Physics of the Riemann Hypothesis

David Orlando Alejandro Alemán Espinosa

Universidad de los Andes

Departamento de física

Advisor: Ph.D. Alonso Botero Mejía

November, 2014

Signature

Advisor: Alonso Botero Mejía

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Abstract

The Hilbert-Polya conjecture suggests the existence of a quantum Hamiltonian whose energies are the numbers t_n where $\frac{1}{2} + it_n$ are the nontrivial zeros of the Riemann zeta function. This could inmediately imply that the Riemann hypothesis is true. The purpose of this thesis is to study some of the different contributions to the problem that has been made during the last century. Specifically, we discuss (a) the Montgomery conjecture which states a relation between the pair correlation functions of the Riemann zeros and the eigenvalues of the Gaussian Unitary Ensemble, and (b) some of the evidence developed by Michael Berry and Jonathan Keating that suggests via the Gutzwiller Trace formula some of the quantum chaotic characteristics that the Riemann Hamiltonian must possess in case that it exists.

Introduction

Bernhard Riemann published a well-known paper in 1859 titled “Uber die Anzahl der Primzahlen unter einer gegebenen Grösse” (“On the Number of Primes Less Than a Given Magnitude”) [1]. In it he studied a prime counting function up to a given point (further discussed in Chapter 1). The zeta function and its analytical continuation to $\mathbb{C} \setminus \{1\}$ plays a major role in the paper. It is in this paper that he conjectured that the zeros of the zeta function whose real part lies between 0 and 1, which are called the non-trivial zeros of the zeta function, have real part equal to $\frac{1}{2}$. To this day this problem, know called the Riemann hypothesis, has resisted the attacks of a vast number of the world's best mathematicians. The trueness or falseness of this hypothesis has deep consequences in different fields of mathematics, especially in number theory, since the zeta function has proved to be deeply connected with the distribution of prime numbers [2]. The Riemann hypothesis is considered by many mathematicians as one if not the most important unresolved problem in pure mathematics.

The Hilbert-Polya conjecture is considered as one of the most promising paths to find a solution to the Riemann Hypothesis. It states that the hypothesis is true because the numbers t_n, where $\dfrac{1}{2} + it_n$ are the nontrivial zeros, correspond to the eigenvalues of a self-adjoint operator which corresponds to the Hamiltonian of some quantum system. The fact that the eigenvalues of self-adjoint matrices are real could inmediately imply that the Riemann hypothesis is true. The formulation of this conjecture is usually atributted to David Hilbert and George Polya indepedently around 1910[3], although the first published mention of it was in 1973 by Hugh Montgomery paper ”On the pair correlation of zeros of the zeta function”[4].

In this thesis we will study some connections between the nontrivial zeros of the Riemann zeta function and the energy levels of certain physical systems. Particularly, we will study the resemblance between the pair correlation functions from both the zeros of the zeta function and the eigenvalues of the Gaussian Unitary Ensemble (GUE).

Later, we will study the relation between the counting functions of the zeros above the real axis, and the energy levels in quantum chaotic systems.

In chapter 1 we will study the Riemann zeta Function and some of its basic properties, such as its analytical continuation to the complex plane, and some facts about the zeros of the function.

In chapter 2 some of the historical background concerning the Riemann Hypothesis and the Hilbert-Polya conjecture will be given, as well as a discussion concerning the importance of proving or disproving the hypothesis, and some of the consequences it will carry.

In chapter 3 we will derive a counting function of the nontrivial zeros, from the real axis up to a certain point in the upper half of the complex plane, which as we shall see, will be suficient as a counting function since the zeros of the zeta funciton are symmetrical with respect to the real axis. It will also include a derivation of the Gutzwiller Trace Formula and the counting function for energy levels in a quantum chaotic system [5]. We will also look at some of the conclusions derived by Berry and Keating regarding the characteristics that the Riemann Hamlitonian must possess based on the relations between the zero counting function and the Gutzwiller Trace Formula [6].

Chapter 4 will be devoted to the Montgomery conjecture regarding the pair correlation function of the nontrivial zeros [4], as well as to deriving the pair correlation function of the eigenvalues of the matrices from the GUE as the dimensions of the matrices tend to infinity, and finally, see how it resembles the result found by Montgomery.

CHAPTER 1

Riemann zeta function

Before we get started, it is necessary to understand some basic properties of the Riemann zeta function. This chapter will be devoted to explain some of its important characteristics, as well as to giving a brief insight into the Riemann Hypothesis. We will follow Edwards in this chapter [2].

1.1 Definition of the Riemann zeta function

The Riemann zeta function is defined on the open half plane $G = \{S \in \mathbb{C} : Re(s) > 1\}$ as:

$$\zeta : G \mapsto \mathbb{C}$$
$$\zeta(s) := \sum_{n=1}^{\infty} \frac{1}{n^s}.$$

This infinite series converges inside G, because it converges absolutely; we have that

$$|n^{-s}| = |n^{-\sigma-it}| = |n^{-\sigma}| \cdot |n^{-it}| = |n^{-\sigma}| \cdot |e^{-itl\kappa n}| = |n^{-\sigma}| = n^{-\sigma}.$$

Where we have used the standard notation $\sigma := Re(s)$ and $t := Im(s)$.

An immediate connection between the Riemann zeta function and the prime numbers arises from the next formula, due to Euler:

Theorem 1.1 (Euler Product formula). *The Riemann zeta function is equal to*

$$\zeta(s) = \prod_{p \text{ prime}} \frac{1}{1-p^{-s}},$$

for $Re(s) > 1$.

Proof. *We have that for $Re(s) > 1$,*

$$\begin{aligned}
\zeta(s) &= \sum_{n=1}^{\infty} \frac{1}{n^s} = 1 + \frac{1}{2^s} + \frac{1}{3^s} + \frac{1}{4^s} + \frac{1}{5^s} + \frac{1}{6^s} + \dots \\
\Rightarrow \frac{1}{2^s}\zeta(s) &= \frac{1}{2^s} + \frac{1}{4^s} + \frac{1}{6^s} + \frac{1}{8^s} + \frac{1}{10^s} + \dots \\
\Rightarrow \left(1 - \frac{1}{2^s}\right)\zeta(s) &= 1 + \frac{1}{3^s} + \frac{1}{5^s} + \frac{1}{7^s} + \frac{1}{9^s} + \frac{1}{11^s} + \dots \\
\Rightarrow \frac{1}{3^s}\left(1 - \frac{1}{2^s}\right)\zeta(s) &= \frac{1}{3^s} + \frac{1}{9^s} + \frac{1}{15^s} + \frac{1}{21^s} + \frac{1}{27^s} + \dots \\
\Rightarrow \left(1 - \frac{1}{3^s}\right)\left(1 - \frac{1}{2^s}\right)\zeta(s) &= 1 + \frac{1}{5^s} + \frac{1}{7^s} + \frac{1}{11^s} + \frac{1}{13^s} + \dots
\end{aligned}$$

