t+\Delta-\gamma)\log x]\, h[(t-\gamma')\log x]\ \mathrm{d}t + O\bigg(\frac{(\Delta+1)\log^2 T}{\log x}\bigg) + O\Big(\sqrt{T}\log^2 T\Big)$$
$$+ O\left(\int_1^T \left|\sum_{\gamma\in I_\Delta} h[(t+\Delta-\gamma)\log x] \sum_{|t-\gamma'|\leqslant\frac{1}{\log x}} h[(t-\gamma')\log x]\right|\ \mathrm{d}t\right). \tag{5.3.11}$$

The next step is different from the steps in the proof of part (a). To bound the last error term in (5.3.11), we will use the Cauchy-Schwarz inequality:

$$\int_1^T \left|\sum_{\gamma\in I_\Delta} h[(t+\Delta-\gamma)\log x] \sum_{|t-\gamma'|\leqslant\frac{1}{\log x}} h[(t-\gamma')\log x]\right|\ \mathrm{d}t$$
$$\leqslant \left\|\sum_{\gamma\in I_\Delta} h[(t+\Delta-\gamma)\log x]\right\|_2 \cdot \left\|\sum_{|t-\gamma'|\leqslant\frac{1}{\log x}} h[(t-\gamma')\log x]\right\|_2$$
$$= J_1\cdot J_2. \tag{5.3.12}$$

To estimate J_1, we expand the integral, apply Cauchy-Schwarz once more, and use that $h\in L^2$ and $|I_\Delta| \ll (\Delta+1)\log T$. This gives

$$\begin{aligned} J_1^2 &= \sum_{\gamma,\,\gamma'\in I_\Delta} \int_0^T h[(t+\Delta-\gamma)\log x] h((t+\Delta-\gamma')\log x)\ \mathrm{d}t \\ &\ll \frac{(\Delta+1)^2\log^2 T}{\log x}. \end{aligned} \tag{5.3.13}$$

To estimate J_2, we use (5.3.6) to extend the sum over zeros to the interval $[0, T+1]$, together with the bound $N(T+1) \ll T\log T$ and the fact that $h\in L^1$. This yields

$$\begin{aligned} J_2^2 &= \sum_{0<\gamma,\,\gamma'\leqslant T+1} \int_1^T h[(t-\gamma)\log x] h[(t-\gamma')\log x]\ \mathrm{d}t + O\big(T\log^2 T\big) \\ &= R_1 + O(T\log^2 T) \\ &\ll T\log^2 T, \end{aligned} \tag{5.3.14}$$

where we used part (a) and part (a) of Lemma 5.16. Combining (5.3.11), (5.3.12), (5.3.13), and (5.3.14), we obtain

$$R_{22} = \sum_{0<\gamma,\gamma'\leqslant T} \int_1^T h[(t+\Delta-\gamma)\log x]\, h[(t-\gamma')\log x]\ \mathrm{d}t + O\Big((\Delta+1)\sqrt{T}\log^2 T\Big).$$

Similarly, the integral above may be extended to $\mathbb{R}$ up to the same error term. The rest of the proof is analogous to part (a). ☐

5.3.3 A modified pair correlation approach

The next step is to introduce the weight function $w(u)$, from (1.3.5), to write R_1 and R_2 in Lemma 5.14 in terms of Montgomery's function $F(\alpha)$ and Chan's function $F_\Delta(\alpha)$.

Lemma 5.15. *Let $T \in \{T_n\}$, where T_n satisfies* (5.3.4)*. Define k as in* (5.3.5)*, and assume RH. For $4 \leqslant x \leqslant T$, and $0 < \Delta \leqslant T$, we have error terms*

(a) $$R_1 = \frac{\pi^2}{\log x} \sum_{0<\gamma,\,\gamma'\leqslant T} \widehat{k}[(\gamma-\gamma')\log x] w(\gamma-\gamma') + O\bigg(\frac{T\log^2 T}{\log^3 x}\bigg).$$

(b) $$R_2 = \frac{2\pi^2}{\log x} \sum_{0<\gamma,\gamma'\leqslant T} \Big\{\widehat{k}[(\gamma-\gamma')\log x] w(\gamma-\gamma') - \widehat{k}\left[(\gamma-\gamma'-\Delta)\log x\right] w\big(\gamma-\gamma'-\Delta\big)\Big\} + O\bigg(\frac{T\log^2 T}{\log^3 x}\bigg).$$

Proof. The proofs of the expressions in parts (a) and (b) are proved using similar methods, but the proof of part (b) is more involved. For this reason, we only work out part (b). Recall that k is the function defined in (5.3.5). We have that $\widehat{k}(y) \ll \min(1, \frac{1}{y^2})$. From this estimate we introduce the weight function $w(u)$, defined in (1.3.5), into the sum over zeros

$$\sum_{0<\gamma,\gamma'\leqslant T} \widehat{k}[(\gamma-\gamma')\log x]$$

using the following argument. We consider the difference

$$D := \widehat{k}\Big[\Big(\gamma-\gamma'-\Delta\Big)\log x\Big] - \widehat{k}\Big[\Big(\gamma-\gamma'-\Delta\Big)\log x\Big] w\Big(\gamma-\gamma'-\Delta\Big).$$

Using the facts that $N(T) \ll T\log T$, there are $O(\log t)$ zeros in any given interval $[t, t+1]$, and that $\Delta \leqslant T$, we have

$$\begin{aligned} D &\ll \frac{1}{\log^2 x} \sum_{0<\gamma'\leqslant T} \sum_{\gamma} \frac{1}{4+(\gamma-\gamma'-\Delta)^2} \\ &\ll \frac{1}{\log^2 x} \sum_{0<\gamma'\leqslant T} \log\big(\gamma'+\Delta\big) \ll \frac{T\log^2 T}{\log^2 x}. \end{aligned}$$

Therefore,

$$\sum_{0<\gamma,\gamma'\leqslant T} \widehat{k}\Big[\big(\gamma-\gamma'-\Delta\big)\log x\Big] = \sum_{0<\gamma,\gamma'\leqslant T} \hat{k}\left[\big(\gamma-\gamma'-\Delta\big)\log x\right] w\Big(\gamma-\gamma'-\Delta\Big) + O\left(\frac{T\log^2 T}{\log^2 x}\right).$$

Similarly, we may introduce the weight $w(u)$ into the the other terms in the representations of R_1 and R_2 in Lemma 5.14 to complete the proof. $\square$

Using Lemma 5.15 and the properties of $F(\alpha)$ and $F_\Delta(\alpha)$, we take $x = T^\beta$ and proceed to estimate R_i.

Lemma 5.16 (Estimates of R_i)**.** *Assume RH. Let $T \in \{T_n\}$, where T_n satisfies* (5.3.4)*. Fix $0 < \beta \leqslant 1$, let g be defined in* (5.2.2)*, and define R_i as in* (5.2.8)*. For $T \geqslant 4$, $x = T^\beta$, and $0 < \Delta = o(\log^2 T)$, we have*

$$\text{(a) } R_1 = \frac{T}{2}\left\{\int_1^\infty \frac{F(\alpha)}{\alpha^2}\,\mathrm{d}\alpha + \int_0^1 v\,g^2(v)\,\mathrm{d}v + \frac{g(0)^2}{2\beta^2} - \log\beta\right\} + o(T).$$

$$\begin{aligned}\text{(b) } R_2 = T\Bigg\{&\int_0^1 v\,g^2(v)\left[1 - w(\Delta)\cos(\Delta v\beta\log T)\right]\mathrm{d}v - \log(\beta)\\ &- w(\Delta)\int_{\Delta\beta\log T}^{\Delta\log T}\frac{\cos(u)}{u}\,\mathrm{d}u + \frac{1}{2}\int_1^\infty \frac{2F(\alpha) - F_\Delta(\alpha) - F_{-\Delta}(\alpha)}{\alpha^2}\,\mathrm{d}\alpha\Bigg\} + o(T),\end{aligned}$$

where the error term on part (a) is of size $O\Big(T\sqrt{\frac{\log\log T}{\log T}}\Big)$, and the error term on part (b) is of size $O\Big(\frac{T}{\sqrt{\log T}}\Big) + O\Big(\frac{\Delta}{\log^2 T}\Big)$.

Proof. Let $T \in \{T_n\}$, fix $0 < \beta \leqslant 1$, and choose $x = T^\beta$ for $T \geqslant 4$.

Part (a). Recall the definition of the function $F(\alpha)$ and $w(u)$ in (1.3.5). Then using the definition of Fourier transform, we manipulate the sum over zeros in the representation formula for R_1 in Lemma 5.15 to yield

$$\begin{aligned}\sum_{0<\gamma,\,\gamma'\leqslant T} \widehat{k}[(\gamma-\gamma')\log x]w(\gamma-\gamma') &= \int_{-\infty}^{\infty} k(u) \sum_{0<\gamma,\gamma'\leqslant T} e^{-2\pi i u(\gamma-\gamma')\log x} w(\gamma-\gamma')\,\mathrm{d}u\\ &= \frac{T\log T}{(2\pi)^2\beta}\int_{-\infty}^{\infty} k\Big(\frac{\alpha}{2\pi\beta}\Big)F(\alpha)\,\mathrm{d}\alpha. \qquad (5.3.15)\end{aligned}$$

Then, inputting (5.3.15) into part (a) of Lemma 5.15 gives

$$R_1 = \frac{\pi^2}{\log x}\sum_{0<\gamma,\,\gamma'\leqslant T}\widehat{k}[(\gamma-\gamma')\log x]w(\gamma-\gamma') + O\Big(\frac{T}{\log T}\Big)$$

$$= \frac{T}{(2\beta)^2} \int_{-\infty}^{\infty} k\Big(\frac{\alpha}{2\pi\beta}\Big) F(\alpha) \, \mathrm{d}\alpha + O\Big(\frac{T}{\log T}\Big). \tag{5.3.16}$$

Recall from (5.3.5) that $k(u)$ is piecewise defined with a transition at $u = \frac{1}{2\pi}$. Thus, we use (5.1.8) and the fact that $F(\alpha)$ and $k(u)$ are both even and non-negative functions to rewrite the above integral over k and F as

$$\int_{-\infty}^{\infty} k\Big(\frac{\alpha}{2\pi\beta}\Big) F(\alpha) \, \mathrm{d}\alpha = 2\int_{0}^{\beta} k\Big(\frac{\alpha}{2\pi\beta}\Big) \big[\alpha + o(1) + T^{-2\alpha} \log T (1 + o(1))\big] \, \mathrm{d}\alpha$$
$$+ 2\int_{\beta}^{1} \Big(\frac{\beta}{\alpha}\Big)^2 \big[\alpha + o(1) + T^{-2\alpha} \log T (1 + o(1))\big] \, \mathrm{d}\alpha + 2\int_{1}^{\infty} \Big(\frac{\beta}{\alpha}\Big)^2 F(\alpha) \, \mathrm{d}\alpha. \tag{5.3.17}$$

For the second integral on the right-hand side in (5.3.17), because β is fixed, we know that

$$2\int_{\beta}^{1} \Big(\frac{\beta}{\alpha}\Big)^2 \big[\alpha + o(1) + T^{-2\alpha} \log T (1 + o(1))\big] \, \mathrm{d}\alpha = -2\beta^2 \log\beta + o(1). \tag{5.3.18}$$

To compute the first integral on the right-hand side of (5.3.17), we use the facts that $k\Big(\frac{\alpha}{2\pi\beta}\Big) = g^2\Big(\frac{\alpha}{\beta}\Big)$ for $0 \leqslant \alpha \leqslant \beta$, that $0 < \beta \leqslant 1$ is fixed, and that k is smooth near the origin and uniformly bounded. By technical yet straightforward manipulations, we find that

$$2\int_{0}^{\beta} k\Big(\frac{\alpha}{2\pi\beta}\Big)\big[\alpha + o(1) + T^{-2\alpha} \log T (1 + o(1))\big] \, \mathrm{d}\alpha = 2\beta^2 \int_{0}^{1} v\, g^2(v) \, \mathrm{d}v + g^2(0) + o(1). \tag{5.3.19}$$

Combining the estimates (5.3.18) and (5.3.19) yields

$$\int_{-\infty}^{\infty} k\Big(\frac{\alpha}{2\pi\beta}\Big) F(\alpha) \, \mathrm{d}\alpha = 2\beta^2 \int_{0}^{1} v\, g^2(v) \, \mathrm{d}v - 2\beta^2 \log\beta + g^2(0) + 2\beta^2 \int_{1}^{\infty} \frac{F(\alpha)}{\alpha^2} \, \mathrm{d}\alpha + o(1). \tag{5.3.20}$$

Inputting (5.3.20) into the representation for R_1 in (5.3.16) concludes the proof of part (a).

Part (b). We consider the definition of the function $F_\Delta(\alpha)$ in (5.1.4). Then using the definition of Fourier transform, we manipulate the sum over zeros in the representation formula for R_2 in Lemma 5.15 to yield

$$\sum_{0<\gamma,\gamma'\leqslant T} \hat{k}\left((\gamma - \gamma' - \Delta) \log x\right) w\Big(\gamma - \gamma' - \Delta\Big)$$

$$= \int_{-\infty}^{\infty} k(u) \sum_{0<\gamma,\gamma'\leqslant T} T^{-2\pi\beta iu(\gamma-\gamma'-\Delta)} w(\gamma-\gamma'-\Delta)\ \mathrm{d}u$$

$$= \frac{T\log T}{(2\pi)^2\beta} \int_{-\infty}^{\infty} k\Big(\frac{\alpha}{2\pi\beta}\Big) F_\Delta(\alpha)\ \mathrm{d}\alpha. \tag{5.3.21}$$

Then, inputting (5.3.15) and (5.3.21) into part (b) of Lemma 5.15 gives

$$R_2 = \frac{T}{2\beta^2}\left\{\int_{-\infty}^{\infty} k\Big(\frac{\alpha}{2\pi\beta}\Big) F(\alpha)\ \mathrm{d}\alpha - \int_{-\infty}^{\infty} k\Big(\frac{\alpha}{2\pi\beta}\Big) F_\Delta(\alpha)\ \mathrm{d}\alpha\right\} + O\Big(\frac{T}{\log T}\Big).$$

By splitting the second integral above using the symmetry relations for F_Δ in (5.1.9), we have

$$-\frac{T}{2\beta^2}\int_{-\infty}^{\infty} k\Big(\frac{\alpha}{2\pi\beta}\Big) F_\Delta(\alpha)\ \mathrm{d}\alpha = -\frac{T}{2\beta^2}\int_{0}^{\infty} k\Big(\frac{\alpha}{2\pi\beta}\Big)[F_\Delta(\alpha)+F_{-\Delta}(\alpha)]\ \mathrm{d}\alpha.$$

Next, we divide the integral over the intervals $(0,\ \beta)$, $(\beta,\ 1)$, and $(1,\ \infty)$, and apply (5.1.10). Consequently, since $k(u)$ is even, $k(0) = g^2(0)$, and $T^{i\alpha\Delta} + T^{-i\alpha\Delta} = 2\cos(\Delta\alpha\log T)$, we obtain

$$-\frac{T}{2\beta^2}\int_{0}^{\beta} k\Big(\frac{\alpha}{2\pi\beta}\Big)[F_\Delta(\alpha)+F_{-\Delta}(\alpha)]\mathrm{d}\alpha = -\frac{Tg^2(0)}{2\beta^2} - Tw(\Delta)\int_0^1 v\, g(v)^2\cos(\Delta v\beta\log T)\ \mathrm{d}v + o(T),$$

and

$$-\frac{T}{2\beta^2}\int_{\beta}^{1} k\Big(\frac{\alpha}{2\pi\beta}\Big)[F_\Delta(\alpha)+F_{-\Delta}(\alpha)]\ \mathrm{d}\alpha = -Tw(\Delta)\int_{\Delta\beta\log T}^{\Delta\log T} \frac{\cos u}{u}\ \mathrm{d}u + o(T).$$

By combining the above integrals, we have that

$$-\frac{T}{2\beta^2}\int_{-\infty}^{\infty} k\Big(\frac{\alpha}{2\pi\beta}\Big) F_\Delta(\alpha)\ \mathrm{d}\alpha = -T\left\{\frac{g^2(0)}{2\beta^2} + w(\Delta)\int_0^1 v\, g(v)^2\cos(\Delta v\beta\log T)\ \mathrm{d}v \right.$$
$$\left. + w(\Delta)\int_{\Delta\beta\log T}^{\Delta\log T}\frac{\cos u}{u}\ \mathrm{d}u + \frac{1}{2}\int_1^{\infty}\frac{F_\Delta(\alpha)+F_{-\Delta}(\alpha)}{\alpha^2}\ \mathrm{d}\alpha\right\} + o(T). \tag{5.3.22}$$

From the proof of part (a) (see (5.3.20)), we know that

$$\frac{T}{2\beta^2}\int_{-\infty}^{\infty} k\Big(\frac{\alpha}{2\pi\beta}\Big)F(\alpha)\ \mathrm{d}\alpha = T\left[\int_0^1 v\,g^2\,(v)\ \ \mathrm{d}v - \log\beta + \frac{g^2(0)}{2\beta^2} + \int_1^{\infty}\frac{F(\alpha)}{\alpha^2}\ \mathrm{d}\alpha\right] + o(T). \tag{5.3.23}$$

By adding (5.3.22) and (5.3.23) together, our asymptotic formula for R_2 reduces to

$$\begin{aligned} R_2 =& T\left[\int_0^1 v\,g^2\,(v)\,(1-w(\Delta)\cos(\Delta v\beta\log T))\ \mathrm{d}v - \log\beta\right.\\ &\left. - w(\Delta)\int_{\Delta\beta\log T}^{\Delta\log T}\frac{\cos u}{u}\,\mathrm{d}u + \frac{1}{2}\int_1^{\infty}\frac{2F(\alpha)-F_{\Delta}(\alpha)-F_{-\Delta}(\alpha)}{\alpha^2}\,\mathrm{d}\alpha\right] + o(T), \end{aligned}$$

which completes the proof. □

5.4 Contributions from the primes

In this section, we estimate the expressions $G_i + H_i$. First, we obtain intermediate expressions for G_i and H_i separately.

5.4.1 Expressions for G_i and H_i

We begin with a useful Lemma that helps estimate the second moment of some trigonometric polynomials.

Lemma 5.17. *Let $T > 0$, and let $\{a_n\}_{n\geqslant 1}$ and $\{h_n\}_{n\geqslant 1}$ be sequences of real numbers such that*
$\sum_{n=1}^{\infty}(n|a_n|^2 + |a_n|) < \infty$. *Denote*

$$C := \sum_{n\geqslant 2}|a_n|\sum_{m\geqslant 2}\frac{|a_m|}{\log m} + \sum_{n=1}^{\infty} n|a_n|^2.$$

Then,

(a) $$\int_0^T\left|\sum_{n=1}^{\infty} a_n\,\cos(t\log n)\right|^2\ \mathrm{d}t = T\,a_1^2 + \frac{T}{2}\sum_{n\geqslant 2}a_n^2 + O(C)$$

(b) $$\int_0^T\left|\sum_{n=1}^{\infty} a_n\,\sin(t\log n)\right|^2\ \mathrm{d}t = \frac{T}{2}\sum_{n\geqslant 2}a_n^2 + O(C)$$

(c) $$\int_0^T\left|\sum_{n=1}^{\infty} a_n\,[\cos((t+h_n)\log n) - \cos(t\log n)]\right|^2\ \mathrm{d}t = T\sum_{n\geqslant 2}a_n^2\,[1-\cos(h_n\log n)] + O(C)$$

(d) $\displaystyle\int_0^T \left|\sum_{n=1}^{\infty} a_n\,[\sin((t+h_n)\log n) - \sin(t\log n)]\right|^2\,\mathrm{d}t = T\sum_{n\geqslant 2} a_n^2\,[1-\cos(h_n\log n)] + O(C)\,.$

The implied constants are universal.

Proof. A classical result of Montgomery and Vaughan [83, Corollary 3] states that, for complex numbers $(b_n)_{n\geqslant 1}$, we have

$$\int_0^T \left|\sum_{n=1}^{\infty} b_n\, n^{-it}\right|^2\,\mathrm{d}t = \sum_{n=1}^{\infty} |b_n|^2\,\big(T+O(n)\big). \tag{5.4.1}$$

For part (a), let $z := \sum_{n=1}^{\infty} a_n\, n^{-it}$, and note that $\operatorname{Re} z = \sum_{n=1}^{\infty} a_n\,\cos(t\log n)$. Consider the identity

$$(\operatorname{Re} z)^2 = \frac{|z|^2 + \operatorname{Re}(z^2)}{2}. \tag{5.4.2}$$

By (5.4.1), we have

$$\int_0^T \frac{|z|^2}{2}\,\mathrm{d}t = \frac{1}{2}\sum_{n\geqslant 1} a_n^2\,\big(T+O(n)\big). \tag{5.4.3}$$

We write $z = a_1 + \sum_{n=2}^{\infty} a_n\, n^{-it}$ and use that, for $n\geqslant 2$, we have $\int n^{-it}\,\mathrm{d}t = in^{-it}/\log n$. This yields

$$\begin{aligned}\int_0^T \frac{z^2}{2}\,\mathrm{d}t &= \frac{a_1^2}{2}T + O\Bigg(|a_1|\sum_{n\geqslant 2}\frac{|a_n|}{\log n}\Bigg) + O\Bigg(\sum_{n,\,m\geqslant 2}\frac{|a_n a_m|}{\log(mn)}\Bigg)\\ &= \frac{a_1^2}{2}T + O\Bigg(C + \sum_{n=1}^{\infty} n|a_n|^2\Bigg)\,.\end{aligned} \tag{5.4.4}$$

Here, we used the Cauchy-Schwarz inequality to obtain

$$|a_1|\sum_{n\geqslant 2}\frac{|a_n|}{\log n} \leqslant |a_1|\sqrt{\sum_{n\geqslant 2}\frac{1}{n\log^2 n}}\cdot\sqrt{\sum_{n\geqslant 2} n|a_n|^2} \ll \sum_{n=1}^{\infty} n|a_n|^2.$$

Combining (5.4.2),(5.4.3), and (5.4.4), we obtain part (a). Part (b) is analogous, using the identity

$$(\operatorname{Im} z)^2 = \frac{|z|^2 - \operatorname{Re}(z^2)}{2}$$

in place of (5.4.2). Note that, since $\sin 0 = 0$, part (a) has an extra contribution from the term a_1 that is not present in part (b). For parts (c) and (d), we use the identities

$$\cos((t+h_n)\log n) - \cos(t\log n) = \operatorname{Re}\,[n^{-it}(n^{-ih_n}-1)],$$

$$\sin((t+h_n)\log n) - \sin(t\log n) = -\operatorname{Im}\,[n^{-it}(n^{-ih_n}-1)]$$

and

$$|n^{-ih_n} - 1|^2 = 2(1 - \cos(h_n \log n)).$$

Then, we apply the same argument above with $z = \sum_{n=1}^{\infty} a_n(n^{-ih_n} - 1)\, n^{-it}$, using Montgomery and Vaughan's result (5.4.1) with $b_n = a_n(n^{-ih_n} - 1)$. $\square$

Using the previous lemma, we obtain the following expressions for G_i.

Lemma 5.18 (G_i)**.** *Let $\Delta > 0$ and $4 \leqslant x \leqslant T$. Let G_1 and G_2 be defined in* (5.2.8)*. Then,*

$$\text{(a) } G_1 = -\frac{T}{2} \sum_{n \leqslant x} \frac{\Lambda(n)^2}{n \log^2 n} f^2\left(\frac{\log n}{\log x}\right) + O\left(\frac{x}{\log x}\right)$$

$$\text{(b) } G_2 = -T \sum_{n \leqslant x} \frac{\Lambda(n)^2}{n \log^2 n} f^2\left(\frac{\log n}{\log x}\right) [1 - \cos(\Delta \log n)] + O\left(\frac{x}{\log x}\right).$$

Next, with the goal of studying H_1 and H_2, we use some estimates of Goldston, together with some trigonometric identities, to obtain expressions for the real and imaginary parts of integrals involving $\log \zeta(1/2 + it)$ times trigonometric functions. Some of these results appear previously in [53] (part (b)) and implicitly in [46] (part (d)). We collect them all in the following lemma, for the reader's convenience.

Lemma 5.19. *Assume RH. Let $T > 1$, let $h \in \mathbb{R}$, and let $n \geqslant 2$ be an integer. Denote*

$$\mathcal{E} = \mathcal{E}(n, T) := n^{1/2} \log\log 3n + \frac{n^{1/2} \log T}{\log n}.$$

Then, the following estimates hold:

$$\text{(a) } \int_1^T \log|\zeta(\tfrac{1}{2} + it)| \cos(t \log n)\, \mathrm{d}t = \frac{T}{2} \frac{\Lambda(n)}{n^{1/2} \log n} + O(\mathcal{E})$$

$$\text{(b) } \int_1^T \pi S(t) \sin(t \log n)\, \mathrm{d}t = -\frac{T}{2} \frac{\Lambda(n)}{n^{1/2} \log n} + O(\mathcal{E})$$

$$\text{(c) } \int_1^T \log|\zeta(\tfrac{1}{2} + it)| \left[\cos((t+h)\log n) + \cos((t-h)\log n) - 2\cos(t \log n)\right] \mathrm{d}t$$
$$= -T\, \frac{\Lambda(n)[1 - \cos(h \log n)]}{n^{1/2} \log n} + O(\mathcal{E})$$

$$\text{(d) } \int_1^T \pi S(t) \left[\sin((t+h)\log n) + \sin((t-h)\log n) - 2\sin(t \log n)\right] \mathrm{d}t$$
$$= T\, \frac{\Lambda(n)[1 - \cos(h \log n)]}{n^{1/2} \log n} + O(\mathcal{E})$$

Proof. Assuming RH, Goldston [53, p. 169], improving upon a contour argument of Titchmarsh [101], showed that

$$\int_0^T \log \zeta(\tfrac{1}{2} + it)\, n^{it}\ \mathrm{d}t = \frac{T\,\Lambda(n)}{n^{1/2}\log n} + O(n^{1/2}\log\log 3n) + O\left(\frac{n^{1/2}\log T}{\log n}\right) \tag{5.4.5}$$

and

$$\int_0^T \log \zeta(\tfrac{1}{2} + it) n^{-it}\ \mathrm{d}t \ll \log T. \tag{5.4.6}$$

Adding (5.4.5) and (5.4.6) and taking real parts yields part (a). Part (b) is [53, Equation (6.3)]. Parts (c) and (d) follow from parts (a) and (b) after applying the trigonometric identities

$$\cos((t+h)\log n) + \cos((t-h)\log n) - 2\cos(t\log n) = -2\cos(t\log n)[1-\cos(h\log n)],$$

and

$$\sin((t+h)\log n) + \sin((t-h)\log n) - 2\sin(t\log n) = -2\sin(t\log n)[1-\cos(h\log n)].$$

This completes the proof of the lemma. □

We now obtain expressions for H_i from the above. As mentioned in the introduction, in the next lemma we will use Theorem 5.1 to control some of the error terms in part (b), which is the part of the lemma that is relevant to Theorem 5.3.

Lemma 5.20 (H_i)**.** *Assume RH. Let $0 < \Delta \leqslant T^b$ with $0 < b < 1$, and $4 \leqslant x \leqslant T$. Let H_1 and H_2 be defined in* (5.2.8)*. Then,*

(a) $H_1 = T \displaystyle\sum_{n\leqslant x} \frac{\Lambda(n)^2}{n\log^2 n} f\left(\frac{\log n}{\log x}\right) + O\left(\frac{x\log\log x\log T}{\log^2 x}\right)$

(b) $H_2 = 2T \displaystyle\sum_{n\leqslant x} \frac{\Lambda(n)^2}{n\log^2 n} f\left(\frac{\log n}{\log x}\right)[1-\cos(\Delta\log n)] + O\left(\frac{x\log\log x\log T}{\log^2 x}\right) + O\left(\frac{T}{\sqrt{\log x}}\right).$

Proof. Part (a) follows from part (a) of Lemma 5.19 and the definition of H_1. For part (b), we rearrange the terms and use a change of variables to find that

$$\begin{aligned} H_2 = &-2\int_1^T \log|\zeta(\tfrac{1}{2}+it)|\,[A(t+\Delta) + A(t-\Delta) - 2A(t)]\ \mathrm{d}t \\ &+ O\left(\int_1^{1+\Delta} |\log|\zeta(\tfrac{1}{2}+it)||\ |A(t) - A(t-\Delta)|\ \mathrm{d}t\right) \end{aligned}$$

$$+ O\left(\int_T^{T+\Delta} |\log|\zeta(\tfrac{1}{2}+it)||\ |A(t)-A(t-\Delta)|\ \mathrm{d}t \right).$$

By Theorem 5.1, with $0 < \Delta \leqslant T^b$, we have

$$\int_T^{T+\Delta} \log^2|\zeta(\tfrac{1}{2}+it)|\ \mathrm{d}t = o(T). \tag{5.4.7}$$

Note that we used Lemma 5.13 to show that the contribution from the constant a in Theorem 5.1 is $o(T)$ over the interval $[T, T+\Delta]$. By Montgomery and Vaughan's result in (5.4.1), we also have

$$\int_T^{T+\Delta} |A(t)-A(t-\Delta)|^2\ \mathrm{d}t \ll \sum_{n\leqslant x} \frac{\Lambda^2(n)}{n\log^2 n}\big(\Delta+n\big) \ll \Delta\log\log x + \frac{x}{\log x}. \tag{5.4.8}$$

We use the Cauchy-Schwarz inequality, (5.4.7), and (5.4.8) to obtain

$$\int_T^{T+\Delta} |\log|\zeta(\tfrac{1}{2}+it)||\ |A(t)-A(t-\Delta)|\ \mathrm{d}t \ll \sqrt{\Delta T\log\log x} + \sqrt{\frac{Tx}{\log x}} \ll \frac{T}{\sqrt{\log x}},$$

since we have $4 \leqslant x \leqslant T$ and $0 < \Delta \leqslant T^b$. The first error term may be treated similarly. This yields

$$H_2 = -2\int_1^T \log|\zeta(\tfrac{1}{2}+it)|\,[A(t+\Delta)+A(t-\Delta)-2A(t)]\ \mathrm{d}t + O\left(\frac{T}{\sqrt{\log x}}\right).$$

The conclusion now follows from part (c) of Lemma 5.19 and the definition of $A(t)$ in (5.2.7). □

5.4.2 Estimating $G_i + H_i$

Starting from the previous results, we proceed to estimate $G_i + H_i$ asymptotically, taking advantage of some cancellations between their sums via the function g (introduced in (5.2.2)). In this section, we will diverge from the strategies of previous work of Fujii to obtain more precise input from the primes, which is necessary for Theorem 5.3.

Lemma 5.21 (Asymptotic estimate of $H_i + G_i$)**.** *Assume RH. Let $T \geqslant 4$, and let $0 < \Delta = o(\log^2 T)$. Fix $0 < \beta \leqslant 1$, and choose $x = T^\beta$. Define the function $c(v)$ as in (5.1.7). Then, as $T \to \infty$, we have*

$$\text{(a)}\ H_1 + G_1 = \frac{T}{2}\left\{ \log\log T + \gamma_0 + \sum_{m=2}^{\infty}\sum_{p\geqslant 2}\frac{1}{p^m}\left(\frac{1}{m^2}-\frac{1}{m}\right) + \log\beta - \int_0^1 \alpha\, g(\alpha)^2\ \mathrm{d}\alpha \right\}$$

$$+ O\left(\frac{T \log\log T}{\log T}\right)$$

(b) $$H_2 + G_2 = T\left\{\int_0^{\Delta\beta \log T} \frac{1-\cos u}{u}\, \mathrm{d}u + c(\Delta) - \int_0^1 \alpha\,[1-\cos(\Delta\beta\log T\alpha)]g^2(\alpha)\ \mathrm{d}\alpha\right\} + o(T),$$

where the error term $o(T)$ in part (b) is actually

$$O\left(\frac{T}{\sqrt{\log T}}\right) + O\left(\frac{T\Delta}{\log^2 T}\right).$$

Proof. We split the proof in the following subsections.

Part (a)

We add Lemma 5.18 and Lemma 5.20 and use that, by Lemma 5.8, $u^2 g(u)^2 = (1-f(u))^2$. This yields

$$G_1 + H_1 = \frac{T}{2}\sum_{n\leqslant x}\frac{\Lambda^2(n)}{n\log^2 n} - \frac{T}{2\log^2 x}\sum_{n\leqslant x}\frac{\Lambda^2(n)}{n} g^2\left(\frac{\log n}{\log x}\right) + O\left(\frac{T\log\log T}{\log T}\right). \tag{5.4.9}$$

For the first term, we separate the primes from the prime powers and use Merten's Theorem, which states

$$\sum_{p\leqslant x}\frac{1}{p} = \log\log x + \gamma_0 - \sum_{m=2}^{\infty}\sum_{p\geqslant 2}\frac{1}{m\,p^m} + O\left(\frac{1}{\log x}\right).$$

Therefore, we see that

$$\sum_{n\leqslant x}\frac{\Lambda^2(n)}{n\log^2 n} = \log\log x + \gamma_0 + \sum_{m=2}^{\infty}\sum_{p\geqslant 2}\frac{1}{p^m}\left(\frac{1}{m^2} - \frac{1}{m}\right) + O\left(\frac{1}{\log x}\right). \tag{5.4.10}$$

For the second term, unconditionally, note that the prime number theorem with error term implies that

$$P(y) := \sum_{n\leqslant y}\frac{\Lambda(n)^2}{n} = \frac{\log^2 y}{2} + O(1).$$

Then, using summation by parts and integration by parts, we obtain

$$\sum_{n\leqslant x}\frac{\Lambda^2(n)}{n} g^2\left(\frac{\log n}{\log x}\right) = \log^2 x\int_0^1 \alpha\, g^2(\alpha)\ \mathrm{d}\alpha + O(\log x)\,. \tag{5.4.11}$$

By inserting (5.4.10) and (5.4.11) into (5.4.9), we obtain part (a).