Note that as a direct consequence of the unique factorization of integer into primes, if we keep repeating this process and multiply $\left(1 - \frac{1}{p_{n+1}^s}\right)$ to the left of $\left(1 - \frac{1}{p_n^s}\right) \dots \left(1 - \frac{1}{2^s}\right)\zeta(s)$, where P_n denotes the $n-th$ prime, all the factors on the right containing an integer divisible by P_{n+1} will vanish. So we conclude that

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

for $Re(s)$, which is equivalent to

$$\zeta(s) = \prod_{p}^{\infty} \frac{1}{1-p^{-s}}. \qquad \square$$

1.2 Meromorphic continuation of $\zeta(s)$ to the complex plane, and the functional equation

The Riemann zeta function is originally defined only for complex numbers whose real part is greater than one since it diverges for other values. It was Riemann who was able to find the meromorphic extension of the zeta function to the entire complex plane whose only pole lies in 1 i.e., he was able to find the meromorphic function on the complex plane which is equal to the zeta function when restricted to $G = \{S \in \mathbb{C} : Re(s) > 1\}$. It can be shown that if two meromorphic functions defined on the complex plane are extensions of a meromorphic function defined on an open set, then these functions are equal [7]. Because of this there will be no ambiguity when we define the meromorphic extension to the complex plane of the zeta function.

First we shall see how the zeta function can be extended to a meromorphic function on $H := \{S \in \mathbb{C} : Re(s) > 0\}$, and then based on a famous functional equation involving the zeta function and the Gamma function we will see how it can be extended to a meromorphic function on the complex plane.

Theorem 1.2. *The Riemann zeta function can be meromorphically extended to* $H := \{S \in \mathbb{C} : Re(s) > 0\}$ *by means of the following relation:*

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

for $0 < Re(s)$*, where* $\{x\} := x - \lfloor x \rfloor$ *is defined as the fractional part of* x *(*$\lfloor x \rfloor$ *is the largest integer not greater than* x*). Where* $1 + \frac{1}{s-1} - s\int_1^\infty \{x\}x^{-s-1}dx$ *is a meromorphic function on* H*. Its only singularity is a simple pole located at* $s = 1$*.*

Proof.

$$
\begin{aligned}
\zeta(s) &= \sum_{n=1}^{\infty} \frac{1}{n^s} \\
&= \sum_{n=1}^{\infty} n(n^{-s} - (n+1)^{-s}) \\
&= \sum_{n=1}^{\infty} ns \int_{n}^{n+1} x^{-s-1} dx \\
&= s \sum_{n=1}^{\infty} \int_{n}^{n+1} \lfloor x \rfloor x^{-s-1} dx \\
&= \int_{1}^{\infty} \lfloor x \rfloor x^{-s-1} dx \\
&= s \int_{1}^{\infty} (x - \{x\}) x^{-s-1} dx \\
&= s \int_{1}^{\infty} x^{-s} dx - s \int_{1}^{\infty} \{x\} x^{-s-1} dx \\
&= \frac{s}{s-1} - s \int_{1}^{\infty} \{x\} x^{-s-1} dx \\
&= 1 + \frac{1}{s-1} - s \int_{1}^{\infty} \{x\} x^{-s-1} dx.
\end{aligned}
$$

Since the integral converges absolutely for $0 < Re(s)$, the above expression defines a meromorphic function for $0 < Re(s)$ whose only singularity is a simple pole coming from the term $\frac{1}{s-1}$. Looking at the left hand side of this equation we see that the function on the right hand side is the meromorphic continuation of $\zeta(s)$ to $H := \{S \in \mathbb{C} : Re(s) > 0\}$.

Now, in order to find the meromorphic extension of the zeta function to the whole complex plane we will need to use the Gamma function, which is defined for $Re(s) > 0$ as:

$$\Gamma(s) := \int_{0}^{\infty} x^{s-1} e^{-x} dx. \tag{1.1}$$

Proposition 1.1. *The Gamma function defines an holomorphic function for $Re(s) > 0$*

Proof. *First, lets prove that the Gamma function converges. Let $\sigma := Re(s)$. The absolute value of the integrand is equal to $|x^{s-1}e^{-x}| = x^{\sigma-1}e^{-x}$. Where we have that:*

$$\int_0^\infty |x^s e^{-x}| dx = \int_0^\infty x^{\sigma-1} e^{-x} dx = \int_0^1 x^{\sigma-1} e^{-x} dx + \int_1^\infty x^{\sigma-1} e^{-x} dx$$
$$\leq \int_0^1 x^{\sigma-1} dx + \int_1^\infty x^{\sigma-1} e^{-x} dx.$$

The first integral converges for $\sigma > 0$ and the second integral converges because of the exponential decay.

To prove the analyticity of the Gamma function we will use a theorem in complex analysis which states that if $f(s)$ is a complex-valued function defined in some open set $A \subseteq \mathbb{C}$, if the first partial derivatives of $f(s)$ with respect to $Re(s)$ and $Im(s)$ exist everywhere inside A, and if these derivatives satisfy the Cauchy-Riemann condition $\frac{\partial f(s)}{\partial Re(s)} = \frac{1}{i}\frac{\partial f(s)}{\partial Im(s)}$ inside A, then f is holomorphic inside A.

Using this theorem we have that the Gamma function is analytic for $0 < Re(s)$, because:

$$\begin{aligned} \frac{\partial \Gamma(\sigma+it)}{\partial \sigma} &= \frac{\partial}{\partial \sigma} \lim_{N\to\infty} \int_0^N x^{\sigma+it-1} e^{-x} dx \\ &= \lim_{N\to\infty} \frac{\partial}{\partial \sigma} \int_0^N x^{\sigma+it-1} e^{-x} dx, \end{aligned}$$

where the derivative and the limit can be interchanged because of the pointwise convergence of the integral and uniform convergence of the derivative

$$\begin{aligned} &= \lim_{N\to\infty} \int_0^N \frac{\partial x^{\sigma+it-1} e^{-x}}{\partial \sigma} dx \ \ \text{(using the Leibniz rule)} \\ &= \lim_{N\to\infty} \int_0^N x^{\sigma+it-1} e^{-x} \ln(x) dx \\ &= \lim_{N\to\infty} \int_0^N \frac{\partial x^{\sigma+it-1} e^{-x}}{\partial (it)} dx \\ &= \frac{1}{i} \lim_{N\to\infty} \int_0^N \frac{\partial x^{\sigma+it-1} e^{-x}}{\partial t} dx \\ &= \frac{1}{i} \lim_{N\to\infty} \frac{\partial}{\partial t} \int_0^N x^{\sigma+it-1} e^{-x} dx \ \ \text{(by the Leibniz rule)} \end{aligned}$$

$$
\begin{aligned}
&= \frac{1}{i}\frac{\partial}{\partial t}\lim_{N\to\infty}\int_0^N x^{\sigma+it-1}e^{-x}dx \\
&= \frac{1}{i}\frac{\partial\Gamma(\sigma+it)}{\partial t}. \qquad \square
\end{aligned}
$$

We now extend the Gamma function to a meromorphic function in the complex plane by means of the so called Reduction formula $\Gamma(s+1) = s\Gamma(s)$.