Part (b): Summing by parts

Similarly, we have

$$\begin{aligned} G_2 + H_2 = & T \sum_{n \leqslant x} \frac{\Lambda^2(n)}{n \log^2 n} [1 - \cos(\Delta \log n)] \\ & - \frac{T}{\log^2 x} \sum_{n \leqslant x} \frac{\Lambda^2(n)}{n} g^2\left(\frac{\log n}{\log x}\right) [1 - \cos(\Delta \log n)] + O\left(\frac{T \log\log T}{\log T}\right). \end{aligned} \tag{5.4.12}$$

Using summation by parts, integration by parts, and the prime number theorem with error term, we obtain

$$\begin{aligned} \sum_{n \leqslant x} \frac{\Lambda^2(n)}{n} g^2\left(\frac{\log n}{\log x}\right)[1 - \cos(\Delta \log n)] &= \sum_{n \leqslant x} \frac{\Lambda(n) \log n}{n} g^2\left(\frac{\log n}{\log x}\right) [1 - \cos(\Delta \log n)] + O(1) \\ &= \log^2 x \int_0^1 \alpha \, [1 - \cos(\Delta \beta \log T \alpha)] \, g^2(\alpha) \, \mathrm{d}\alpha + O(\Delta + 1) \, . \end{aligned} \tag{5.4.13}$$

To estimate the first term on the right-hand side of (5.4.12), consider the quantity

$$M(y) := \sum_{n \leqslant y} \Lambda^2(n) = y \log y - y + E(y),$$

so that $\mathrm{d}M(y) = \log y \; \mathrm{d}y + \mathrm{d}E(y)$ and $E(y) = O_N\left(\frac{y}{\log^N y}\right)$ is defined in (5.1.6). For this, we let $1 < \ell < 2$ be a parameter. We anticipate that we will eventually take $\ell \to 1^+$. Then, the sum in the first term of (5.4.12) is

$$\begin{aligned} \sum_{n \leqslant x} \frac{\Lambda^2(n)}{n \log^2 n}[1 - \cos(\Delta \log n)] &= \int_{\ell}^{x^+} \frac{1 - \cos(\Delta \log y)}{y \log^2 y} \, \mathrm{d}M(y) \\ &= \int_{\ell}^{x^+} \frac{1 - \cos(\Delta \log y)}{y \log y} \, \mathrm{d}y + \int_{\ell}^{x^+} \frac{1 - \cos(\Delta \log y)}{y \log^2 y} \, \mathrm{d}E(y). \end{aligned}$$

We use the change of variables $u = \Delta \log y$ in the first integral. For the second integral, we integrate by parts and use that $E(\ell) = \ell - \ell \log \ell$ to find that

$$\begin{aligned} & T \sum_{n \leqslant x} \frac{\Lambda^2(n)}{n \log^2 n}[1 - \cos(\Delta \log n)] \\ & \quad = T \Bigg\{ \int_{\Delta \log \ell}^{\Delta \log x} \frac{1 - \cos u}{u} \, \mathrm{d}u + (1 - \cos(\Delta \log \ell)) \left(\frac{\log \ell - 1}{\log^2 \ell}\right) \\ & \qquad + \int_{\ell}^{\infty} \frac{E(y)}{y^2 \log^3 y}[-\Delta \log y \sin(\Delta \log y) + (1 - \cos(\Delta \log y))(\log y + 2)] \, \mathrm{d}y \Bigg\} \end{aligned}$$

$$+ O\left(\frac{(\Delta+1)T}{\log^{N+1} x}\right). \tag{5.4.14}$$

Here, we used that $E(y) \ll_N \dfrac{y}{\log^N y}$ (for any $N > 0$) to extend the last integral to infinity, up to an error term. Now, we let $\ell \to 1^+$. Note that

$$\lim_{\ell \to 1}(1 - \cos(\Delta \log \ell))\left(\frac{\log \ell - 1}{\log^2 \ell}\right) = -\frac{\Delta^2}{2}.$$

Additionally, since $E(y) = y - y\log y$ for all $1 \leqslant y < 2$, the second integrand above satisfies, in this range,

$$\frac{E(y)}{y^2 \log^3 y}[-\Delta \log y \sin(\Delta \log y) + (1 - \cos(\Delta \log y))(\log y + 2)] = \frac{\Delta^2}{2} + O\big(\Delta^2(y-1)\big).$$

This shows that the second integral is absolutely convergent on $(1, \infty)$. Therefore, recalling that $x = T^\beta$ and $\Delta \ll \log^2 T$, we may let $\ell \to 1^+$ in (5.4.14) to find that

$$T \sum_{n \leqslant x} \frac{\Lambda^2(n)}{n \log^2 n}\,[1 - \cos(\Delta \log n)] = T\left\{ \int_0^{\Delta\beta \log T} \frac{1 - \cos u}{u}\, \mathrm{d}u + c(\Delta) \right\} + O\left(\frac{T}{\log T}\right), \tag{5.4.15}$$

where $c(v)$ is defined in (5.1.7). By combining (5.4.12), (5.4.13), and (5.4.15), we complete the proof of Lemma 5.21. We remark that the restriction $\Delta = o(\log^2 T)$ comes from the sum over primes in equation (5.4.13). $\square$

5.5 Proofs of main theorems

We now explain how Theorems 5.1, 5.2, 5.3 and 5.4 follow from the combination of our previous lemmas.

5.5.1 Proof of Theorem 5.1

For all $T \in \{T_n\}$, the proof of Theorem 5.1 follows from inputting part (a) of Lemmas 5.21 and 5.16 into the representation formula for $\log|\zeta(\frac{1}{2} + it)|$, which we proved in part (a) of Lemma 5.10. Some of the integrals in these results are over the interval $[1, T]$, but these can easily be extended to $[0, T]$ since

$$\int_0^1 \log^2 |\zeta(\tfrac{1}{2} + it)|\, \mathrm{d}t \ll 1.$$

In particular, Theorem 5.1 holds for all $T \in \{T_n\}$ such that $T \geqslant 4$. We now extend this result to hold for all $T \geqslant 4$.

Assume $T_n \leqslant T \leqslant T_{n+1}$. Since the integrand in Theorem 5.1 is positive, we know that

$$\int_0^{T_n} \log^2 \left|\zeta\left(\tfrac{1}{2}+it\right)\right| \, \mathrm{d}t \leqslant \int_0^{T} \log^2 \left|\zeta\left(\tfrac{1}{2}+it\right)\right| \, \mathrm{d}t \leqslant \int_0^{T_{n+1}} \log^2 \left|\zeta\left(\tfrac{1}{2}+it\right)\right| \, \mathrm{d}t$$

Moreover, because both T_n and T_{n+1} are at most 1 away from T and Theorem 5.1 holds for T_n and T_{n+1}, by part (a) of Lemma 5.13, it follows that

$$\int_0^{T} \log^2 \left|\zeta\left(\tfrac{1}{2}+it\right)\right| \, \mathrm{d}t = \frac{T}{2}\log\log T + aT + o(T),$$

which completes the proof of Theorem 5.1 for all $T \geqslant 4$.

5.5.2 Proof of Theorems 5.3 and 5.4

For the proof of Theorem 5.3, when we input part (b) of Lemmas 5.21 and 5.16 into part (b) of Lemma 5.10, we get

$$\begin{aligned}
&\int_1^{T} \left[\log\left|\zeta\left(\tfrac{1}{2}+it+i\Delta\right)\right| - \log\left|\zeta\left(\tfrac{1}{2}+it\right)\right|\right]^2 \mathrm{d}t \\
&= T\left\{ \int_0^{\Delta\beta\log T} \frac{1-\cos u}{u}\,\mathrm{d}u - w(\Delta)\int_{\Delta\beta\log T}^{\Delta\log T} \frac{\cos u}{u}\,\mathrm{d}u - \log\beta \right. \\
&\qquad + \int_0^1 v\, g^2(v)\cos(\Delta v\beta\log T)\left(1-w(\Delta)\right)\mathrm{d}v \\
&\qquad \left. + c(\Delta) + \frac{1}{2}\int_1^{\infty} \frac{2F(\alpha)-F_{\Delta}(\alpha)-F_{-\Delta}(\alpha)}{\alpha^2}\,\mathrm{d}\alpha \right\} + o(T).
\end{aligned} \tag{5.5.1}$$

Because our results hold independently of our choice of β, there should be no β dependence in our final result. First, note that, by analyzing separately the cases $\Delta \ll 1$ and $\Delta \gg 1$ and using the definition of $w(u)$, we have

$$\frac{|1-w(\Delta)|}{\Delta\log T} \ll \frac{1}{\log T},$$

uniformly for $\Delta > 0$. We use this fact and combine the first three terms on the right-hand side of (5.5.1) to yield

$$\int_0^{\Delta\beta\log T} \frac{1-\cos u}{u}\,\mathrm{d}u - w(\Delta)\int_{\Delta\beta\log T}^{\Delta\log T} \frac{\cos u}{u}\,\mathrm{d}u - \log\beta$$

$$= \int_0^{\Delta \log T} \frac{1-\cos u}{u}\,\mathrm{d}u - (w(\Delta)-1)\int_{\Delta\beta\log T}^{\Delta\log T} \frac{\cos u}{u}\,\mathrm{d}u$$
$$= \int_0^1 \frac{1-\cos(\Delta\alpha\log T)}{\alpha}\,\mathrm{d}\alpha + O\Big(\frac{1}{\log T}\Big),$$

where we used integration by parts in the last line. Next we consider the integral involving $g^2(v)$ on the right-hand side of (5.5.1). Using integration by parts, we similarly see that

$$\int_0^1 v\ g^2(v)\cos(\Delta v\beta\log T)\,(1-w(\Delta))\ \mathrm{d}v \ll \frac{1}{\log T}.$$

Combining these simplified expressions together gives

$$\int_1^T \big[\log\big|\zeta\big(\tfrac12+it+i\Delta\big)\big| - \log\big|\zeta\big(\tfrac12+it\big)\big|\big]^2\ \mathrm{d}t$$
$$= T\left\{\int_0^1 \frac{1-\cos(\Delta\alpha\log T)}{\alpha}\ \mathrm{d}\alpha + \frac12\int_1^\infty \frac{2F(\alpha)-F_\Delta(\alpha)-F_{-\Delta}(\alpha)}{\alpha^2}\ \mathrm{d}\alpha\right\} + T\,c(\Delta) + o(T).$$

We then extend the range of integration to $[0,T]$ since, by Theorem 5.1 and the Cauchy-Schwarz inequality, we have

$$\int_0^1 \big[\log\big|\zeta\big(\tfrac12+it+i\Delta\big)\big| - \log\big|\zeta\big(\tfrac12+it\big)\big|\big]^2\ \mathrm{d}t \ll (1+\Delta)\log\log(3+\Delta).$$

This completes the proof of Theorem 5.3 for $T\in\{T_n\}$. Since the integrand is non-negative, this result can be extended to all $T \geqslant 4$ using the same argument as in the proof of Theorem 5.1 along with part (b) of Lemma 5.13. Finally, to prove Theorem 5.4, recall that (5.4.15) implies that

$$T\sum_{n\leqslant T}\frac{\Lambda(n)^2}{n\log^2 n}\,[1-\cos(\Delta\log n)] = T\left\{\int_0^1 \frac{1-\cos\Delta u\log T}{u}\,\mathrm{d}u + c(\Delta)\right\} + O\Big(\frac{T}{\log T}\Big),$$

where $c(v)$ is defined in (5.1.7). Therefore, Theorem 5.4 is equivalent to Theorem 5.3.

5.5.3 Proof of Theorem 5.2

To prove Theorem 5.2, we need to express the sum over primes in terms of the logarithmic derivative of $\zeta(s)$ near $s=1$.

Lemma 5.22. *Assume RH. Let $x \geqslant 2$ and $u \in i\mathbb{R}$ with $0 < |u| \leqslant \sqrt{x}$. Then,*

$$-\frac{\zeta'}{\zeta}(1+u) = \sum_{n \leqslant x} \frac{\Lambda(n)}{n^{1+u}} + \frac{x^{-u}}{u} + O\left(\frac{\log^2 x}{\sqrt{x}}\right),$$

where the implied constant is universal.

Proof. This can be established using classical arguments in a similar manner to the proof of the Prime Number Theorem (assuming RH), e.g. [84, Chapter 13]. □

Clearly,

$$\sum_{n \leqslant T} \frac{\Lambda(n)^2}{n \log^2 n} (1 - \cos(\Delta \log n)) = \widetilde{C}(\Delta) + \sum_{n \leqslant T} \frac{\Lambda(n)}{n \log n} (1 - \cos(\Delta \log n)) + O\left(\frac{1}{T}\right), \tag{5.5.2}$$

where $\widetilde{C}(v)$ is defined in (5.1.5). Also, note that

$$\frac{1 - \cos(\Delta \log n)}{\log n} = -\frac{1}{2} \int_0^{i\Delta} n^u - n^{-u} \, du.$$

Therefore, Lemma 5.22 yields

$$\begin{aligned} \sum_{n \leqslant T} \frac{\Lambda(n)}{n \log n}(1 - \cos(\Delta \log n)) &= -\int_0^{i\Delta} \sum_{n \leqslant T} \frac{\Lambda(n)}{n^{1-u}} - \sum_{n \leqslant T} \frac{\Lambda(n)}{n^{1+u}} \, du \\ &= \int_0^{i\Delta} \frac{\zeta'}{\zeta}(1-u) - \frac{\zeta'}{\zeta}(1+u) - \frac{T^{-u} + T^u}{u} \, du + O\left(\frac{\Delta \log^2 T}{\sqrt{T}}\right). \end{aligned} \tag{5.5.3}$$

Theorem 5.2 now follows from Theorem 5.4, (5.5.2), (5.5.3) and a change of variables.

5.6 Transition between ranges

In this section, we prove Corollary 5.7 in both ranges. We begin by showing how Theorem 5.3 reduces to Fujii's theorem when $\Delta = o(1)$.

Proposition 5.23. *Assume RH. Let $T \geqslant 4$ and $\Delta = O(1)$. Then*

$$\frac{1}{2} \int_1^{\infty} \frac{2F(\alpha) - F_{\Delta}(\alpha) - F_{-\Delta}(\alpha)}{\alpha^2} \, d\alpha = \int_1^{\infty} \frac{F(\alpha)\left[1 - \cos(\Delta \alpha \log T)\right]}{\alpha^2} \, d\alpha + O(\Delta),$$

as $T \to \infty$.

Proof. Consider the identity

$$\begin{aligned}
2F(\alpha)-&F_{\Delta}(\alpha)-F_{-\Delta}(\alpha)\\
&=\frac{8\pi^2}{T\log T}\int_{-\infty}^{\infty} e^{-4\pi|u|}\left[1-\cos(\Delta\alpha\log T+2\pi\Delta u)\right]\left|\sum_{0<\gamma\leqslant T} T^{i\alpha\gamma}e^{2\pi iu\gamma}\right|^2 \mathrm{d}u \qquad (5.6.1)\\
&\geqslant 0.
\end{aligned}$$

By the mean value theorem, $\cos(\Delta\alpha\log T+2\pi\Delta u)=\cos(\Delta\alpha\log T)+O(\Delta|u|)$. We also have the identity

$$F(\alpha)=\frac{4\pi^2}{T\log T}\int_{-\infty}^{\infty} e^{-4\pi|u|}\left|\sum_{0<\gamma\leqslant T} T^{i\alpha\gamma}e^{2\pi iu\gamma}\right|^2 \mathrm{d}u\geqslant 0.$$

Therefore, we obtain

$$\begin{aligned}
2F(\alpha)-F_{\Delta}(\alpha)-F_{-\Delta}(\alpha)=&F(\alpha)\left[1-\cos(\Delta\alpha\log T)\right]\\
&+O\left(\Delta\int_{-\infty}^{\infty} e^{-4\pi|u|}|u|\left|\sum_{0<\gamma\leqslant T} T^{i\alpha\gamma}e^{2\pi iu\gamma}\right|^2 \mathrm{d}u\right).
\end{aligned}$$

The rest of the proof consists of controlling this last error term. This requires a technical but straightforward modification of Montgomery's arguments and definitions in [81], which we define and prove in Appendix B. In particular, we define $\widetilde{F}_{\sigma_0}(\alpha)$ in (7.0.10), which is a modification of $F(\alpha)$ by using a slightly different weight. Using the estimate $|u|\ll e^{4\pi|u|\varepsilon}$ for $\varepsilon>0$ and the identity (7.0.11) for $\widetilde{F}_{\sigma_0}(\alpha)$, we find that

$$2F(\alpha)-F_{\Delta}(\alpha)-F_{-\Delta}(\alpha)=F(\alpha)\left[1-\cos(\Delta\alpha\log T)\right]+O\Big(\Delta\widetilde{F}_{\sigma_0}(\alpha)\Big),$$

where $\sigma_0=1-\varepsilon$ (we may take any $0<\varepsilon<\frac{1}{2}$). Now, Proposition 7.4 implies that

$$\int_{1}^{\infty}\frac{\widetilde{F}_{\sigma_0}(\alpha)}{\alpha^2}\,\mathrm{d}\alpha\ll 1.$$

Hence the desired result now follows. □

Remark. By (5.6.1), we know that $2F(\alpha)-F_{\Delta}(\alpha)-F_{-\Delta}(\alpha)\geqslant 0$. Modifying an argument of Goldston [53, Lemma A] in a straightforward manner, it can be shown that, for $\Delta=o(\log^2 T)$, as $T\to\infty$, we have

$$\int_{1}^{\infty}\frac{2F(\alpha)-F_{\Delta}(\alpha)-F_{-\Delta}(\alpha)}{\alpha^2}\,\mathrm{d}\alpha\ll 1.$$

Proof of Corollary 5.7. Note that, by Proposition 5.23, since Theorem 5.3 reduces to Fujii's theorem when $\Delta = o(1)$, part (a) follows from Fujii's remarks [46, Section 3]. For part (b), let $\Delta \gg 1$. We want to show that

$$\pi^2 \int_0^T [S(t+\Delta) - S(t)]^2 \, \mathrm{d}t = T\left[\sum_{n \leqslant T} \frac{\Lambda^2(n)}{n \log^2 n}(1 - \cos(\Delta \log n)) + 1\right] + o(T).$$

To prove part (b) of Conjecture 5.5, by Theorem 5.4, it is enough to show that

$$\frac{1}{2}\int_1^\infty \frac{2F(\alpha) - F_\Delta(\alpha) - F_{-\Delta}(\alpha)}{\alpha^2} \, \mathrm{d}\alpha = 1 + o(1).$$

By Conjecture 5.6, we have

$$\frac{1}{2}\int_1^\infty \frac{2F(\alpha) - F_\Delta(\alpha) - F_{-\Delta}(\alpha)}{\alpha^2} \, \mathrm{d}\alpha = \int_1^\infty \frac{1 - \cos\left(\Delta\alpha \log T\right) w\left(\Delta\right)}{\alpha^2} \, \mathrm{d}\alpha + o(1).$$

Now note that

$$\int_1^\infty \frac{1}{\alpha^2} \, \mathrm{d}\alpha = 1.$$

Then, integrating by parts, we find that

$$\int_1^\infty \frac{\cos(\Delta\alpha \log T)\, w(\Delta)}{\alpha^2} \, \mathrm{d}\alpha = O\left(\frac{1}{\Delta \log T}\right) = O\left(\frac{1}{\log T}\right),$$

as we wanted. This completes the proof. $\square$

Chapter 6

Zeros of families of L-functions

This chapter is comprised of the paper [A5]. We study the q-analogue of the average of Montgomery's function $F(\alpha, T)$ (defined in (1.3.5)) over bounded intervals. Assuming GRH, our goal is to obtain upper and lower bounds for this average over an interval that are as close as possible to the pointwise conjectured value of 1. To compute our bounds, we extend a Fourier analysis approach of Carneiro, Chandee, Chirre and Milinovich [16], and apply computational methods of non-smooth programming.

6.1 Introduction

The pair correlation conjecture (1.3.4), and similarly, the behaviour of Montgomery's function $F(\alpha)$ in larger ranges of α, have since proved to be deep and difficult questions, being related to important problems such as the behavior of primes in short intervals [58]. Recall, as mentioned in Section 1.3.7, that the pair correlation conjecture is equivalent to the statement

$$\frac{1}{\ell}\int_{b}^{b+\ell} F(\alpha, T)\ \mathrm{d}\alpha \sim 1,$$

as $T \to \infty$, for any fixed $b \geqslant 1$ and $\ell > 0$, where F is defined in (1.3.5). For further background on the pair correlation conjecture and its equivalences, see, for instance, [16], and the references therein. For a gentle introduction to the pair correlation conjecture and its relation to prime numbers, see the notes [55].

6.1.1 Bounds via Fourier optimization

Recently, Carneiro, Chandee, Chirre, and Milinovich [16] studied these averages of F over bounded intervals, by developing a general theoretical framework that relates them to some extremal problems in Fourier analysis. This was inspired by some constructions of Goldston [53] and Goldston and Gonek [56]. For example, let $\mathcal{A}_1$ be the class of continuous, even, and non-negative functions $g \in L^1(\mathbb{R})$ such that supp $\widehat{g} \subset [-1, 1]$. Consider the following extremal problems:[1]

Extremal Problem 6.0.1 (EP1)**.** *Find*

$$\mathbf{C}^+ := \inf_{g\in\mathcal{A}_1\setminus\{0\}} \frac{\widehat{g}(0) + 2\int_0^1 \alpha\, \widehat{g}(\alpha)\ \mathrm{d}\alpha}{\min_{0\leqslant\alpha\leqslant 1} |\widehat{g}(\alpha) + \widehat{g}(1-\alpha)|}.$$

Extremal Problem 6.0.2 (EP2)**.** *Define the constant*

$$c_0 := \min_{x\in\mathbb{R}\setminus\{0\}} \frac{\sin x}{x} = -0.2172336282\ldots \tag{6.1.1}$$

Find

$$\mathbf{C}^- := \sup_{\substack{g\in\mathcal{A}_1\\ g(0)>0}} \frac{(1-c_0)g(0) + c_0\left(\widehat{g}(0) + 2\int_0^1 \alpha\, \widehat{g}(\alpha)\ \mathrm{d}\alpha\right)}{\max_{0\leqslant\alpha\leqslant 1}\left(|\widehat{g}(\alpha)| + |\widehat{g}(1-\alpha)|\right)}.$$

As a consequence of their general framework, they obtain the following:

Theorem 6.1 (c.f. [16, Theorem 1])**.** *Assume RH, let $b \geqslant 1$, and let $\varepsilon > 0$. For sufficiently large fixed ℓ (possibly depending on b and ε), as $T \to \infty$, we have*

$$\mathbf{C}^- - \varepsilon + o(1) \leqslant \frac{1}{\ell}\int_b^{b+\ell} F(\alpha, T)\ \mathrm{d}\alpha \leqslant \mathbf{C}^+ + \varepsilon + o(1).$$

Additionally, they establish the bounds (see [16, Corollary 2] and the numerical examples in p.18 and p.20)

$$0.927818 < \mathbf{C}^- \leqslant \mathbf{C}^+ < 1.330174, \tag{6.1.2}$$

which give the respective numerical lower and upper bounds for the left-hand side of (1.3.13).

6.1.2 q-analogues: an average over Dirichlet $L-$functions

Montgomery [81] also suggested the investigation of the pair correlation of zeros of a family of Dirichlet $L-$functions in the q-aspect. One wishes to study the distribution of the low-lying zeros of $L(s,\chi)$, on average over Dirichlet characters χ (mod q), and over $Q \leqslant q \leqslant 2Q$. By taking these averages, one can obtain improvements over what is known for the Riemann zeta-function, and this provides heuristic evidence for the original case. In [27, 89], the authors obtained improvements over (1.3.6) for these q-analogues, and used this to obtain lower bounds for the average proportion of simple zeros of Dirichlet L-functions. Later, in [17], the authors introduced the idea of relating the pair correlation of zeros of $\zeta(s)$, and its q-analogue, to some Hilbert spaces of entire functions. Sono [97] used this idea to improve the aforementioned lower bounds on the proportion of simple zeros. These were

[1] In [16], the authors work with a larger class of functions instead of $\mathcal{A}_1$. See Section 6.3.1 for further comments. Note that our class $\mathcal{A}_1$ is called $\mathcal{A}_0$ in [16]. We make this change of notation since, in Section 6.2, other classes $\mathcal{A}_\Delta$ will naturally appear, where the support $[-1, 1]$ is replaced by $[-\Delta, \Delta]$ for a parameter Δ.

further improved in [30], by using a different class of functions and sophisticated numerical optimization methods (see Section 6.3.1).

To define these q-analogues, we must introduce some notation. We use the framework established in [27], and follow the notation in [17, Section 6]. Assume GRH for Dirichlet L-functions (GRH). Let Φ be a real-valued function with compact support in (a, b), where $0 < a < b$. Denote by

$$\widetilde{\Phi}(s) := \int_0^\infty \Phi(x)x^{s-1}\,\mathrm{d}x$$

its Mellin transform. Additionally, assume that $\Phi(x^{-1}) = \Phi(x)$ for all $x \in \mathbb{R}\backslash\{0\}$, that $\widetilde{\Phi}(it) \geqslant 0$ for all $t \in \mathbb{R}$, and that $|\widetilde{\Phi}(it)| \ll |t|^{-2}$ as $|t| \to \infty$. For instance, a possible choice satisfying all conditions (see [17]) is Φ such that

$$\widetilde{\Phi}(s) = \left(\frac{e^s - e^{-s}}{2s}\right)^2.$$

Finally, let W be a smooth, non-negative function with compact support in (1, 2). We can now define the q-analogue of $N(T)$ as

$$N_\Phi(Q) := \sum_q \frac{W(q/Q)}{\phi(q)} \sideset{}{^*}\sum_{\chi\,(\mathrm{mod}\,q)} \sum_{\gamma_\chi} |\widetilde{\Phi}(i\gamma_\chi)|^2, \tag{6.1.3}$$

where the second sum (indicated by the superscript *) is over all primitive Dirichlet characters (mod q), and the last sum is over all non-trivial zeros $1/2 + i\gamma_\chi$ of $L(s, \chi)$. Define the q-analogue of $F(\alpha, T)$ as

$$F_\Phi(\alpha) = F_\Phi(\alpha, Q) := \frac{1}{N_\Phi(Q)} \sum_q \frac{W(q/Q)}{\phi(q)} \sideset{}{^*}\sum_{\chi\,(\mathrm{mod}\,q)} \sum_{\gamma_\chi} |\widetilde{\Phi}(i\gamma_\chi)Q^{i\alpha\gamma_\chi}|^2. \tag{6.1.4}$$

Chandee, Lee, Liu and Radziwiłł [27] proved an asymptotic formula for $F_\Phi(\alpha)$ similar to (1.3.6) for $|\alpha| < 2$, showing, in particular, that $F_\Phi(\alpha) \sim 1$ when $1 \leqslant |\alpha| < 2$ (see Lemma 6.3 below for a full statement). Moreover, they conjectured that $F_\Phi(\alpha) \sim 1$ for all $|\alpha| \geqslant 1$, in analogy with Montgomery's original conjecture for $F(\alpha, T)$. We may now state our main result, which gives evidence for this conjecture.

Theorem 6.2. *Assume GRH, and let $b \geqslant 1$. For sufficiently large fixed ℓ (possibly depending on b), as $Q \to \infty$, we have*

$$0.982144 + o(1) < \frac{1}{\ell}\int_b^{b+\ell} F_\Phi(\alpha, Q)\,\mathrm{d}\alpha < 1.077542 + o(1).$$

We highlight that our upper and lower bounds are very close to the conjectured value of 1. We also remark that while the size of ℓ in the lower bound may depend on b, the size of ℓ in the upper bound is independent of b. A similar situation occurs in Theorem 6.1. For effective bounds that hold for any given b and ℓ, see Section 6.2.1.

To prove Theorem 6.2, we develop a framework for estimating these integrals over bounded intervals via Fourier analysis, extending that of [16]. We take advantage of the new information available when $|\alpha| \in [1, 2)$, from [27]. This leads to slightly different Fourier extremal problems. For instance, with $\mathcal{A}_1$ and c_0 as above, consider the following:

Extremal Problem 6.2.1 (EP3)**.** *Find*

$$\mathbf{D}^+ := \inf_{g \in \mathcal{A}_1 \setminus \{0\}} \frac{\widehat{g}(0) + 8\int_0^{1/2} \alpha\, \widehat{g}(\alpha)\ \mathrm{d}\alpha + 4\int_{1/2}^{1} \widehat{g}(\alpha)\ \mathrm{d}\alpha}{2\min_{0 \leqslant \alpha \leqslant 1} |\widehat{g}(\alpha) + \widehat{g}(1-\alpha)|}.$$

Extremal Problem 6.2.2 (EP4)**.** *Find*

$$\mathbf{D}^- := \sup_{\substack{g \in \mathcal{A}_1 \\ g(0) > 0}} \frac{(1-c_0)g(0) + \frac{c_0}{2}\left(\widehat{g}(0) + 8\int_0^{1/2} \alpha\, \widehat{g}(\alpha)\ \mathrm{d}\alpha + 4\int_{1/2}^{1} \widehat{g}(\alpha)\ \mathrm{d}\alpha\right)}{\max_{0 \leqslant \alpha \leqslant 1} \left(|\widehat{g}(\alpha)| + |\widehat{g}(1-\alpha)|\right)}.$$

We show that $\mathbf{D}^- - \varepsilon$ and $\mathbf{D}^+ + \varepsilon$ are lower and upper bounds for the average in Theorem 6.2, respectively (see Lemma 6.6 below). The simple choice of test function $\widehat{g}(\alpha) = \max\{(1 - |\alpha|), 0\}$ already shows that

$$0.981897 < \mathbf{D}^- \quad \text{and} \quad \mathbf{D}^+ < 1.083334.$$

To go further, we then numerically optimize the bounds. Note that the functionals in the above extremal problems are not smooth, due to the maximum and minimum in the denominators. Hence, we apply the principal axis method of Brent [13], which is an algorithm for unconstrained non-smooth optimization. We also applied our optimization routine to the problems (EP1) and (EP2), and found a minor refinement in the fifth and sixth decimal digits in the bounds (6.1.2) from [16, Corollary 2]. It seems that these are very close to the sharp values for the Fourier optimization problems. Under the hypotheses of Theorem 6.1, we find

$$0.927819 + o(1) < \frac{1}{\ell}\int_b^{b+\ell} F(\alpha, T)\ \mathrm{d}\alpha < 1.330144 + o(1).$$

In Section 6.2, we prove a general result relating the integrals of $F_\Phi(\alpha)$ to some extremal problems, extending [16, Theorem 7]. Subsequently, we use it to relate the problems (EP3) and (EP4) to Theorem 6.2. Furthermore, we provide effective bounds for the integral of $F_\Phi(\alpha)$ over any arbitrary interval, in Theorem 6.5. In Section 6.3, we show how to numerically optimize the bounds for (EP1)-(EP4), completing the proof of Theorem 6.2.

Remark. Analogues of Montgomery's function $F(\alpha)$ have also been studied for other families of L-functions. Recently, Chandee, Klinger-Logan and Li [26] proved an analogue of (1.3.6) for an average over a family of $\Gamma_1(q)$ L-functions, in the range $|\alpha| < 2$. Therefore, assuming GRH for this family and for Dirichlet L-functions, the conclusion of Theorem 6.2 also holds for this family, as $q \to \infty$. See Section 6.2.3 for more details.

6.2 Fourier optimization and the average of $F_\Phi(\alpha)$

For $\Delta \geqslant 1$, let $\mathcal{A}_\Delta$ be the class of continuous, even, and non-negative functions $g \in L^1(\mathbb{R})$ such that $\operatorname{supp} \widehat{g} \subset [-\Delta, \Delta]$. For $g \in \mathcal{A}_\Delta$, denote

$$\rho_\Delta(g) := \widehat{g}(0) + 2\int_0^1 \alpha\, \widehat{g}(\alpha)\ \mathrm{d}\alpha + 2\int_1^\Delta \widehat{g}(\alpha)\ \mathrm{d}\alpha. \tag{6.2.1}$$

From the definition of $F_\Phi(\alpha)$ in (6.1.4) and Fourier inversion, we have the convolution formula, for $R \in L^1(\mathbb{R})$ with $\widehat{R} \in L^1(\mathbb{R})$:

$$\sum_q \frac{W(q/Q)}{\phi(q)} \sideset{}{^*}\sum_{\chi \,(\mathrm{mod}\, q)} \sum_{\gamma_\chi, \gamma_\chi'} R\left(\frac{(\gamma_\chi - \gamma_\chi')\log Q}{2\pi}\right) \widetilde{\Phi}(i\gamma_\chi)\widetilde{\Phi}(i\gamma_\chi') = N_\Phi(Q)\int_{-\infty}^{\infty} F_\Phi(\alpha)\, \widehat{R}(\alpha)\ \mathrm{d}\alpha. \tag{6.2.2}$$

A crucial tool is the asymptotic formula of Chandee, Lee, Liu and Radziwiłł:

Lemma 6.3 (c.f. [27, Theorem 1.2])**.** *Assume GRH. Let $\varepsilon > 0$. Then*

$$\begin{aligned} F_\Phi(\alpha, Q) =& (1 + o(1))\left(f(\alpha) + \Phi(Q^{-|\alpha|})^2 \log Q \left(\frac{1}{2\pi}\int_{-\infty}^{\infty} |\widetilde{\Phi}(ix)|^2\ \mathrm{d}x\right)^{-1}\right) \\ &+ O\left(\Phi(Q^{-|\alpha|})\sqrt{f(\alpha)\log Q}\right), \end{aligned}$$

uniformly for $|\alpha| \leqslant 2 - \varepsilon$, as $Q \to \infty$, where $f(\alpha) = \begin{cases} |\alpha|, & \textit{for} \ \ |\alpha| \leqslant 1, \\ 1, & \textit{for} \ \ |\alpha| > 1. \end{cases}$

By Plancherel's theorem for the Mellin transform, the term

$$\Phi(Q^{-|\alpha|})^2 \log Q \left(\frac{1}{2\pi}\int_{-\infty}^{\infty} |\widetilde{\Phi}(ix)|^2\ \mathrm{d}x\right)^{-1}$$

behaves like a Dirac delta at the origin (see the argument in [27, pp. 82–83]). Therefore, for any fixed $1 \leqslant \Delta < 2$ and $g \in \mathcal{A}_\Delta$, from (6.2.2), we obtain

$$\frac{1}{N_\Phi(Q)} \sum_q \frac{W(q/Q)}{\phi(q)} \sideset{}{^*}\sum_{\chi \,(\mathrm{mod}\, q)} \sum_{\gamma_\chi, \gamma_\chi'} g\left(\frac{(\gamma_\chi - \gamma_\chi')\log Q}{2\pi}\right) \widetilde{\Phi}(i\gamma_\chi)\widetilde{\Phi}(i\gamma_\chi') = \rho_\Delta(g) + o(1), \tag{6.2.3}$$

as $Q \to \infty$.