Proposition 1.2 (Reduction Formula)**.** *The Gamma function satisfies the functional equation* $\Gamma(s+1) = s\Gamma(s)$*, for* $\sigma > 0$*.*

Proof. *We have:*

$$
\begin{aligned}
\Gamma(s+1) &= \int_0^\infty e^{-t}t^s dt \\
&= -\int_0^\infty t^s d(e^{-t}) \\
&= -t^s e^{-t}\ |_0^\infty + \int_0^\infty e^{-t}st^{s-1}dt \\
&= s\int_0^\infty e^{-t}t^{s-1}dt \\
&= s\Gamma(s) \qquad \square
\end{aligned}
$$

Looking at the reduction formula we can define $\Gamma(s)$ for $-1 < Re(s) \leq 0$ by $\Gamma(s) = \frac{\Gamma(s+1)}{s}$. And in general define it for $-(n+1) < Re(s) \leq -n$, $n \in \mathbb{N}$, by:

$$\Gamma(s) = \frac{\Gamma(s+n+1)}{\prod_{m=0}^{n}(s+m)}. \tag{1.2}$$

Therefore the meromorphic extension of the Gamma function has simple poles at all negative integers. It can also be proved that the Gamma function has no zeros in $\mathbb{C}$ [2].

Before we meromorphically extend $\zeta(s)$ to the complex plane, we need to consider the Theta function defined by:

$$\Theta : \mathbb{R}^+ \longrightarrow \mathbb{R},$$

$$\Theta(t) := \sum_{n=-\infty}^{\infty} e^{-\pi n^2 t}.$$

We need to use a functional equation for $\Theta(t)$, which can be derived using the following theorem.

Theorem 1.3 (Poisson summation formula)**.** *Suppose f is a function of a complex* *variable such that*

(i) The function f is analytic in a horizontal strip

$$S_a := \{z \in \mathbb{C} : |Im(z)| < a\},$$

for some a.

(ii) There exists a constant $A > 0$ such that $|f(\sigma + it)| \leq \frac{A}{1+\sigma^2}$, for all $\sigma \in \mathbb{R}$ and $|t| < a$ for some a.

Then

$$\sum_{n=-\infty}^{\infty} f(n) = \sum_{-\infty}^{\infty} \hat{f}(n),$$

where $\hat{f}(n)$ denotes the Fourier transform of f, $\hat{f}(n) = \int_{-\infty}^{\infty} f(x)e^{-2\pi ixn}dx$.

Proof. *See [8].*

Note that $f(z) := e^{-\pi z^2 t}$ for fixed $t > 0$ is entire i.e., analytic over $\mathbb{C}$, and for $|y| < 1$, $x \in \mathbb{R}$,

$$|f(x + iy)| = e^{-\pi(x^2 - y^2)t} < e^{-\pi x^2 t} \cdot e^{\pi t} < \frac{e^{2\pi t}}{1 + x^2},$$

where the last inequality can be derived after few calculations. We can therefore apply the last theorem to the Theta function.

The Fourier transform of $f(n) = e^{-\pi n^2 t}$, $n \in \mathbb{N}$, is equal to

$$\begin{aligned} \hat{f}(n) &= \int_{-\infty}^{\infty} e^{-\pi x^2 t} \cdot e^{-2\pi ixn} dx \\ &= \sqrt{\frac{\pi}{\pi t}} e^{\frac{-4\pi^2 n^2}{4\pi t}} \\ &= t^{-\frac{1}{2}} e^{-\frac{\pi n^2}{t}}, \end{aligned}$$

where we have used the identity for integrals of Gaussian functions

$$\int_{-\infty}^{\infty} e^{-ax^2 + bx} = \sqrt{\frac{\pi}{a}} e^{\frac{b^2}{4a}},$$

which holds when $Re(a) > 0$. Hence, by the Poisson summation formula we have

$$\Theta(t) = \sum_{n=-\infty}^{\infty} e^{-\pi n^2 t} = \sum t^{-\frac{1}{2}} e^{-\frac{\pi n^2}{t}} = t^{-\frac{1}{2}} \Theta\left(\frac{1}{t}\right),$$

for all $t > 0$. This functional equation for $\Theta(t)$,

$$\Theta(t) = t^{-\frac{1}{2}}\Theta\left(\frac{1}{t}\right), \tag{1.3}$$

will be very useful in the proof of the following theorem.

Theorem 1.4. *The Riemann xi function defined for $Re(s) > 0$ by:*

$$\xi(s) := \frac{1}{2}s(s-1)\pi^{-\frac{s}{2}}\Gamma\left(\frac{s}{2}\right)\zeta(s), \tag{1.4}$$

has an analytic extension to the complex plane, which satisfies the functional equation

$$\xi(s) = \xi(1-s). \tag{1.5}$$

Proof. *If we substitute x by $n^2\pi y$ inside the Gamma function we get, for $Re(s) > 0$,*

$$\begin{aligned}
\Gamma\left(\frac{s}{2}\right) &= \int_0^\infty x^{\frac{s}{2}-1}e^{-x}dx \\
&= \int_0^\infty (n^2\pi y)^{\frac{s}{2}-1}e^{-n^2\pi y}n^2\pi dy \\
&= n^s\pi^{\frac{s}{2}}\int_0^\infty y^{\frac{s}{2}-1}e^{-n^2\pi y}dy.
\end{aligned}$$

If we now substitute this expression into $\xi(s)$ it gives for $Re(s) > 1$,

$$\begin{aligned}
\frac{2}{s(s-1)}\xi(s) &= \pi^{-\frac{s}{2}}\Gamma\left(\frac{s}{2}\right)\zeta(s) \\
&= \sum_{n=1}^\infty \pi^{-\frac{s}{2}}\Gamma\left(\frac{s}{2}\right)\frac{1}{n^s} \\
&= \sum_{n=1}^\infty \int_0^\infty y^{\frac{s}{2}-1}e^{-n^2\pi y}dy \\
&= \int_0^\infty y^{\frac{s}{2}-1}\left(\sum_{n=1}^\infty e^{-n^2\pi y}\right)dy \\
&= \int_0^\infty y^{\frac{s}{2}-1}w(y)dy, \qquad (1.6)
\end{aligned}$$

where we have interchanged the summation and the integral by the monotone convergence theorem, see [9], and where we have defined $w(y) := \sum_{n=1}^\infty e^{-\pi n^2 y}$. Noticing *that* $\Theta(y) = 2w(y) + 1$ *and using the functional equation for* $\Theta(y)$ (1.3), *we get that* $2w(y) + 1 = y^{-\frac{1}{2}}\left(2w\left(\frac{1}{y}\right) + 1\right)$, *which implies that*

$$w\left(\frac{1}{y}\right) = \sqrt{y}w(y) + \frac{\sqrt{y}}{2} - \frac{1}{2}. \tag{1.7}$$