The following problems are essentially those considered in [16, Section 2.1.1], which correspond to the case $\Delta = 1$. For any $\Delta \geqslant 1$, we may consider the following variations:

Extremal Problem 6.3.1 (EP5)**.** *Let $\ell > 0$ and $\Delta \geqslant 1$. Find*

$$\mathcal{W}_\Delta^+(\ell) := \inf \sum_{j=1}^N \rho_\Delta(g_j),$$

where the infimum is taken over N and all collections $g_1, g_2, \ldots, g_N \in \mathcal{A}_\Delta$ such that there exist points $\xi_1, \xi_2, \ldots, \xi_N \in \mathbb{R}$, with

$$\sum_{j=1}^{N} \widehat{g}_j(\alpha - \xi_j) \geqslant \mathbb{I}_{[0,\,\ell]}(\alpha) \tag{6.2.4}$$

for all $\alpha \in \mathbb{R}$.

Extremal Problem 6.3.2 (EP6)**.** *Let $\ell > 0$ and $\Delta \geqslant 1$. Find*

$$\mathcal{W}_\Delta^-(\ell) := \sup \sum_{j=1}^{N} (2g_j(0) - \rho_\Delta(g_j)), \tag{6.2.5}$$

where the supremum is taken over N and all collections $g_1, g_2, \ldots, g_N \in \mathcal{A}_\Delta$ such that there exist points $\xi_1, \xi_2, \ldots, \xi_N \in \mathbb{R}$, with

$$\sum_{j=1}^{N} \widehat{g}_j(\alpha - \xi_j) \leqslant \mathbb{I}_{[0,\,\ell]}(\alpha) \tag{6.2.6}$$

for all $\alpha \in \mathbb{R}$.

Extremal Problem 6.3.3 (EP7)**.** *Let $b, \beta \in \mathbb{R}$ with $b < \beta$, and $\Delta \geqslant 1$. Find*

$$\mathcal{W}_{*,\,\Delta}^-(b, \beta) := \sup \sum_{j=1}^{N} (g_j(0) + \tau_j(\rho_\Delta(g_j) - g_j(0))), \tag{6.2.7}$$

where the supremum is taken over N and all collections $g_1, g_2, \ldots, g_N \in \mathcal{A}_\Delta$ such that there exist points $\eta_1, \eta_2, \ldots, \eta_N \in \mathbb{R}$ and values $\tau_1, \tau_2, \ldots, \tau_N \leqslant 1$, such that

$$\sum_{j=1}^{N} \widehat{g}_j(\alpha - \eta_j) \leqslant \mathbb{I}_{[b,\,\beta]}(\alpha) \tag{6.2.8}$$

for all $\alpha \in \mathbb{R}$, and

$$\mathrm{Re}\left(\sum_{j=1}^{N} e^{2\pi i \eta_j x} g_j(x)\right) \geqslant \sum_{j=1}^{N} \tau_j g_j(x), \tag{6.2.9}$$

for all $x \in \mathbb{R}$.

The following result relates the problem of estimating integrals of $F_\Phi(\alpha)$ to the above problems in Fourier analysis. This general result will allow us to obtain all our bounds for these integrals. As we shall see, while the abstract formulation of these problems and the general result in Lemma 6.4 are analogous to those in [16], the novelty lies in the way we may explore them, by taking advantage of the new possibilities with $1 < \Delta < 2$, and its interplay with the other parameters. We anticipate that, when applying Lemma 6.4, we will usually have in mind the limit $\Delta \to 2^-$.

Lemma 6.4. *Assume GRH, let $b \in \mathbb{R}$ and $\ell > 0$. Let $1 \leqslant \Delta < 2$. Then, as $Q \to \infty$, we have*

$$\mathcal{W}^{-}_{\Delta}(\ell) + o(1) \leqslant \mathcal{W}^{-}_{*,\Delta}(b,\, b+\ell) + o(1) \leqslant \int_b^{b+\ell} F_\Phi(\alpha, Q)\, \mathrm{d}\alpha \leqslant \mathcal{W}^{+}_{\Delta}(\ell) + o(1). \qquad (6.2.10)$$

The proof is essentially that of [16, Theorem 7], where the authors prove the analogous result for integrals of $F(\alpha, T)$, with $\Delta = 1$. We reproduce it below, in our context, for the reader's convenience.

Proof. Assume that the bound (6.2.4) holds. We use it, combined with the convolution formula (6.2.2) and (6.2.3), to find

$$\begin{aligned}
&\int_b^{b+\ell} F_\Phi(\alpha)\, \mathrm{d}\alpha \\
&\leqslant \sum_{j=1}^{N} \int_{\mathbb{R}} F_\Phi(\alpha)\, \widehat{g}_j(\alpha - b - \xi_j)\, \mathrm{d}\alpha \\
&= \frac{1}{N_\Phi(Q)} \sum_{j=1}^{N} \sum_q \frac{W(q/Q)}{\phi(q)} \sideset{}{^*}\sum_{\chi\,(\mathrm{mod}\,q)} \sum_{\gamma_\chi,\gamma'_\chi} Q^{i(b+\xi_j)(\gamma_\chi-\gamma'_\chi)} g_j\left(\frac{(\gamma_\chi-\gamma'_\chi)\log Q}{2\pi}\right) \widetilde{\Phi}(i\gamma_\chi)\widetilde{\Phi}(i\gamma'_\chi) \\
&\leqslant \frac{1}{N_\Phi(Q)} \sum_{j=1}^{N} \sum_q \frac{W(q/Q)}{\phi(q)} \sideset{}{^*}\sum_{\chi\,(\mathrm{mod}\,q)} \sum_{\gamma_\chi,\gamma'_\chi} g_j\left(\frac{(\gamma_\chi-\gamma'_\chi)\log Q}{2\pi}\right) \widetilde{\Phi}(i\gamma_\chi)\widetilde{\Phi}(i\gamma'_\chi) \\
&= \sum_{j=1}^{N} \rho_\Delta(g_j) + o(1).
\end{aligned}$$

This implies the upper bound in (6.2.10). To obtain the last inequality, we used the fact that $W(t)$, $g_j(t)$, and $\widetilde{\Phi}(it)$ are all non-negative (for $t \in \mathbb{R}$).

For the lower bound, we first note that $\mathcal{W}^{-}_{\Delta}(\ell) \leqslant \mathcal{W}^{-}_{*,\Delta}(b,\, b+\ell)$. To see this, take a configuration that satisfies (6.2.6). Let $\beta = b+\ell$. Then, taking $\eta_j = \xi_j + b$, (6.2.8) is verified, and choosing $\tau_j = -1$ for all j, (6.2.9) is also verified. With these choices, (6.2.7) reduces to (6.2.5), as desired. It remains to show that $\mathcal{W}^{-}_{*,\Delta}(b,\, b+\ell) + o(1) \leqslant \int_b^{b+\ell} F_\Phi(\alpha, Q)\, \mathrm{d}\alpha$. Given a zero $\frac{1}{2} + i\gamma_\chi$ of $L(s,\chi)$ of multiplicity m_{γ_χ}, denote $\kappa_{\gamma_\chi} := m_{\gamma_\chi}\widetilde{\Phi}(i\gamma_\chi)^2$. Assume that (6.2.8) and (6.2.9) hold. We again use them with (6.2.2) and (6.2.3) to obtain

$$\begin{aligned}
&\int_b^{b+\ell} F_\Phi(\alpha)\, \mathrm{d}\alpha \\
&\geqslant \sum_{j=1}^{N} \int_{\mathbb{R}} F_\Phi(\alpha)\, \widehat{g}_j(\alpha - \eta_j)\, \mathrm{d}\alpha \\
&= \frac{1}{N_\Phi(Q)} \sum_{j=1}^{N} \sum_q \frac{W(q/Q)}{\phi(q)} \sideset{}{^*}\sum_{\chi\,(\mathrm{mod}\,q)} \sum_{\gamma_\chi,\gamma'_\chi} Q^{i\eta_j(\gamma_\chi-\gamma'_\chi)} g_j\left(\frac{(\gamma_\chi-\gamma'_\chi)\log Q}{2\pi}\right) \widetilde{\Phi}(i\gamma_\chi)\widetilde{\Phi}(i\gamma'_\chi) \\
&= \frac{1}{N_\Phi(Q)} \sum_{j=1}^{N} \sum_q \frac{W(q/Q)}{\phi(q)} \sideset{}{^*}\sum_{\chi\,(\mathrm{mod}\,q)} \Bigg\{ g_j(0) \sum_{\gamma_\chi} \kappa_{\gamma_\chi}
\end{aligned}$$

$$
\begin{aligned}
&\qquad\qquad + \sum_{\gamma_\chi \neq \gamma'_\chi} Q^{i\eta_j(\gamma_\chi - \gamma'_\chi)} g_j\left(\frac{(\gamma_\chi - \gamma'_\chi)\log Q}{2\pi}\right)\widetilde{\Phi}(i\gamma_\chi)\widetilde{\Phi}(i\gamma'_\chi)\Bigg\} \\
&\geqslant \frac{1}{N_\Phi(Q)}\sum_{j=1}^{N}\sum_q \frac{W(q/Q)}{\phi(q)}\sideset{}{^*}\sum_{\chi\,(\mathrm{mod}\,q)}\Bigg\{g_j(0)(1-\tau_j)\sum_{\gamma_\chi}\kappa_{\gamma_\chi} \\
&\qquad\qquad + \tau_j\sum_{\gamma_\chi,\,\gamma'_\chi} g_j\left(\frac{(\gamma_\chi - \gamma'_\chi)\log Q}{2\pi}\right)\widetilde{\Phi}(i\gamma_\chi)\widetilde{\Phi}(i\gamma'_\chi)\Bigg\} \\
&\geqslant \sum_{j=1}^{N}(g_j(0) + \tau_j(\rho_\Delta(g_j) - g_j(0))) + o(1).
\end{aligned}
$$

This gives the desired lower bound. To obtain the last inequality, we used that, by (6.1.3),

$$
\sum_q \frac{W(q/Q)}{\phi(q)}\sideset{}{^*}\sum_{\chi\,(\mathrm{mod}\,q)}\sum_{\gamma_\chi}\kappa_{\gamma_\chi} \geqslant \sum_q \frac{W(q/Q)}{\phi(q)}\sideset{}{^*}\sum_{\chi\,(\mathrm{mod}\,q)}\sum_{\gamma_\chi}\widetilde{\Phi}(i\gamma_\chi)^2 = N_\Phi(Q).
$$

□

Remark. Note that if $\Delta_1 \leqslant \Delta_2$, then $\mathcal{A}_{\Delta_1} \subset \mathcal{A}_{\Delta_2}$. Therefore, $\mathcal{W}^+_\Delta(\ell)$ is non-increasing with Δ, while $\mathcal{W}^-_\Delta(\ell)$ and $\mathcal{W}^-_{*,\Delta}(b,\beta)$ are non-decreasing with Δ. For some properties regarding monotonicity, subadditivity, and other basic facts on the above functions $\mathcal{W}^\pm_\Delta$, we refer to [16, Proposition 6], which continues to hold for any $\Delta \geqslant 1$. Also, note that in the statement of Lemma 6.4, the parameters b, ℓ and Δ are all free and independent. Here and henceforth, the error term $o(1)$ should be regarded as a function of Q, which may depend on all other fixed parameters (b, ℓ and Δ).

6.2.1 Triangle bounds

Here, we give simple, effective bounds for the integral of $F_\Phi(\alpha)$ over an arbitrary interval, by using (EP5) and (EP6) with the functions $\widehat{g}_j$ chosen as triangles. Our bounds have the property of being continuous and non-decreasing with ℓ. To begin, let $\Delta \geqslant 1$. For $0 < \delta \leqslant \Delta$, let

$$
K_\delta(x) = \delta\left(\frac{\sin \pi\delta x}{\pi\delta x}\right)^2 \quad \text{and} \quad \widehat{K_\delta}(\alpha) = \left(1 - \frac{|\alpha|}{\delta}\right)_+. \tag{6.2.11}
$$

Note that

$$
\rho_\Delta(K_\delta) = \begin{cases} 1 + \frac{\delta^2}{3}, & \text{if } \ 0 < \delta \leqslant 1, \\ \delta + \frac{1}{3\delta}, & \text{if } \ 1 < \delta \leqslant \Delta. \end{cases} \tag{6.2.12}
$$

Theorem 6.5. *Assume GRH, let $b \geqslant 1$, and let $\ell > 0$. Then, as $Q \to \infty$, we have*

$$
\mathcal{C}^-(\ell) + o(1) \leqslant \int_b^{b+\ell} F_\Phi(\alpha, Q)\,\mathrm{d}\alpha \leqslant \mathcal{C}^+(\ell) + o(1),
$$

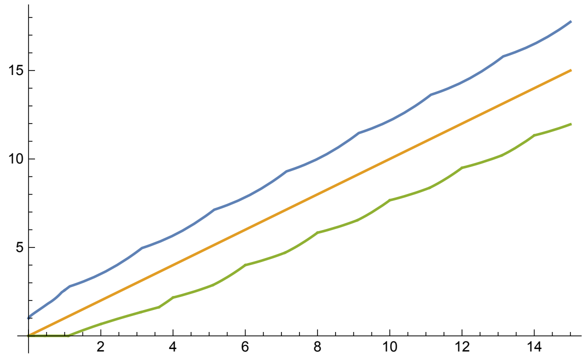

Figure 6.1: The upper bound (in blue) and the lower bound (in green) given in Theorem 6.5, compared with the q-analogue of the pair correlation conjecture (in yellow).

where

$$\mathcal{C}^{+}(\ell)=\begin{cases}\frac{13(\ell+2)}{12}+\frac{1}{3}\left\{\frac{\ell}{2}\right\}^3-\frac{7}{6}\left\{\frac{\ell}{2}\right\}-\frac{1}{6}\left(2\left\{\frac{\ell}{2}\right\}^3-6\left\{\frac{\ell}{2}\right\}^2-6\left\{\frac{\ell}{2}\right\}+5\right)_+, & \text{if } \ell\geqslant 1,\\ \min\left\{\frac{13(\ell+2)}{12}+\frac{1}{3}\left\{\frac{\ell}{2}\right\}^3-\frac{7}{6}\left\{\frac{\ell}{2}\right\}-\frac{1}{6}\left(2\left\{\frac{\ell}{2}\right\}^3-6\left\{\frac{\ell}{2}\right\}^2-6\left\{\frac{\ell}{2}\right\}+5\right)_+\right.\\ \qquad\left.;\ (1+c)\left(1+\frac{\ell^2(1+c)^2}{12c^2}\right)\right\}, & \text{if } 0<\ell<1,\ \text{with } c=\max\left\{6^{-1/3}\ell^{2/3}\,;\,\frac{\ell}{2-\ell}\right\};\end{cases} \tag{6.2.13}$$

and

$$\mathcal{C}^{-}(\ell)=\begin{cases}\max\left\{\frac{11(\ell-2)}{12}+\frac{1}{2}\left\{\frac{\ell}{2}\right\}^2-\frac{5}{6}\left\{\frac{\ell}{2}\right\}+\frac{1}{3}+\frac{1}{6}\left\{\frac{\ell}{2}\right\}\left(-\left\{\frac{\ell}{2}\right\}^2+6\left\{\frac{\ell}{2}\right\}-3\right)_+\right.\\ \qquad\qquad\left.;\ \frac{1}{2}\ell-\frac{2}{3\ell}\right\}, & \text{if } \ell\geqslant 2,\\ \left(\ell-1-\frac{\ell^2}{12}\right)_+, & \text{if } 0<\ell\leqslant 2.\end{cases} \tag{6.2.14}$$

Proof. We would like to apply Lemma 6.4 with $\Delta\to 2$. To achieve this, we must obtain continuous bounds for an arbitrary $\Delta\in(1,2)$. For simplicity, we will additionally assume that $\frac{4}{3}\leqslant\Delta<2$ throughout the proof.

Upper bound. Following the strategy in [16], we choose $n\geqslant 0$ large triangles, with two additional small triangles at the beginning and end. In (EP5), we take $N=n+2$, $\widehat{g}_j=K_\Delta$ for $2\leqslant j\leqslant n+1$, and $\widehat{g}_1=\widehat{g}_{N+2}=\frac{\delta}{\Delta}\widehat{K}_\delta$. These are the similar triangles with base 2Δ and height 1, and base 2δ and height $\frac{\delta}{\Delta}$, respectively. Moreover, let

$$\Delta(n-1)+2\delta=\ell, \tag{6.2.15}$$

and consider the translates given by $\xi_1=0$, $\xi_j=\delta+\Delta(j-2)$ for $2\leqslant j\leqslant n+1$, and $\xi_{n+2}=\Delta(n-1)+2\delta=\ell$. Then, condition (6.2.4) is satisfied. We must now choose n and δ in terms of ℓ and Δ, such that (6.2.15) holds. If $\frac{\ell}{\Delta}\in\mathbb{N}$, we may take $(n,\delta)=(\frac{\ell}{\Delta},\frac{\Delta}{2})$. This gives the upper bound

$$\left(1+\frac{1}{3\Delta^2}\right)\ell+\frac{\Delta^2}{12}+1.$$

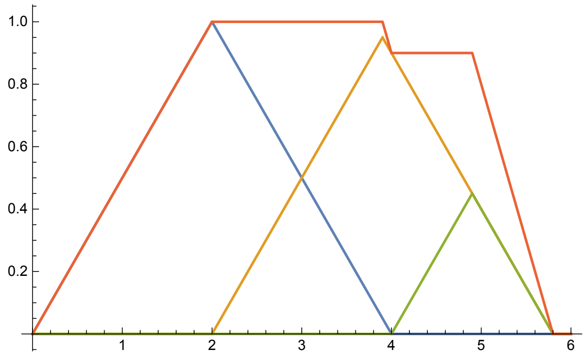

Figure 6.2: A superposition of triangles of three different sizes gives a minorant of $\mathbb{I}_{[0,\ell]}$, producing a continuous lower bound. This is the construction for $\ell = 5.8$, when $\Delta \to 2^-$.

If $\frac{\ell}{\Delta} \notin \mathbb{N}$, we have the choices $(n, \delta) = \left(\lfloor \frac{\ell}{\Delta} \rfloor + 1, \frac{\Delta}{2}\left\{\frac{\ell}{\Delta}\right\}\right)$ or $\left(\lfloor \frac{\ell}{\Delta} \rfloor, \frac{\Delta}{2} + \frac{\Delta}{2}\left\{\frac{\ell}{\Delta}\right\}\right)$. Note that the first choice implies $0 < \delta < \frac{\Delta}{2} < 1$, while the second choice implies $\frac{\Delta}{2} < \delta < \Delta < 2$. We take the minimum of both possibilities, and we must further divide the second choice in cases, depending on whether or not $\delta \geqslant 1$, to apply (6.2.12). Note that $\delta \geqslant 1$ if and only if $\left\{\frac{\ell}{\Delta}\right\} \geqslant \frac{2}{\Delta} - 1$. This yields the upper bound $\mathcal{W}_\Delta^+(\ell) \leqslant C_\Delta^+(\ell)$, where

$$C_\Delta^+(\ell) = \begin{cases} \left(\frac{1}{3\Delta^2} + 1\right)(\Delta + \ell) + p_\Delta(\{\ell/\Delta\}), & \text{if } \left\{\frac{\ell}{\Delta}\right\} < \frac{2}{\Delta} - 1, \\ \left(\frac{1}{3\Delta^2} + 1\right)(\Delta + \ell) + q_\Delta(\{\ell/\Delta\}) - r_\Delta(\{\ell/\Delta\})_+, & \text{if } \left\{\frac{\ell}{\Delta}\right\} \geqslant \frac{2}{\Delta} - 1; \end{cases} \tag{6.2.16}$$

$$p_\Delta(x) := \frac{(x+1)\left(\Delta^3(x+1)^2 - 12\Delta^2 + 12\Delta - 4\right)}{12\Delta}, \qquad q_\Delta(x) := \frac{\Delta^2 x^3}{12} + x\left(1 - \Delta - \frac{1}{3\Delta}\right)$$

and

$$r_\Delta(x) := \frac{\Delta^2 x^3}{12} - \frac{\Delta x^2}{2} + (1-\Delta)x + \frac{\Delta}{2} - \frac{1}{3\Delta}.$$

One can verify that, for all $1 \leqslant \Delta \leqslant 2$, $r_\Delta(x)$ has a unique root in the interval $(0, 1)$, and, if $\Delta \geqslant \frac{4}{3}$, this root is always greater than $\frac{2}{\Delta} - 1$, since $r_\Delta\left(\frac{2}{\Delta} - 1\right) > 0$ and $r_\Delta(1) < 0$. This root denotes the transition between the two choices of n and δ above. In particular, for $\Delta \geqslant 4/3$ and $\ell > 0$, note that $C_\Delta^+(\ell)$ is a continuous function of ℓ and Δ. Therefore, for fixed ℓ, and separately analyzing the cases $\frac{\ell}{2} \in \mathbb{N}$ and $\frac{\ell}{2} \notin \mathbb{N}$, we may let $\Delta \to 2$ in (6.2.16) and Lemma 6.4 to obtain the upper bound in Theorem 6.5, in the case $\ell \geqslant 1$. The upper bound for $0 < \ell < 1$ follows from taking $\Delta = 1$ in Lemma 6.4, and applying directly the bounds for $\mathcal{W}_1^+(\ell)$ in [16, Theorem 9].

Lower bound. If $0 < \ell \leqslant 2\Delta$, we may take the single triangle $\widehat{g}_1 = \widehat{K}_{\ell/2}$, with $\xi_1 = \ell/2$. This gives the lower bound $\mathcal{W}_\Delta^-(\ell) \geqslant (\ell - 1 - \frac{\ell^2}{12})_+$ if $\ell \leqslant 2$ (where we have the trivial bound of zero for $\ell \leqslant 6 - 2\sqrt{6} = 1.101\ldots$), and $\mathcal{W}_\Delta^-(\ell) \geqslant \frac{1}{2}\ell - \frac{2}{3\ell}$ if $2 < \ell \leqslant 2\Delta$. Letting $\Delta \to 2$, we obtain these same lower bounds in Lemma 6.4 for any $0 < \ell < 4$.

In the next step, we must diverge slightly from the strategy in [16] to obtain bounds that are continuous, with respect to ℓ and Δ. For any $\ell \geqslant \Delta$, we combine triangles of three different sizes, instead of two as before. First, we take $n \geqslant 0$ big triangles, followed by one medium triangle, and possibly one last small triangle. Let $n = \lfloor \frac{\ell}{\Delta} \rfloor - 1$, $\delta_1 = \frac{\Delta}{2}\left(1 + \{\frac{\ell}{\Delta}\}\right)$, and $\delta_2 = \frac{\Delta}{2}\{\frac{\ell}{\Delta}\}$. Consider the functions $\widehat{g}_j = \widehat{K_2}$ for $1 \leqslant j \leqslant n$, $\widehat{g_{n+1}} = \frac{\delta_1}{\Delta}\widehat{K_{\delta_1}}$, and $\widehat{g_{n+2}} = \frac{\delta_2}{\Delta}\widehat{K_{\delta_2}}$. Take $\xi_j = \Delta j$ for $1 \leqslant j \leqslant n$, $\xi_{n+1} = \Delta n + \delta_1$, and $\xi_{n+2} = \Delta(n+1) + \delta_2$. The last pair $(\widehat{g_{n+2}}, \xi_{n+2})$ is only included when $2K_{\delta_2}(0) - \rho(K_{\delta_2}) > 0$, that is, when $\{\frac{\ell}{\Delta}\} > \frac{6-2\sqrt{6}}{\Delta}$. Note that, when $\Delta \geqslant \frac{4}{3}$, we have $\delta_1 \geqslant \frac{\Delta}{2} \geqslant \frac{2}{3}$, so that $2K_{\delta_1}(0) - \rho(K_{\delta_1})$ is always positive in this range. Additionally, note that $\ell = \Delta n + 2\delta_1 = \Delta(n+1) + 2\delta_2$, and (6.2.6) is satisfied.

The above configuration, in (EP6), yields $\mathcal{W}_\Delta^-(\ell) \geqslant C_\Delta^-(\ell)$, where

$$C_\Delta^-(\ell) = \begin{cases} \left(\frac{1}{3\Delta^2} + 1\right)(\Delta + \ell) + u_\Delta(\{\ell/\Delta\}), & \text{if } \{\frac{\ell}{\Delta}\} < \frac{2}{\Delta} - 1, \\ \left(\frac{1}{3\Delta^2} + 1\right)(\Delta + \ell) + v_\Delta(\{\ell/\Delta\}) + w_\Delta(\{\ell/\Delta\})_+, & \text{if } \{\frac{\ell}{\Delta}\} \geqslant \frac{2}{\Delta} - 1; \end{cases} \tag{6.2.17}$$

$$u_\Delta(x) = \frac{-\frac{1}{4}\Delta^3(x+1)^3 + 3\Delta^2\left(x^2+1\right) - 3\Delta(x+1) + 2x}{6\Delta};$$

$$v_\Delta(x) = \frac{(x-1)\left(3\Delta^2(x-1)+4\right)}{12\Delta}; \quad \text{and} \quad w_\Delta(x) = \frac{6\Delta x\left(-\frac{1}{12}\Delta^2x^2 + \Delta x - 1\right)}{12\Delta}.$$

Note that, for $0 \leqslant x \leqslant 1$ and $1 \leqslant \Delta \leqslant 2$, $w_\Delta(x) > 0$ if and only if $x > \frac{6-2\sqrt{6}}{\Delta}$. Moreover, we have that $0 \leqslant \frac{2}{\Delta} - 1 < \frac{6-2\sqrt{6}}{\Delta} < 1$. In particular, $C_\Delta^-(\ell)$ is a continuous function of ℓ and Δ, and we may take $\Delta \to 2$ to obtain the lower bounds in Theorem 6.5. In the lower bound for $\ell > 2$, the maximum is attained by the second function for $2 < \ell \leqslant \ell_1$, and by the first function for $\ell > \ell_1$, where $\ell_1 = 3.609\ldots$ □

Remark. An important technical feature of the bounds in Theorem 6.5 is their continuity, which helps to take $\Delta \to 2$. To achieve this continuity for an arbitrary $\Delta \in (4/3, 2)$, we must take precise configurations of triangles, slightly different from those considered in [16], and take care with the cases that arise depending on the size of Δ. As $\ell \to \infty$, it is clearly convenient to take Δ as large as possible, as we have the multiplying factors $(1 \pm \frac{1}{3\Delta^2})$. However, for some fixed values of ℓ, one could do slightly better than stated in Theorem 6.5, by using the general bounds in (6.2.16) and (6.2.17) and choosing an optimal Δ in (4/3, 2).

6.2.2 Asymptotic bounds

Recall that

$$\mathbf{D}^+ := \inf_{g \in \mathcal{A}_1 \setminus \{0\}} \frac{\widehat{g}(0) + 8\int_0^{1/2} \alpha\, \widehat{g}(\alpha)\, \mathrm{d}\alpha + 4\int_{1/2}^1 \widehat{g}(\alpha)\, \mathrm{d}\alpha}{2\min_{0\leqslant\alpha\leqslant1} |\widehat{g}(\alpha) + \widehat{g}(1-\alpha)|}$$

and

$$\mathbf{D}^- := \sup_{\substack{g \in \mathcal{A}_1 \\ g(0)>0}} \frac{(1-c_0)g(0) + \frac{c_0}{2}\left[\widehat{g}(0) + 8\int_0^{1/2} \alpha\, \widehat{g}(\alpha)\, \mathrm{d}\alpha + 4\int_{1/2}^1 \widehat{g}(\alpha)\, \mathrm{d}\alpha\right]}{\max_{0\leqslant\alpha\leqslant1}\left(|\widehat{g}(\alpha)| + |\widehat{g}(1-\alpha)|\right)}.$$

In this section, we begin the proof of Theorem 6.2, by connecting the integrals of $F_\Phi(\alpha)$ to the above extremal problems. The main idea is to consider, in (EP5) and (EP7), copies of a single function $\widehat{g}$, instead of a triangle, so that we may then optimize over admissible functions.

Lemma 6.6. *Assume GRH, and let $b \geqslant 1$. For sufficiently large fixed ℓ, as $Q \to \infty$, we have*

$$\mathbf{D}^- - \varepsilon + o(1) < \frac{1}{\ell}\int_b^{b+\ell} F_\Phi(\alpha, Q)\, \mathrm{d}\alpha < \mathbf{D}^+ + \varepsilon + o(1).$$

Proof. Throughout the proof, let $g \in \mathcal{A}_1$, so that $\operatorname{supp}\widehat{g} \subset [-1,1]$. For $1 < \Delta < 2$, consider the dilation $g_\Delta(\alpha) = \Delta g(\Delta\alpha)$, so that $g_\Delta \in \mathcal{A}_\Delta$. Again, we must first obtain bounds for an arbitrary $\Delta \in (1, 2)$, with the goal of taking $\Delta \to 2^-$ at the end.

Upper bound

Assume that $\min_{0\leqslant\alpha\leqslant 1} |\widehat{g}(\alpha) + \widehat{g}(1-\alpha)| \neq 0$. Then, since $\widehat{g}(0) > 0$ and $\widehat{g}$ is continuous, we must have $\widehat{g}(\alpha) + \widehat{g}(1-\alpha) > 0$ for all $\alpha \in [0, 1]$, and by multiplying by an appropriate constant, we may assume that

$$\min_{0\leqslant\alpha\leqslant 1} (\widehat{g}(\alpha) + \widehat{g}(1-\alpha)) = 1. \tag{6.2.18}$$

In (EP5), given ℓ, let $N = \left\lceil \frac{\ell}{\Delta} \right\rceil + 1$. Consider the N functions $\widehat{g_j} = \widehat{g_\Delta}$, for $1 \leqslant j \leqslant N$, and take the translates $\xi_j = \Delta(j-1)$. Then, by (6.2.18), the fact that $\operatorname{supp}\widehat{g} \in [-1,1]$, and that $\widehat{g}$ is even, we obtain

$$\begin{aligned}\sum_{j=1}^{N} \widehat{g_j}(\alpha - \xi_j) &= \sum_{j=1}^{N} \widehat{g}\left(\frac{\alpha}{\Delta} - j + 1\right) \\ &= \widehat{g}\left(\left\{\frac{\alpha}{\Delta}\right\}\right) + \widehat{g}\left(1 - \left\{\frac{\alpha}{\Delta}\right\}\right) \\ &\geqslant 1,\end{aligned} \tag{6.2.19}$$

for all $0 \leqslant \alpha \leqslant \Delta\left\lceil \frac{\ell}{\Delta} \right\rceil$, in particular for $0 \leqslant \alpha \leqslant \ell$. By an argument of Carneiro, Chandee, Chirre, and Milinovich (adding a finite number of triangles if necessary, see [16, p. 18]) we may assume that this sum is non-negative for all α, and therefore (6.2.4) is satisfied. This gives the bound

$$\mathcal{W}^+{}_\Delta(\ell) \leqslant \frac{\rho_\Delta(g_\Delta)}{\Delta}\,\ell + O(1),$$

where the implied constant may depend on g, but not on ℓ or Δ. Note that the function

$$\Delta \mapsto \frac{\rho_\Delta(g_\Delta)}{\Delta} = \frac{1}{\Delta}\left(\widehat{g}(0) + 2\Delta^2\int_0^{\frac{1}{\Delta}} \alpha\,\widehat{g}(\alpha)\, \mathrm{d}\alpha + 2\Delta\int_{\frac{1}{\Delta}}^{1} \widehat{g}(\alpha)\, \mathrm{d}\alpha\right)$$

is continuous for $1 \leqslant \Delta \leqslant 2$. Then, we may take $\Delta \to 2$ in Lemma 6.4 with the above bound, to obtain, for any fixed $\varepsilon > 0$ and ℓ sufficiently large,

$$\int_b^{b+\ell} F_\Phi(\alpha, Q)\, \mathrm{d}\alpha \leqslant \ell\,(\mathbf{D}^+ + \varepsilon) + o(1),$$

as $Q \to \infty$. This proves the upper bound in Lemma 6.6.