Now, splitting the integral in equation (1.6) *and making the change of variables* $y \mapsto \frac{1}{y}$ *on one of the integrals, yields*

$$\begin{aligned}
\frac{2}{s(s-1)}\xi(s) &= \int_0^1 y^{\frac{s}{2}-1}w(y)dy + \int_1^\infty y^{\frac{s}{2}-1}w(y)dy \\
&= \int_1^\infty y^{-\frac{s}{2}-1}w\left(\frac{1}{y}\right)dy + \int_1^\infty y^{\frac{s}{2}-1}w(y)dy \\
&= \int_1^\infty y^{-\frac{s}{2}-1}\left(\sqrt{y}w(y) + \frac{\sqrt{y}}{2} - \frac{1}{2}\right)dy + \int_1^\infty y^{\frac{s}{2}-1}w(y)dy.
\end{aligned}$$

If we now integrate the terms of the last equation not involving $w(y)$, *we get*

$$\begin{aligned}
\frac{2}{s(s-1)}\xi(s) &= \left(\frac{y^{-\frac{s}{2}+\frac{1}{2}}}{-s+1} - \frac{y^{-\frac{s}{2}}}{-s}\right|_1^\infty + \int_1^\infty (y^{-\frac{s}{2}-\frac{1}{2}} + y^{\frac{s}{2}-1})w(y)dy \\
&= \frac{1}{s-1} - \frac{1}{s} + \int_1^\infty (y^{-\frac{s}{2}-\frac{1}{2}} + y^{\frac{s}{2}-1})w(y)dy.
\end{aligned}$$

This implies that

$$\xi(s) = \frac{1}{2} + \frac{s(s-1)}{2}\int_1^\infty (y^{-\frac{s}{2}-\frac{1}{2}} + y^{\frac{s}{2}-1})w(y)dy, \tag{1.8}$$

for $Re(s) > 1$. *Since* $w(y) = O(e^{-\pi y})$ *as* $y \to \infty$, *the integral on the right hand side of equation* (1.8) *converges absolutely for any* s. *This implies that this expression defines the analytical continuation of* $\xi(s)$ *to the whole complex plane. Furthermore, this expression is invariant under the change of variables* $s \mapsto s - 1$.

So we have the following functional equation:

$$\xi(s) = \xi(1-s). \quad \square$$

Looking again at equation (1.8), we get for $Re(s) > 0$

$$\zeta(s) = \frac{\pi^{\frac{s}{2}}}{\Gamma\left(\frac{s}{2}\right)}\left(\frac{1}{s(s-1)} + \int_1^\infty (x^{\frac{1}{2}s-1} + x^{-\frac{1}{2}s-\frac{1}{2}})w(x)dx\right), \tag{1.9}$$

which is meromorphic in $\mathbb{C}$ since is the product of an analytic function with a meromorphic function, (notice that $\frac{\pi^{\frac{s}{2}}}{\Gamma(\frac{s}{2})}$ is analytic because $\Gamma(s)$ has no zeros). We conclude that this expression is the meromorphic continuation of the zeta function. Analogously, $\zeta(s)$ can be defined for $Re(s) \leq 0$, via the functional equation of $\xi(s)$,

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

which implies that

$$\xi(s) = \frac{\pi^{-\frac{1}{2}+s}\Gamma\left(\frac{1-s}{2}\right)\xi(1-s)}{\Gamma\left(\frac{s}{2}\right)}. \tag{1.10}$$

Where we recall that $\xi(1-s)$ was defined for $Re(s) < 1$ in theorem 1.2.

From equation (1.9) it is immediate that the only pole of the extended zeta function is $s = 1$, since: the simple pole in $\frac{1}{s}$ cancels with the simple zero in $\Gamma\left(\frac{s}{2}\right)$ at $s = 0$, the Gamma function has no zeros, $\pi^{\frac{s}{2}}$ has no poles, and the improper integral at the right converges absolutely.

1.3 Zeros of the Riemann zeta function

In this section we will prove some facts about the zeros of the extended Riemann zeta function, which from now on we will simply call the zeta function and will be denoted by $\zeta(s)$. The functional equation for $\xi(s)$ will be very useful in later proofs. We begin with the following propositions.

Proposition 1.3. *The zeta function has no zeros for $Re(s) > 1$.*

Proof. *Let $s = \sigma + it$, with $\sigma > 1$. Recalling the Euler product for $\sigma > 1$, we have*

$$\begin{aligned} |\zeta(s)| = \prod_{p \text{ prime}} \frac{1}{|1-p^{-s}|} \quad &\geq \quad \prod_{p} \frac{1}{1+|p^{-s}|} = \prod_{p} \frac{1}{1+p^{-\sigma}} \\ = e^{-\sum_p \ln(1+p^{-\sigma})} \quad &> \quad e^{-\sum_p p^{-\sigma}} > 0. \end{aligned}$$

Here we used the fact that $\ln(1+x) < x$ for $|x| < 1$. Since $|\zeta(s)| > 0$ for $\sigma > 0$ we conclude that $\zeta(s) \neq 0$ for $\sigma > 0$ $\square$

Proposition 1.4. *The zeta function only has zeros in the negative even integers for $Re(s) < 0$. These zeros are simple.*

Proof. *From equation* (1.10) *we have that* $\zeta(s)$ *is defined for* $Re(s) < 0$*, by the functional equation*

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

Now, $\pi^{-\frac{1}{2}+s}$ *is never zero and from the last proposition* $\zeta(1-s)$ *has no zeros for* $Re(s) < 0$*. Recall also that* $\Gamma(s)$ *has no zeros in the complex plane. Therefore, the only zeros* $\zeta(s)$ *has are the poles for* $\left(\frac{s}{2}\right)$ *for* $Re(s) < 0$*. From equation* (1.2) *these poles are the negative integers which are in particular simple poles. We conclude that the zeros of* $\zeta(s)$ *for* $Re(s) < 0$ *are simple zeros located at the negative integers.* $\square$

These zeros of $\zeta(s)$ for $Re(s) < 0$ are commonly called the trivial zeros of the zeta function since their existence is immediately derived from the poles of $\Gamma\left(\frac{s}{2}\right)$. It can be shown through some number-theoretic arguments that $\zeta(s)$ has no zeros on the line $Re(s) = 1$. From which is immediate using the functional equation (1.10) that there are no zeros on the line $Re(s) = 0$ either. Before we go on a further discussion about the other zeros of $\zeta(s)$ in the next section, we will show some other useful properties of $\zeta(s)$ and $\xi(s)$.