Lower bound

Here, we will use the framework of (EP7). We may assume, without loss of generality, that $g(0) > 0$, and that $\max_{0 \leqslant \alpha \leqslant 1} |\widehat{g}(\alpha)| + |\widehat{g}(1-\alpha)| = 1$. For a fixed $b \geqslant 1$ and large ℓ, let $\beta = b + \ell$, and write

$$\int_b^{b+\ell} F_\Phi(\alpha, Q)\, \mathrm{d}\alpha = 1/2 \int_{-\beta}^{\beta} F_\Phi(\alpha, Q)\, \mathrm{d}\alpha - \int_0^b F_\Phi(\alpha, Q)\, \mathrm{d}\alpha. \tag{6.2.20}$$

Let $n = \left\lfloor \frac{\beta}{\Delta} \right\rfloor$. In (EP7), let $N = 2n-1$, and take $\widehat{g_j} = \widehat{g_\Delta}$ and $\eta_j = \Delta(n-j)$, for $1 \leqslant j \leqslant N$. Define

$$\mathfrak{m}(n) = \min_{x \in \mathbb{R}} D_n(x),$$

where

$$D_n(x) = \sum_{k=-n}^{n} e^{ikx} = \frac{\sin((n+1/2)x)}{\sin(x/2)}$$

is the Dirichlet kernel. From [16, Equation (2.37)], it is known that

$$\lim_{n \to \infty} \frac{\mathfrak{m}(n)}{n} = 2c_0, \quad \text{and moreover,} \quad \left| \frac{\mathfrak{m}(n)}{n} - 2c_0 \right| \ll \frac{1}{n}, \tag{6.2.21}$$

where c_0 is defined in (6.1.1). Let

$$\tau_j = \inf_{\substack{x \in \mathbb{R} \\ g(x) \neq 0}} \frac{g(x) \mathrm{Re} \left(\sum_{j=1}^{2n-1} e^{2\pi i \Delta(n-j)x} \right)}{(2n-1) g(x)} = \frac{\mathfrak{m}(n-1)}{2n-1}.$$

Then, (6.2.9) is automatically satisfied, and we can verify (6.2.8) (where $b = -\beta$). This gives the bound

$$\mathcal{W}^-_{*,\Delta}(-\beta, \beta) \geqslant (2n-1) \left(\Delta g(0) - \frac{\mathfrak{m}(n-1)}{2n-1} (\rho_\Delta(g_\Delta) - \Delta g(0)) \right).$$

This implies, by (6.2.21), that

$$\frac{\mathcal{W}^-_{*,\Delta}(-\beta, \beta)}{2} \geqslant \frac{\beta}{\Delta} \left(\Delta g(0)(1 - c_0) + c_0\, \rho_\Delta(g_\Delta) \right) - O(1),$$

where the implied constant may depend on g but not on Δ or β (note that $\rho_\Delta(g_\Delta)$ can be bounded in terms of g, uniformly in Δ). Now, we apply Lemma 6.4 and (6.2.20), and let $\Delta \to 2$ as before. For any fixed $\varepsilon > 0$ and $b \geqslant 1$, we obtain, for sufficiently large fixed ℓ, that

$$\int_b^{b+\ell} F_\Phi(\alpha, Q)\, \mathrm{d}\alpha \geqslant \ell\, (\mathbf{D}^- - \varepsilon) + o(1),$$

as $Q \to \infty$, as desired. $\square$

6.2.3 $\Gamma_1(q)$-analogues: an average over automorphic L-functions

In this section, for the convenience of the reader, we briefly define the $\Gamma_1(q)$-analogue of $F(\alpha)$, and show how it also satisfies the conclusions of Theorem 6.2 and Theorem 6.5. This is the framework of Chandee, Klinger-Logan and Li in [26], to which we refer for more details. The authors consider a large family of $GL(2)$ L-functions, as follows. Let k and q be positive integers, with $k \geqslant 3$. Consider the subgroups of $GL_2(\mathbb{Z})$

$$\Gamma_0(q) = \left\{ \begin{pmatrix} a & b \\ c & d \end{pmatrix} : \, ad - bc = 1, \, c \equiv 0 \, (\mathrm{mod}\, q) \right\},$$

and

$$\Gamma_1(q) = \left\{ \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \Gamma_0(q) : \, a \equiv d \equiv 1 \, (\mathrm{mod}\, q) \right\}.$$

Let $S_k(\Gamma_0(q), \, \chi)$ be the space of cusp forms of weight $k \geqslant 3$ for $\Gamma_0(q)$ and nebentypus character χ (mod q). Let $\mathcal{H}_\chi \subset S_k(\Gamma_0(q), \, \chi)$ be an orthogonal basis of $S_k(\Gamma_0(q), \, \chi)$ consisting of Hecke cusp forms, normalized so that the first Fourier coefficient is 1. It is known that each $f \in \mathcal{H}_\chi$ has an associated L-function $L(s, \, f)$. Assume GRH for all the $L(s, \, f)$ and for all Dirichlet L-functions. Then, we define the $\Gamma_1(q)$-analogue of $F(\alpha)$ as

$$F_\Phi^*(\alpha, \, q) := \frac{2\,\Gamma(k-1)}{N_\Phi^*(q)\,\phi(q)\,(4\pi)^{k-1}} \sum_{\substack{\chi \ (\mathrm{mod}\ q) \\ \chi(-1)=(-1)^k}} \sum_{f \in \mathcal{H}_\chi} \frac{1}{\|f\|^2} \left| \sum_{\gamma_f} \widetilde{\Phi}(i\gamma_f)\, q^{i\gamma_f \alpha} \right|^2,$$

where

$$N_\Phi^*(q) := \frac{2\,\Gamma(k-1)}{\phi(q)\,(4\pi)^{k-1}} \sum_{\substack{\chi \ (\mathrm{mod}\ q) \\ \chi(-1)=(-1)^k}} \sum_{f \in \mathcal{H}_\chi} \frac{1}{\|f\|^2} \sum_{\gamma_f} \left| \widetilde{\Phi}(i\gamma_f) \right|^2,$$

and the inner sums run over the ordinates of all non-trivial zeros $\frac{1}{2} + i\gamma_f$ of $L(s, \, f)$. Note that

$$S_k(\Gamma_1(q)) = \bigoplus_{\chi \, (\mathrm{mod}\ q)} S_k(\Gamma_0(q), \chi),$$

where $S_k(\Gamma_1(q))$ is the space of holomorphic cusp forms for $\Gamma_1(q)$. Therefore, we may think of $F_\Phi^*(\alpha, \, q)$ as the $\Gamma_1(q)$-analogue of $F(\alpha)$.

In [26, Theorem 1.1], the authors show that the same asymptotic formula in Lemma 6.3 holds, with $F_\Phi^*(\alpha, \, q)$ replacing $F_\Phi(\alpha, Q)$, as $q \to \infty$. Fourier inversion yields, as in (6.2.2),

$$\begin{aligned} \frac{2\,\Gamma(k-1)}{\phi(q)\,(4\pi)^{k-1}} & \sum_{\substack{\chi \ (\mathrm{mod}\ q) \\ \chi(-1)=(-1)^k}} \sum_{f \in \mathcal{H}_\chi} \frac{1}{\|f\|^2} \sum_{\gamma_f, \gamma_f'} R\left(\frac{(\gamma_f - \gamma_f')\log q}{2\pi} \right) \widetilde{\Phi}(i\gamma_f) \widetilde{\Phi}(i\gamma_f') \\ & = N_\Phi^*(q) \int_{\mathbb{R}} F_\Phi^*(\alpha, \, q)\, \widehat{R}(\alpha)\, \mathrm{d}\alpha. \end{aligned}$$

Then, the same argument in the proof of Lemma 6.4 shows that, for any fixed $b \geqslant 1$, $\ell > b$, and $1 \leqslant \Delta < 2$,

$$\mathcal{W}^-_{*,\Delta}(b, b+\ell) + o(1) \leqslant \int_b^{b+\ell} F^*_\Phi(\alpha, q)\, \mathrm{d}\alpha \leqslant \mathcal{W}^+_\Delta(\ell) + o(1),$$

as $q \to \infty$. The bounds for $\mathcal{W}^\pm_\Delta(\ell)$ and $\mathcal{W}^-_{*,\Delta}(\ell)$, given in the proofs of Theorem 6.2 and Theorem 6.5, now immediately imply the analogous theorems for $F^*_\Phi(\alpha, q)$, with the same constants.

6.3 Numerically optimizing the bounds

We must optimize the functionals given in (EP1)-(EP4), over functions in the class $\mathcal{A}_1$. First, we transform these optimization problems over $\mathcal{A}_1$ into unrestricted optimization problems over $\mathbb{R}^{d+1}$, where $d \in \mathbb{N}$. By a result of Krein [1, p. 154], if $g \in \mathcal{A}_1$, then $g(x) = |h(x)|^2$, for some $h \in L^2(\mathbb{R})$ with $\operatorname{supp} \widehat{h} \subset [-\frac{1}{2}, \frac{1}{2}]$. We may then search over functions of the form $\widehat{h}(x) = p(x)\mathbb{I}_{[-\frac{1}{2},\frac{1}{2}]}$, where

$$p(x) := \sum_{i=0}^{d} a_i x^i$$

is a polynomial of degree d. The numerators in (EP1)-(EP4) are now bilinear forms

$$\sum_{i,j=0}^{d} c_{ij} a_i a_j$$

in the coefficients of p. To implement these bilinear forms, one may compute the values of c_{ij} by numerically evaluating the numerators of the functionals on the polynomials $p_{ij}(x) := x^i + x^j$, for $0 \leqslant i, j \leqslant d$. The maxima and minima in the denominators in (EP1)-(EP4) may be computed via a simple 1-dimensional optimization routine.

We proceed to optimize over the coefficients a_i via the principal axis method of Brent [13]. This is an iterative algorithm without derivatives, which requires two initial values for all coefficients a_i. We take $d \leqslant 12$, run the algorithm with many different randomly-chosen initializations, and additionally run it with initializations found previously from running this procedure with lower degrees. In this way, we found the following functions:

$$p_1(x) = 200x^{12} + 815x^{10} - 152x^8 - 59x^6 + \frac{69x^4}{10} - \frac{157x^2}{1000} + 1,$$

which shows $\mathbf{D}^+ < 1.077542$ in (EP3); and

$$p_2(x) = -x^2 + 5,$$

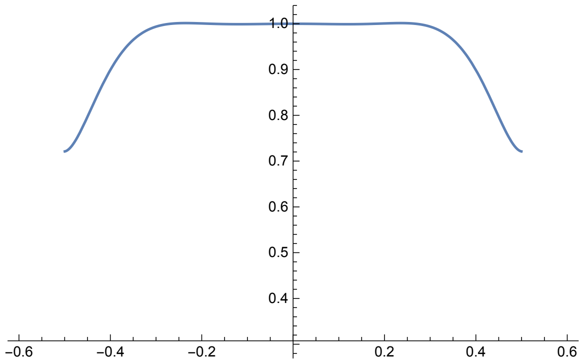

Figure 6.3: The function $\widehat{h}(x) = p_1(x)\mathbb{I}_{[-1/2,\,1/2]}$ is a perturbation of $\mathbb{I}_{[-1/2,\,1/2]}$.

which shows $\mathbf{D}^- > 0.982144$ in (EP4). This proves[2] Theorem 6.2. We also found

$$p_3(x) = -3855x^{12} + 2203x^{10} - \frac{2743x^8}{10} - \frac{152x^6}{5} + \frac{303x^4}{100} - \frac{7x^2}{250} + 1,$$

which shows $\mathbf{C}^+ < 1.330144$ in (EP1); and

$$p_2(x) = -x^2 + \frac{250}{47},$$

which shows $\mathbf{C}^- > 0.927819$ in (EP2). We also ran this routine with $d = 14$, and found no improvement in the first six decimal digits with respect to the above functions.

6.3.1 Remarks on a larger class of functions

Let $\mathcal{A}$ be the class of continuous, even, and non-negative functions $g \in L^1(\mathbb{R})$, such that $\widehat{g}(\alpha) \leqslant 0$ for $|\alpha| \geqslant 1$. Note that $\mathcal{A}_1 \subset \mathcal{A}$. Cohn and Elkies [34] first used this class $\mathcal{A}$ to obtain upper bounds for the sphere packing problem. Recently, Chirre, Gonçalves, and de Laat [30] also used it to sharpen bounds in the theory of the Riemann zeta and other L-functions. With this more general framework, the problems considered in [30] are reduced to convex optimization problems, which the authors solve numerically via semidefinite programming (see [7] for background on semidefinite programming). Furthermore, Chirre, Pereira, and de Laat [33] used a similar framework, with semidefinite programming, to obtain fine estimates for primes in arithmetic progressions, following a Fourier optimization approach by Carneiro, Milinovich, and Soundararajan [22]. In all these works, the authors use these numerical techniques to construct test functions of the form $g(x) = p(x)e^{-\pi x^2}$, where p is a polynomial of a certain degree.

In [16], the authors also build their theoretical framework using this larger class $\mathcal{A}$, while working with the simpler class $\mathcal{A}_1$ to obtain their bounds. We explored the optimizations problems with this larger class, with the purpose of refining Theorem 6.1 and Theorem 6.2,

[2] The numerators in the functionals can be computed exactly in rational arithmetic, in terms of c_0. The maximum and minimum in the denominators, and the value of c_0 given in (6.1.1), may be easily verified to the desired precision, for instance by first isolating the critical points and then applying the bisection method, using interval arithmetic.

using the semidefinite programming methods described in [30]. However, this did not lead to any improvement over the results obtained with bandlimited functions in $\mathcal{A}_1$, even after using polynomials of large degrees, and significantly larger than the degree used in [30]. A similar situation occurred in Chapter 3, where the aforementioned results in [22] and [33] were further extended to primes represented by quadratic forms. Therein, bandlimited functions also outperform polynomials times gaussians, unless one uses much larger degrees, which might not be feasible.

Nevertheless, for completeness, we will briefly describe how to construct these functions with semidefinite programming in the present framework, and the results obtained. Henceforth, assume GRH. In [57], the authors show that, for any fixed, small $\delta > 0$, we have

$$F(\alpha, T) \geqslant \frac{3}{2} - |\alpha| - o(1), \tag{6.3.1}$$

uniformly for $1 \leqslant |\alpha| \leqslant \frac{3}{2} - \delta$, as $T \to \infty$. This gives a conditional improvement over the asymptotic formula (1.3.6), and has been used to refine some estimates under GRH (e.g. in [30, 57]). Using (6.3.1), by an argument similar to that of Section 6.2.2 and [16, Section 2.4], we find the following: for fixed $b \geqslant 1$ and ℓ sufficiently large,

$$\frac{1}{\ell} \int_b^{b+\ell} F(\alpha, T)\, \mathrm{d}\alpha \geqslant J_1(g) - \varepsilon + o(1),$$

as $T \to \infty$, and

$$\frac{1}{\ell} \int_b^{b+\ell} F_\Phi(\alpha, Q)\, \mathrm{d}\alpha \geqslant J_2(g) - \varepsilon + o(1),$$

as $Q \to \infty$, for any $g \in \mathcal{A}$. Here, we denote

$$J_1(g) := \frac{(1 - c_0) g(0) + c_0 \left(\rho_1(g) + 2 \int_1^{3/2} \left(\frac{3}{2} - \alpha \right) \widehat{g}(\alpha)\, \mathrm{d}\alpha \right)}{\max_{0 \leqslant \alpha \leqslant 1} \sum_{n=0}^{m} |\widehat{g}(n - \alpha)|}, \tag{6.3.2}$$

and

$$J_2(g) := \frac{(1 - c_0) g(0) + \frac{c_0}{2} \left(\widehat{g}(0) + 8 \int_0^{1/2} \alpha\, \widehat{g}(\alpha)\, \mathrm{d}\alpha + 4 \int_{1/2}^{1} \widehat{g}(\alpha)\, \mathrm{d}\alpha \right)}{\max_{0 \leqslant \alpha \leqslant 1} \sum_{n=0}^{m} |\widehat{g}(n - \alpha)|}. \tag{6.3.3}$$

We may take the parameter m to be any positive integer, and, as in [16, Section 2.4.2], the bounds improve as $m \to \infty$. Note that, if $g \in \mathcal{A}_1$, then J_1 and J_2 simplify to the functionals in (EP2) and (EP4), respectively. Furthermore, note that, since (6.3.1) is an inequality (instead of an asymptotic equality as in (1.3.6) and Lemma 6.3), we used the sign restrictions of $g \in \mathcal{A}$ to obtain the above bound with (6.3.2).

In contrast to [30], the objectives J_1 and J_2 are not linear (or even smooth). To transform it into a semidefinite program, we approximate our problem by one with a linear objective and additional linear inequality constraints. Let N be a positive integer, and let $\{\alpha_1, \alpha_2, \ldots, \alpha_N\}$ be a partition of the interval $[0, 1]$. Then, multiplying g by an appropriate

d	20	40	60	70	$\widehat{g}(\alpha) = (1 - \lvert\alpha\rvert)_+$
$J_1(g)$	0.9211...	0.9236...	0.9245...	0.9248...	0.9275...
$J_2(g)$	0.9748...	0.9774...	0.9784...	0.9788...	0.9818...

Table 6.1: Semidefinite programming bounds for the approximations (with $m = 3$ and $N = 55$) of J_1 and J_2, for several parameters d, compared with a simple triangle bound. The constructed polynomials have degree $4d + 2$.

constant, we may replace the denominators of (6.3.2) and (6.3.3) by 1, and incorporate the system of inequality constraints

$$\sum_{n=0}^{m} \widehat{g}(n - \alpha_j) \leqslant 1, \quad \text{for} \quad 1 \leqslant j \leqslant N.$$

When N is sufficiently large, this results in a reasonable approximation in practice.

We now follow the notation and argument in [30, Section 4], to which we refer for details. By taking dilations, we may relax the condition $\widehat{g} \leqslant 0$ for $|\alpha| \geqslant 1$, to the same condition over $|\alpha| \geqslant R$, where $R \geqslant 1$ is some parameter (after also taking dilations in the definitions of J_1 and J_2), and we may assume $\widehat{g}(0) = 1$. We see this as a bilevel optimization problem, where the outer problem is a 1-dimensional problem over $R \geqslant 1$, and the inner problem optimizes over such a function $g(x) = p(x)e^{-\pi x^2}$, where, as before, p is an even polynomial. For a fixed R, functions g of this form, that are non-positive in $[R, \infty)$, and whose Fourier transform is non-negative, can be written in terms of positive-semidefinite matrices, as follows.

Let $d \in \mathbb{N}$. Let X_2, X_3, X_4 be positive-semidefinite matrices of size $(d + 1)$, and let

$$v(u) := \left(L_0^{-1/2}(\pi u), \ldots, L_d^{-1/2}(\pi u)\right) \in \mathbb{R}^{d+1},$$

where $L_k^{-1/2}$ is the Laguerre polynomial of degree k with parameter -1/2. Then, we may write

$$g(x) = (R^2 - x^2)\, v(x^2)^T X_2\, v(x^2)\, e^{-\pi x^2}\,;\; \widehat{g}(x) = \left(v(x^2)^T X_3\, v(x^2) + x^2\, v(x^2)^T X_4\, v(x^2)\right) e^{-\pi x^2}.$$

Note that g is a polynomial of degree $4d + 2$, times a Gaussian function. The fact that $\widehat{g}(x)$ is the Fourier transform of g is a linear condition over the entries of X_2, X_3, and X_4 in $\mathbb{R}^{d+1}$, which we also write in terms of the Laguerre basis $v(u)$.