First notice that from definition of $\xi(s) = \frac{1}{2}s(s-1)\pi^{-\frac{s}{2}}\Gamma\left(\frac{s}{2}\right)\zeta(s)$ and by the last proposition, we see that the zeros of $\xi(s)$ are exactly the zeros of $\zeta(s)$ such that $0 < Re(s) < 1$ (often called non-trivial zeros). Since the trivial zeros of $\zeta(s)$ cancel with the poles of $\Gamma\left(\frac{s}{2}\right)$ for $Re(s) < 0$, the zero from s at $s = 0$, the zero from $s-1$ at $s = 1$ cancel with the pole of $\zeta(s)$ at $s = 1$ and because $\pi^{-\frac{s}{2}}$ has no zeros. So from the functional equation $\xi(s) = \xi(1-s)$, and the above considerations we see that the non-trivial zeros of the zeta function are symmetric with respect to the line $Im(s) = \frac{1}{2}$.

Next, we will use the following theorem to show that they are also symmetric with respect to the real axis.

Theorem 1.5 (Reflection formula)**.** *Suppose that* f *is analytic in some domain* D*, i.e. open connected set, which contains a segment of the real axis and whose lower half is the reflection of the upper half with respect to that axis. Then*

$$\overline{f(z)} = f(\bar{z}),$$

for each $z \in D$ *if and only if* $f(x)$ *is real for each point* x *on the segment.*

Proof. *See [7].*

Since $\xi(s)$ is analytic over $D = \{s \in \mathbb{C} : 0 < Re(s) < 1\}$, and because

$$\begin{aligned}\xi(x) &= \frac{1}{2}x(x-1)\pi^{-\frac{x}{2}}\Gamma\left(\frac{x}{2}\right)\zeta(x) \\ &= \frac{1}{2}x(x-1)\pi^{-\frac{x}{2}}\left(\int_0^\infty t^{\frac{x}{2}-1}e^{-\frac{x}{2}}dt\right)\left(1+\frac{1}{x-1}-x\int_1^\infty \{t\}t^{-x-1}dt\right),\end{aligned}$$

$\xi(s)$ is clearly real in D (note that we have used the definition of $\zeta(s)$ for $Re(s) > 0$ in theorem 1.2), we conclude that $\overline{\xi(s)} = \xi(\bar{s})$ in D, which implies that all the non-trivial zeros are symmetric with respect to the real axis. We summarize this results in a theorem.

Theorem 1.6. *The non-trivial zeros of $\zeta(s)$ are symmetric with respect to the lines $Re(s) = \frac{1}{2}$ and $Im(s) = 0$. The zeros of $\xi(s)$ are the non-trivial zeros of $\zeta(s)$. Also, $\xi(s)$ satisfy the relation $\xi(\bar{s}) = \xi(\bar{s})$ for $0 < Re(s) < 1$.*

1.4 Riemann Hypothesis

Now, what about the non-trivial zeros i.e., the zeros of the zeta function whose real part lies between 0 and 1. Their behavior has proven to be intrinsically complicated and mysterious. As a matter of fact, they led Riemann to conjecture what is considered today by many, the most important unresolved problem in mathematics[1]:

The Riemann Hypothesis:
All the non-trivial zeros of $\zeta(s)$ have real part equal to $\frac{1}{2}$.

As we mentioned earlier the Riemann Hypothesis made its first appearance in Riemann's celebrated 1859 paper entitled (in german) "On the Number of Primes Less Than a Given Magnitude"[1]. As its name indicates, the purpose of the paper was to study the number of prime numbers less than a fixed real number x. This quantity is usually denoted as $\pi(x)$. The principal result in the paper was a formula for $\pi(x)$ given by

$$\pi(x) = \sum(-1)^\mu \frac{1}{m} f(x^{\frac{1}{m}}), \tag{1.11}$$

where the summation is over the positive integers, the number of prime factors of m is denoted by μ and $f(x)$ is given by

$$f(x) = L_i(x) - \sum^{\alpha}(L_i(x^{\frac{1}{2}+\alpha i}) + Li(x^{\frac{1}{2}-\alpha i})) + \int_x^{\infty} \frac{1}{x^2-1}\frac{dx}{x\log x} + \log\xi(0), \quad (1.12)$$

where $L_i(x) := \int_2^x \frac{dt}{\ln t}$ denotes the logarithmic derivative, the summation is over the nontrivial zeros of $\zeta(s)$ and the $\xi(t)$ function of a complex variable he is using is a slightly modified version of the $\xi(s)$ function we defined, given by

$$\xi(t) := s(s-1)\pi^{-\frac{s}{2}}\Gamma\left(\frac{s}{2}\right)\zeta(s), \quad (1.13)$$

where $s = \frac{1}{2} + it$. He then proceeded to affirm that since $L_i(x)$ is by far the largest term of the first summation, then the conjectured approximation $\pi(x) = L_i(x)$ was valid for sufficiently large x. But, Riemann's proof of this result was inadequate since it is not clear from his arguments that the infinite series for $\pi(x)$ even converges. Also, it was not clear from his arguments that $L_i(x)$ dominates in the series for large x.

What immortalized this paper was not its final result, but the methods it used, which included the definition of $\zeta(s)$ and its meromorphic extension to the complex plane, Fourier and Möbius inversions, functional equations which arise from automorphic forms, contour integration, analytic continuation, and finding exact representations in infinite series for functions as complicated as $\pi(x)$, among other important techniques[10].

It seems it took more than 30 years for the mathematical community to digest the ideas in these eight pages, as Edwards notes [2], because there was no progress at all in the field of analytic number theory for almost 30 years. Then, in a very short period of time a great deal of theorems were proved which used Riemann's ideas in his paper such as a correct proof of the formula for $\pi(x)$ above and two independent proofs by Jacques Hadamard and Charles Jean de la Vallée-Poussin of the very important Prime Number theorem, which states that $\lim_{x\to\infty}\pi(x)logx/x = 1$. Although it was the only paper that Riemann published regarding analytic number theory, it revolutionized many aspects in the field. Since then, this rather intranscendent field of mathematics at the time had a dramatic expansion.

However, what turns out to be the most important point in the paper lies in this short passage:

"...this integral however is equal to the number of roots of $\xi(t) = 0$ lying within in this region, multiplied by $2\pi i$. One now finds indeed approximately this number of

real roots within these limits, and it is very probable that all roots are real. Certainly one would wish for a stricter proof here; I have meanwhile temporarily put aside the search for this after some fleeting futile attempts, as it appears unnecessary for the next objective of my investigation.[11]"

Here, $\xi(t)$ is as given by (1.13), and the region he is referring to is $-\frac{1}{2}i < Im(t) < \frac{1}{2}i$. A short examination based on the previous results of this chapter shows that this is equivalent to the nontrivial zeros of $\zeta(s)$ having real part equal to $\frac{1}{2}$. This conjecture, now named *The Riemann Hypothesis*, turns out to have vast consequences in many fields, especially in number theory, depending on whether it is true or not.

The zeta function has proved to be intrinsically connected to the prime numbers, which are the primordial topic of study in number theory, whose properties do not only stay in the theoretical frame. As a matter of fact, internet security schemes rely heavily on cryptographic methods using the properties of primes, for example. They are the fundamental pieces from which all arithmetic is based. Understanding the distribution of the zeros on the critical line, should the Riemann Hypothesis be true, will give significant insights into understanding the distribution of the primes and their apparent chaotic behaviour. Conversely, if proved false it will not only leave us far away in the road of understanding the intrinsic properties of arithmetic, but will also shatter to the ground the literally thousands of theorems which rely on the trueness of the Riemann Hypothesis [10].

Not in vain the Riemann hypothesis is called by many the most important unresolved problem in mathematics.

CHAPTER 2

The Hilbert-Polya conjecture

As we mentioned in the introduction, around 1910 David Hilbert and George Polya suggested an idea that with the passing decades took more and more strength; namely, that there exists an hermitic operator H such that the eigenvalues of the operator $G = \frac{1}{2} + iH$ are all the nontrivial zeros of the Riemann Zeta function. The hermiticity of H would imply that its eigenvalues are real, and therefore the very existence of this operator would immediately prove the Riemann Hypothesis. This conjecture though, was never published by either of them [3].

Andrew Odlyzko, a mathematician who computed hundreds of millions of Riemann zeros at very large heights [12][13][14], finding numerical confirmation that the statistical properties of the nontrivial zeros were very similar to those of the eigenvalues of the Gaussian Unitary Ensemble discussed in chapter 4, interchanged letters with George Polya, which we will reproduce here, trying to investigate about the origins and motivations of the conjecture [15].

Andrew Odlyzko to George Polya, December 8, 1981: *Dear Professor Polya:*

I have heard on several occasions that you and Hilbert had independently conjectured that the zeros of the Riemann zeta function correspond to the eigenvalues of a self-adjoint hermitian operator. Could you provide me with any references? Could you also tell me when this conjecture was made, and what was your reasoning behind this conjecture at that time?

The reason for my questions is that I am planning to write a survey paper on the distribution of zeros of the zeta function. In addition to some theoretical results, I have performed extensive computations of zeros of the zeta function, comparing their distri-

bution to that of random hermitian matrices, which have been studied very seriously by physicists. If a hermitian operator associated to the zeta function exists, then in some respects we might expect it to behave like a random hermitian operator, which in turn ought to resemble a random hermitian matrix. I have discovered that the distribution of zeros of the zeta function does indeed resemble the distribution of eigenvalues of random hermitian matrices of unitary type.

Any information or comments you might care to provide would be greatly appreciated.

Sincerely yours,

Andrew Odlyzko

George Polya to Andrew Odlyzko, January 3, 1982: *Dear Mr. Odlyzko:*

Many thanks for your letter of December 8. I can only tell you what happened to me.

I spent two years in Goettingen ending around the begin of 1914. I tried to learn analytic number theory from Landau. He asked me one day: "You know some physics. Do you know a physical reason that the Riemann hypothesis should be true." This would be the case, I answered, if the nontrivial zeros of the Xi-function were so connected with the physical problem that the Riemann hypothesis would be equivalent to the fact that all the eigenvalues of the physical problem are real.

I never published this remark, but somehow it became known and it is still remembered.

With best regards.

Your sincerely,

George Polya

Odlyzko also contacted Olga Taussky-Todd who had worked extensively with David Hilbert, since he had already passed away by then, and asked if she knew anything about the origins of the conjecture. But she did not knew anything about it [15].

Despite being a rather vague conjecture initially, the hope of finding a proof for the Riemann Hypothesis, via a physical path, has increased substantially over the years. Since the conjecture was made, numerous lines of attack to the problem have arisen, which give evidence for the spectral interpretation of the zeros from the zeta function. We will enunciate and explain some of the most transcendent physical approaches to the Riemann Hypothesis. This rapid historical review will be based on [3] and [16].

Perhaps, the most important approach to the Hilbert Polya conjecture comes from Random Matrix Theory (RMT) [3], which has proved to be a powerful tool in various fields of physics, ever since it turned out to be very efficient in the prediction of ensemble averages of observables of heavy nuclei, where it first emerged [17]. The degrees of freedom of a large nucleus transform into a gigantic analytical and numerical task which exceeds our actual computational capabilities. Because of this, Eugene Wigner first suggested that a statistical treatment for the description of nuclei should be made; in which the behaviour of nuclei could be statistically explained using random matrices selected from certain ensembles. Since then, RMT has been employed in numerous areas of physics.

Now the question arises as to how to choose a suitable random matrix ensemble for representing the Riemann zeta function operator. As it turns out, the symmetries of a physical system intrinsically determine the properties of the corresponding Hamiltonian describing the system. That is, by Noether's theorem, if the system has a symmetry, it will imply that there exists a corresponding conserved quantity. And these symmetries will narrow the possible Hamiltonians the system could have.

Consider for instance an integrable system. As Stöckmann notes [18], from the symmetry considerations the Hamiltonian could be diagonalized, in which case the eigenvalues will make symmetry classes of their own, which will lead to the assumption that the eigenvalues are totally uncorrelated. And in this case, assuming that the average spacing between eigenvalues is one, the probability distribution of nearest neighbour spacings $p(s)$ is equal to a Poisson distribution with parameter equal to 1; that is, $p(s)ds = \exp^{-s} ds$ is the probability of finding an eigenvalue at a distance between s and $s+ds$ from a given eigenvalue, with no other eigenvalues in between. Oriol Bohigas conjectured that if the classical dynamics of a system is integrable then $p(s)$ corresponds to a Poisson distribution [19]. And if the system is a chaotic one, then $p(s)$ corresponds to the respective quantity associated with a certain ensemble of random matrices.

What is interesting is that in 1973 Hugh Montgomery[4], assuming the Riemann Hypothesis to be true, showed that the pair correlation function of the imaginary part of the nontrivial zeros of the zeta function, in the asymptotic limit on the critical line and properly normalized, is

$$r_2(x) = 1 - \left(\frac{sin(\pi x)}{\pi x}\right)^2. \tag{2.1}$$

This result is known as the *Montgomery Pair Correlation Conjecture*. It was latter pointed out to him, by Freeman Dyson [20], that this was the same pair correlation function of random matrices from the Gaussian Unitary Ensemble (GUE), discussed in chapter 4, as the size of the matrices tends to infinity and when the eigenvalues are suitably normalized. Andrew Odlyzko, who we mentioned earlier, computed hundreds of millions of zeros, and was able to show a great resemblance between the data and the Montgomery conjecture, strongly suggesting the validity of it. Later, Zeév Rudnick and Peter Sarnack proved a more general result for the n-th order correlation function ($n \geq 2$) [21]. The work of Rudnick and Zarnak is beyond the scope of this work, and only the Montgomery conjecture and the pair correlation function from the GUE will be treated, in this respect.

All of these results seem to give evidence that the Riemann Hamiltonian and its corresponding physical system, if it exists, should possess similar qualities as those of physical systems the matrices from the GUE represent, which are strongly chaotic systems without time-reversal symmetry.