This is now a semidefinite program, for which we use the high-precision solver sdpa-gmp [85]. In Table 1, we show the maxima of (6.3.2) and (6.3.3) for several values of d, compared with the bound from the triangle function $\widehat{g}(\alpha) = (1 - |\alpha|)_+ \in \mathcal{A}_1$. In our computations, we take $m = 3$ in the definitions of J_1 and J_2, and $N = 55$ in the partition of $[0, 1]$. Further experiments with other values of m and N did not significantly alter the results. For comparison, the authors use $d = 40$ in [30].

Chapter 7

Appendices

Appendix A: Some useful estimates

Lemma 7.1. *Let $x, y \geqslant 1$ be two parameters. Consider the radial function $G : \mathbb{R}^2 \to \mathbb{R}$ defined by*

$$G(r) = \begin{cases} \min\left\{r^2, 1, \dfrac{x+y-r^2}{y}\right\}, & \text{if } 0 \leqslant r \leqslant (x+y)^{1/2}; \\ 0, & \text{if } r > (x+y)^{1/2}. \end{cases}$$

Then $G \in L^1(\mathbb{R}^2)$, and its Fourier transform $\widehat{G}$ satisfies the following properties:

1. *For $\xi \in \mathbb{R}^2$ and $\xi \neq 0$,*
$$\left|\widehat{G}(\xi)\right| \ll \frac{(x+y)^{1/4}}{|\xi|^{3/2}}. \tag{7.0.1}$$

2. *For $\xi \in \mathbb{R}^2$ and $|\xi| \geqslant 1$,*
$$\left|\widehat{G}(\xi)\right| \ll \frac{1}{|\xi|^{5/2}}\left(1 + \frac{x^{3/4}}{y}\right). \tag{7.0.2}$$

3. *For $\xi = 0$,*
$$\widehat{G}(0) = \left(x + \frac{y}{2}\right)\pi - \frac{\pi}{2}, \tag{7.0.3}$$

Proof. It is clear that $G \in L^1(\mathbb{R}^2)$. Since G is a radial function, it follows that (see [65, p. 429]),

$$\widehat{G}(\xi) = 2\pi \int_0^{\infty} r\, G(r)\, J_0(2\pi r|\xi|)\, \mathrm{d}r, \tag{7.0.4}$$

for $\xi \in \mathbb{R}^2$, where J_0 is the Bessel function of order 0. Since $J_0(0) = 1$, a simple computation shows (7.0.3). Let us start proving the estimate (7.0.1). For $\xi \neq 0$, we split the integral in (7.0.4) into the ranges $0 \leqslant r < 1/|\xi|$ and $1/|\xi| \leqslant r < \infty$. Using the estimates $|J_0(t)| \ll 1$ and $|G(r)| \leqslant 1$, it follows that

$$\left| \int_0^{1/|\xi|} r\, G(r)\, J_0(2\pi r|\xi|)\, \mathrm{d}r \right| \ll \frac{1}{|\xi|^2}. \tag{7.0.5}$$

To estimate the second integral, by [64, 8.451-1] we recall that

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

for $|t| \gg 1$. Then, using that $|G(r)| \leqslant 1$, $\int_0^\infty G(r)/r^{3/2}\, \mathrm{d}r < \infty$, and integration by parts:

$$\begin{aligned}
&\int_{1/|\xi|}^{\infty} r\, G(r)\, J_0(2\pi r|\xi|)\, \mathrm{d}r \\
&\qquad = -\frac{1}{2\pi^2 |\xi|^{3/2}} \int_{1/|\xi|}^{\infty} (r^{1/2} G(r))' \sin(2\pi r|\xi| - \tfrac{\pi}{4})\, \mathrm{d}r \\
&\qquad\quad + \frac{1}{32\pi^3 |\xi|^{5/2}} \int_{1/|\xi|}^{\infty} \left(\frac{G(r)}{r^{1/2}}\right)' \cos(2\pi r|\xi| - \tfrac{\pi}{4})\, \mathrm{d}r + O\left(\min\left\{ \frac{1}{|\xi|^{5/2}}, \frac{1}{|\xi|^2} \right\} \right).
\end{aligned} \tag{7.0.6}$$

Therefore,

$$\begin{aligned}
&\left| \int_{1/|\xi|}^{\infty} r\, G(r)\, J_0(2\pi r|\xi|)\, \mathrm{d}r \right| \\
&\qquad \ll \frac{1}{|\xi|^{3/2}} \int_{1/|\xi|}^{\infty} \left|(r^{1/2} G(r))'\right| \mathrm{d}r + \frac{1}{|\xi|^{5/2}} \int_{1/|\xi|}^{\infty} \left| \left(\frac{G(r)}{r^{1/2}}\right)' \right| \mathrm{d}r + \min\left\{ \frac{1}{|\xi|^{5/2}}, \frac{1}{|\xi|^2} \right\} \\
&\qquad \ll \frac{1}{|\xi|^{3/2}} \int_0^\infty \left| \frac{G(r)}{r^{1/2}} \right| \mathrm{d}r + \frac{1}{|\xi|^{3/2}} \int_0^\infty \left| r^{1/2} G'(r) \right| \mathrm{d}r + \frac{1}{|\xi|^2}.
\end{aligned}$$

Spliting the above integrals according to the definition of G, and using the mean value theorem, it follows that, for $1/|\xi| \leqslant \sqrt{x+y}$, we have

$$\left| \int_{1/|\xi|}^{\infty} r\, G(r)\, J_0(2\pi r|\xi|)\, \mathrm{d}r \right| \ll \frac{(x+y)^{1/4}}{|\xi|^{3/2}}. \tag{7.0.7}$$

Combining (7.0.5) and (7.0.7) we obtain (7.0.1) in the case $1/|\xi| \leqslant (x+y)^{1/2}$. When $1/|\xi| > (x+y)^{1/2}$, we bound as in (7.0.5) to obtain

$$\left|\widehat{G}(\xi)\right| = \left| 2\pi \int_0^{(x+y)^{1/2}} r\, G(r)\, J_0(2\pi r|\xi|)\, \mathrm{d}r \right| \ll x + y \ll \frac{(x+y)^{1/4}}{|\xi|^{3/2}}.$$

This conclude the proof of the estimate (7.0.1). Now, let us prove (7.0.2). Suppose that $|\xi| \geqslant 1$. We split the integral in (7.0.4) as in the previous case, and we bound the first integral as follows:

$$\left| \int_0^{1/|\xi|} r\, G(r)\, J_0(2\pi r|\xi|)\, \mathrm{d}r \right| \ll \int_0^{1/|\xi|} r^3\, \mathrm{d}r \ll \frac{1}{|\xi|^4}. \tag{7.0.8}$$

On the other hand, in (7.0.6) we split the last integrals (depending on the value of $1/|\xi| \leqslant 1$)

and use integration by parts (one more time). In this way, we obtain that

$$\left| \int_{1/|\xi|}^{\infty} r\, G(r)\, J_0(2\pi r|\xi|)\, \mathrm{d}r \right| \ll \frac{1}{|\xi|^{5/2}} \left(1 + \frac{x^{3/4}}{y} \right). \tag{7.0.9}$$

Then, combining (7.0.8) and (7.0.9) we obtain (7.0.2). □

Lemma 7.2. *Let K be an imaginary quadratic field, and let $\mathfrak{q}$ be an integral ideal. Then,*

$$\sum_{\mathfrak{p}|\mathfrak{q},\, k\geqslant 1} \frac{\log \mathrm{N}\mathfrak{p}}{(\mathrm{N}\mathfrak{p})^{k/2}} \ll \sqrt{\log \mathrm{N}\mathfrak{q}}.$$

Proof. Using the factorization law of primes in imaginary quadratic fields [69, p. 57], one can see that, for each $k \geqslant 1$,

$$\sum_{\mathfrak{p}|\mathfrak{q}} \frac{\log \mathrm{N}\mathfrak{p}}{(\mathrm{N}\mathfrak{p})^{k/2}} = \sum_{p} \left(\sum_{\substack{\mathfrak{p}|\mathfrak{q} \\ \mathrm{N}\mathfrak{p}=p}} \frac{\log \mathrm{N}\mathfrak{p}}{(\mathrm{N}\mathfrak{p})^{k/2}} \right) + \sum_{p} \left(\sum_{\substack{\mathfrak{p}|\mathfrak{q} \\ \mathrm{N}\mathfrak{p}=p^2}} \frac{\log \mathrm{N}\mathfrak{p}}{(\mathrm{N}\mathfrak{p})^{k/2}} \right) \ll \sum_{p|\mathrm{N}\mathfrak{q}} \frac{\log p}{p^{k/2}}.$$

It is clear that the sum over $k \geqslant 3$ in the above expression contributes $O(1)$, and the sum when $k = 2$ is bounded by the sum when $k = 1$. Let us analyze the latter case. Assume that $\mathrm{N}\mathfrak{q} \geqslant 3$. We denote by $\omega(n)$ the number of distinct positive integer prime factors of n, and by p_n the n-th prime number. Since $p_n \leqslant Cn \log n$ for some $C > 0$, and the function $y \mapsto y^{-k/2} \log y$ is eventually decreasing, it follows that

$$\sum_{p|\mathrm{N}\mathfrak{q}} \frac{\log p}{\sqrt{p}} \ll \sum_{p\leqslant p_{\omega(\mathrm{N}\mathfrak{q})}} \frac{\log p}{\sqrt{p}} \ll \sum_{p\leqslant C\omega(\mathrm{N}\mathfrak{q})\log(\omega(\mathrm{N}\mathfrak{q}))} \frac{\log p}{\sqrt{p}} \ll \sqrt{\omega(\mathrm{N}\mathfrak{q}) \log(\omega(\mathrm{N}\mathfrak{q}))},$$

where we used integration by parts in the last step. We conclude our desired result using the classical estimate for $\omega(n)$ (see [84, Theorem 2.10]):

$$\omega(n) \ll \frac{\log n}{\log\log n}.$$

□

Appendix B: Variations of Montgomery's weight

Assume RH. Let $\frac{1}{2} < \sigma_0 < \frac{3}{2}$, and define

$$w_{\sigma_0}(u) := \frac{4\sigma_0^2}{4\sigma_0^2 + u^2} \quad \text{and} \quad \widetilde{F}_{\sigma_0}(\alpha) := \frac{2\pi}{T\log T} \sum_{0<\gamma,\,\gamma'\leqslant T} T^{i\alpha(\gamma-\gamma')} w_{\sigma_0}(\gamma - \gamma'). \tag{7.0.10}$$

Note that we recover Montgomery's function $F(\alpha)$ by taking $\sigma_0 = 1$. Since

$$\widehat{w_{\sigma_0}}(y) = 2\pi\sigma_0 e^{-4\pi\sigma_0|y|},$$

we have the identity

$$\widetilde{F}_{\sigma_0}(\alpha) = \frac{4\pi^2\sigma_0}{T\log T}\int_{-\infty}^{\infty} e^{-4\pi\sigma_0|y|}\left|\sum_{0<\gamma\leqslant T} T^{i\alpha\gamma}e^{2\pi y\gamma}\right|^2 \,dy. \tag{7.0.11}$$

In particular, $\widetilde{F}_{\sigma_0}(\alpha) \geqslant 0$, and $\widetilde{F}_{\sigma_0}$ is even. Following Montgomery [81] (see also [58]), we have the following asymptotic formula for $\widetilde{F}_{\sigma_0}(\alpha)$.

Proposition 7.3. *Let $\frac{1}{2} < \sigma_0 < \frac{3}{2}$, and define $\widetilde{F}_{\sigma_0}(\alpha)$ as in (7.0.10). We have*

$$\widetilde{F}_{\sigma_0}(\alpha) = \sigma_0 T^{-2|\alpha|\sigma_0}\log T(1+o(1)) + |\alpha| + o(1),$$

uniformly for $0 \leqslant |\alpha| \leqslant 1$, as $T \to \infty$.

Proof. In Montgomery's explicit formula, we take $\sigma = \frac{1}{2} + \sigma_0$ to obtain, for any $\frac{1}{2} < \sigma_0 < \frac{3}{2}$ and $x \geqslant 1$,

$$\begin{aligned}2\sigma_0\sum_\gamma \frac{x^{i\gamma}}{\sigma_0^2+(t-\gamma)^2} = &-x^{-\sigma_0}\sum_{n\leqslant x}\frac{\Lambda(n)n^{\sigma_0-1/2}}{n^{it}} - x^{\sigma_0}\sum_{n>x}\frac{\Lambda(n)}{n^{1/2+\sigma_0+it}}\\ &+ x^{-\sigma_0+it}(\log\tau + O(1)) + O(x^{1/2}\tau^{-1}),\end{aligned}$$

where $\tau = |t|+2$, and the implied constants depend only on σ_0 (which we henceforth assume to be fixed). We write the above as $L(x,\, t) = R(x,\, T)$. Note that

$$\int_{-\infty}^{\infty}\frac{1}{[\sigma_0^2+(t-\gamma)^2][\sigma_0^2+(t-\gamma')^2]}\,dt = \frac{2\pi}{\sigma_0}\cdot\frac{1}{4\sigma_0^2+(\gamma-\gamma')^2} = \frac{2\pi}{4\sigma_0^3}\,w_{\sigma_0}(\gamma-\gamma').$$

Then, taking the absolute value, squaring, and integrating, following Montgomery we obtain

$$\int_0^T |L(x,\, T)|^2\,dt = \frac{2\pi}{\sigma_0}\sum_{0<\gamma,\,\gamma'\leqslant T} x^{i(\gamma-\gamma')}w_{\sigma_0}(\gamma-\gamma') + O(\log^3 T) = \frac{1}{\sigma_0}\widetilde{F}_{\sigma_0}(\alpha)\,T\log T + O(\log^3 T). \tag{7.0.12}$$

Now, let us analyze $\int_0^T |R(x,\, T)|^2$. For the Dirichlet series, using [83, Corollary 3], we obtain

$$\begin{aligned}\int_0^T\left|-x^{-\sigma_0}\sum_{n\leqslant x}\frac{\Lambda(n)n^{\sigma_0-1/2}}{n^{it}} - x^{\sigma_0}\sum_{n>x}\frac{\Lambda(n)}{n^{1/2+\sigma_0+it}}\right|^2 dt =& x^{-2\sigma_0}\sum_{n\leqslant x}\frac{\Lambda(n)^2}{n^{1-2\sigma_0}}(T+O(n))\\ &+ x^{2\sigma_0}\sum_{n>x}\frac{\Lambda(n)^2}{n^{1+2\sigma_0}}(T+O(n)).\end{aligned} \tag{7.0.13}$$

Note that

$$\int_1^x y^{2\sigma_0-1}\log y \; \mathrm{d}y = \frac{x^{2\sigma_0}(2\sigma_0\log x - 1)+1}{4\sigma_0^2} \quad \text{and} \quad \int_x^\infty y^{-1-2\sigma_0}\log y \; \mathrm{d}y = \frac{x^{-2\sigma_0}(2\sigma_0\log x + 1)}{4\sigma_0^2}.$$

Then, by the prime number theorem with error term, (7.0.13) equals

$$\frac{T\log x}{\sigma_0} + O(T) + O(x\log x).$$

We note that on the left-hand side of (7.0.13), we may use an estimate of Goldston and Montgomery [58, Lemma 7] instead of [83, Corollary 3] to replace the error term $O(x\log x)$ with $O(T\sqrt{\log x})$. Continuing with our proof, we have

$$\int_0^T \left|x^{-\sigma_0+it}(\log \tau + O(1))\right|^2 \; \mathrm{d}t = \frac{T\log^2 T + O(T\log T)}{x^{2\sigma_0}}.$$

If we choose $x = T^\alpha$ for $0 \leqslant \alpha \leqslant 1-\varepsilon$, then following Montgomery's argument the above estimates imply that

$$R(T^\alpha, T) = T\log T\left(T^{-2\alpha\sigma_0}\log T\,(1+o(1)) + \frac{\alpha}{\sigma_0} + o(1)\right).$$

We combine this with (7.0.12) to obtain the desired result for $|\alpha| \leqslant 1-\varepsilon$. As remarked above, by the argument of Goldston and Montgomery [58, Lemma 7], this can be extended uniformly to $|\alpha| \leqslant 1$. $\square$

We also note that the following estimate holds.

Proposition 7.4. *Let $\frac{1}{2} < \sigma_0 < \frac{3}{2}$, $\beta > 1$, and define $\widetilde{F}_{\sigma_0}(\alpha)$ as in* (7.0.10). *Then,*

$$\int_1^\beta \widetilde{F}_{\sigma_0}(\alpha) \; \mathrm{d}\alpha \ll \beta.$$

Proof. Using an argument of Goldston [53, Lemma A], this follows from Proposition 7.3 and the fact that $\widetilde{F}_{\sigma_0}(\alpha) \geqslant 0$. $\square$

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