Furthermore, consider for instance the number of nontrivial zeros from the real axis up to a certain height T, in the complex plane. The counting function for this zeros $N(T)$ i.e., $N(T) = |\sigma + it \in \mathbb{C} : \zeta\sigma + it = 0, 0 < \sigma < 1|$, which we will derive in Chapter 4, can be expressed as the sum of two functions; one smooth $\langle N(T) \rangle$ corresponding to the mean of the function, and the other one a fluctuating function $N_{fl}(T)$ around their average values. The same holds for the counting function $\mathcal{N}(E)$, due to Gutzwiller [5], of energy levels in quantum chaotic systems up to a given energy E, which will be derived also in Chapter 4. Regarding the two fluctuation functions, Berry and Keating were able to find a resemblance between them[6]. The fluctuations for the nontrivial zeros are given by

$$N_{fl}(T) = -\frac{1}{\pi} \sum_{p \in \mathbb{P}} \sum_{m=1}^{\infty} \frac{e^{-\frac{1}{2} m \ln(p)}}{m} \sin(mT \ln(p)), \tag{2.2}$$

where the first summation runs over the prime numbers. Similarly, the fluctuations of the energy levels of a quantum chaotic system are given by

$$\mathcal{N}_{fl}(E) \sim \frac{1}{\pi} \sum_{p} \sum_{m=1}^{\infty} \frac{e^{-\frac{1}{2} m \lambda_p T_p}}{m} \sin\left(\frac{m S_p(E)}{\hbar} - \frac{1}{2} \pi m \mu_p \right), \tag{2.3}$$

where the first summation runs over the classical primitive periodic orbits of the system with length greater than zero, i.e. classically allowed orbits for the particle to travel across, which are only traversed once; the second summation is over the repetitions of those orbits; the lambda term λ_p its the Lyapunov exponent, which describes the rate of separation of infinitesimally close trajectories in a dynamical system, and accounts for its stability or instability; The period of the primitive orbit is denoted by T_p; the Maslov index, denoted by μ_p, is the number of conjugate points on the orbit plus the number of negative eigenvalues of the corresponding Monodromy matrix, discussed in Appendix C, of the orbit. We will explain both formulas more carefully in chapter 4.

Based on these similarities, Berry and Keating suggested the existence of a quantum chaotic system, containing in its spectrum the nontrivial zeros minus $\frac{1}{2}$, which also must satisfy various properties based on the resemblance of both formulas, such as: not having time reversal symmetry; the Riemann dynamics must be homogeneously unstable i.e., all of its orbits are unstable; the classical periodic orbits must be independent of the energy, and must be given by the logarithms of prime numbers; it can be approximated by a one dimensional system, among other important qualities. We will explain them with more details at the end of chapter 4.

The smooth parts of the counting functions, on the other hand, are given by:

$$\langle N(T)\rangle = \frac{T}{2\pi}\log\left(\frac{T}{2\pi}\right) - \frac{T}{2\pi} + \frac{7}{8} + O\left(\frac{1}{T}\right), \tag{2.4}$$

for the nontrivial zeros, and

$$\mathcal{N}_0(E) = \left(\frac{1}{2\pi\hbar}\right)^d \int\int \mathcal{U}(E - H(p,q))dpdq, \tag{2.5}$$

for the energy levels, where d denotes the dimensions of the system, the Hamiltonian is denoted by H, the position and momentum of the particle is denoted by q and p respectively, and $\mathcal{U}$ denotes the unitary step function. The smooth part of the counting function $\mathcal{N}_0(E)$ can be seen as the number of states located in the subset of phase space corresponding to the classical part of the system, the reason being that $\mathcal{U}(E-H(p,q)) = 0$ for $H(p,q) > E$. So, if one is going to look for a Hamiltonian suitable for the Riemann zeros it will be convenient that the number of classical states of the system up to a given energy E, will be similar to that given by $\langle N(T)\rangle$.

As a matter of fact, this led Berry and Keating to propose a Hamiltonian of the form [22]:

$$H = \frac{px + xp}{2}, \tag{2.6}$$

which seemed to satisfy the equation for $\mathcal{N}_0(E)$, as well as others characteristics predicted, based on the similiraties of the fluctuating parts of the counting functions.

However, it presented some aspects that were not in concordance with what the Riemann Hamiltonian should be. For instance, the prime numbers where not associated with the physical orbits of the system, and this must be a primordial requirement independent of the similarities of the counting functions, since the primes are intimately related with $\zeta(s)$. Nevertheless, it was a good starting point that led some physicists to start looking at modified versions of the Hamiltonian proposed by Berry and Keating. See for instance [23], [24], [25], [26], [27]. As it is today, this is quite an active field of research. Hopefully, in the near future they succeed in the quest of the Riemann Hamiltonian.

In the next two chapters we will derive the important results concerning the Montgomery pair correlation conjecture, as well as the connections between the zea function and quantum chaos based on the similarities of the counting functions.

CHAPTER 3

Random matrix correspondence of the pair correlation functions

In this chapter we will reproduce Montgomery's ideas in [4], in order to show that the pair correlation function $r_2(x)$ from the zeros of $\zeta(s)$ in the asymptotic limit, assuming both the Riemann Hypothesis (RH) and the Hardy-Littlewood 2-tuple conjecture, regarding the distribution of twin primes, resembles that from the eigenvalues of the Gaussian Unitary Ensemble as the range of the matrix is very large. More specifically, that they are both equivalent to

$$r_2(x) = 1 - \left(\frac{sin(\pi x)}{\pi x}\right)^2,$$

in the asymptotic limit when a proper normalization is given, where $r_2(x)dx$ is the probability of finding two eigenvalues from the GUE (or imaginary parts of two nontrivial zeros) y and z, such that $|y - z| := x$ lies in $[x, x + dx]$.

3.1 Montgomery's Pair Correlation Conjecture

We will start with the zeta function. We will follow Montgomery [4] and Goldston [28]. Before we study the probability distribution of the spacings between the nontrivial zeros of the zeta function, we need to define the following function.

Definition 3.1. *Define for $\alpha, T \in \mathbb{R}$, $T \geq 2$:*

$$F : \mathbb{R}^2 \longrightarrow \mathbb{C},$$

$$F(\alpha) = F(\alpha, T) = \left(\frac{T}{2\pi}\log T\right)^{-1} \sum_{y,y' \in [0,T]} T^{i\alpha(y-y')} w(y-y'),$$

where y, y' are the imaginary parts of nontrivial zeros of the zeta function, $w(u)$ is a weighting function given by $w(u) = \frac{4}{4+u^2}$ and T represents the height on the line $Re(s) = \frac{1}{2}$, $Im(s) > 0$.

Theorem 3.1 (Montgomety's theorem)**.** *Assume the Riemann Hypothesis to be true. Let $\alpha \in \mathbb{R}$ and $T \geq 2$. Then $F(\alpha)$ is real and even, for $\epsilon > 0$ there is $T_\epsilon > 0$ such that if $T > T_\epsilon$ then $F(\epsilon) \geq -\epsilon$ for all α, and as $T \to \infty$ we have*

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

uniformly for $0 \leq \alpha \leq 1 - \epsilon$

This theorem has three assertions. The first of them i.e., that $F(\alpha)$ is real and even, is straightforward to prove. The function is real because the imaginary part of each $T^{i\alpha(y-y')}$ term cancels with the imaginary part of $T^{i\alpha(y'-y)}$ for any two $y', y \in [0, T]$. And it is even because $T^{i\alpha(y-y')} + T^{i\alpha(y'-y)} = T^{i(-\alpha)(y-y')} + T^{i(-\alpha)(y'-y)}$ for any two $y', y \in [0, T]$. The other two assertions are quite more problematic. We will prove them in the next sections, but first we need to know some definitions and results.

3.1.1 Preliminary results for understanding Montgomery's ideas

We make the following definition

Definition 3.2. *Define $\Lambda : \mathbb{N} \longrightarrow \mathbb{R}$ by*

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

We will make use of the following identity for $\Lambda(n)$ in later proofs.

Proposition 3.1. *For Re$(s) > 1$ we have:*

$$\frac{\zeta'(s)}{\zeta(s)} = -\sum_{n=1}^{\infty} \frac{\Lambda(n)}{n^s}. \tag{3.1}$$

Proof. *By the Euler product, we have for Re$(s) > 1$*

$$\zeta(s) = \prod_{p \text{ prime}} \frac{1}{1-p^{-1}}.$$

Now, taking the logarithmic derivative on both sides we obtain

$$\begin{aligned}
\frac{\zeta'(s)}{\zeta(s)} &= \sum_p \frac{p^{-s}\log p}{1-p^{-s}} \\
&= -\sum_p \log p \frac{1}{1-p^s} \\
&= -\sum_p \log p \sum_{\kappa=0}^{\infty} \left(\frac{1}{p^s}\right)^{\kappa} \\
&= -\sum_{p,\kappa} \frac{\log p}{p^{\kappa s}} \\
&= -\sum_{n=1}^{\infty} \frac{\Lambda(n)}{n^s} \quad . \quad \square
\end{aligned}$$

Now, we prove a formula that connects the nontrivial zeros of the zeta function and the primes, which will be very useful for proving Montgomery's theorem:

Proposition 3.2. *Assume RH. If $1 < \sigma < 2$ and $x \geq 1$ $1-\sigma+it \in \mathbb{R}$, then*

$$\begin{aligned}
&(2\sigma-1)\sum_\gamma \frac{x^{i\gamma}}{\left(\sigma-\frac{1}{2}\right)^2+(t-\gamma)^2} \\
= \quad & -x^{-\frac{1}{2}}\left(\sum_{n\leq x}\Lambda(n)\left(\frac{x}{n}\right)^{1-\sigma+it}+\sum_{n>x}\Lambda(n)\left(\frac{x}{n}\right)^{\sigma+it}\right) \\
&+x^{\frac{1}{2}-\sigma+it}(\log\tau+O(1))+O(x^{\frac{1}{2}}\tau^{-1}).
\end{aligned} \tag{3.2}$$

where the first sum runs over all the imaginary parts ot the nontrivial zeros of $\zeta(s)$ above the real axis and $\tau = |t| + 2$.

Proof. *We will prove this proposition by using an explicit formula for $\zeta(s)$ proved in*

Landau's 1909 Handbuch [29]. It states that for real $x > 1$, $x \neq p^n$, $s = \sigma + it \in \mathbb{C}$ with $s \neq 1$, $s \neq \rho$, $s \neq -2n$,

$$\sum_{n \leq x} \frac{\Lambda(n)}{n^s} = -\frac{\zeta'(s)}{\zeta(s)} + \frac{x^{1-s}}{1-s} - \sum_{p} \frac{x^{p-s}}{p-s} + \sum_{n=1}^{\infty} \frac{x^{-2n-s}}{2n+s}, \tag{3.3}$$

where the first sum on the right hand side of equation (3.3) runs over all zeros p of $\zeta(s)$ in the critical strip above the real axis.

Now, assuming RH, we can write $p = \frac{1}{2} + i\gamma$, and then proceed to rearrange equation (3.3) to obtain:

$$\sum_{\gamma} \frac{x^{\frac{1}{2}+i\gamma-(\sigma+it)}}{\frac{1}{2}+i\gamma-(\sigma+it)} = -\left(\frac{\zeta'(s)}{\zeta(s)} + \sum_{n \leq x} \frac{\Lambda(n)}{n^s} - \frac{x^{1-s}}{1-s} - \sum_{n=1}^{\infty} \frac{x^{-2n-s}}{2n+s}\right).$$

$$\sum_{\gamma} \frac{x^{i\gamma-it}}{\sigma-\frac{1}{2}+it-i\gamma} = x^{\sigma-\frac{1}{2}}\left(\frac{\zeta'(\sigma+it)}{\zeta(\sigma+it)} + \sum_{n \leq x} \frac{\Lambda(n)}{n^{\sigma+it}} - \frac{x^{1-\sigma-it}}{1-\sigma-it} - \sum_{n=1}^{\infty} \frac{x^{-2n-\sigma-it}}{2n+\sigma+it}\right). \tag{3.4}$$

Now, if we replace $s = \sigma + it$ by $s = 1 - \sigma + it$, we obtain:

$$\begin{aligned} &\sum_{\gamma} \frac{x^{i\gamma-it}}{\frac{1}{2}-\sigma+it-i\gamma} \\ = \;& x^{\frac{1}{2}-\sigma}\left(\frac{\zeta'(1-\sigma+it)}{\zeta(1-\sigma+it)} + \sum_{n \leq x} \frac{\Lambda(n)}{n^{1-\sigma+it}} - \frac{x^{\sigma-it}}{\sigma-it} - \sum_{n=1}^{\infty} \frac{x^{-2n-1+\sigma-it}}{2n+1-\sigma+it}\right). \end{aligned} \tag{3.5}$$

We then subtract equation (3.5) from equation (3.4), use identity (3.1) on the right hand side and simplify both sides to obtain the following explicit formula:

$$\begin{aligned} &(2\sigma-1)\sum_{\gamma} \frac{x^{i\gamma}}{\left(\sigma-\frac{1}{2}\right)^2+(t-\gamma)^2} \\ = \;& -x^{-\frac{1}{2}}\left(\sum_{n \leq x} \Lambda(n)\left(\frac{x}{n}\right)^{1-\sigma+it} + \sum_{n > x} \Lambda(n)\left(\frac{x}{n}\right)^{\sigma+it}\right) - x^{\frac{1}{2}-\sigma+it}\frac{\zeta'(1-\sigma+it)}{\zeta(1-\sigma+it)} \\ &+ \frac{x^{\frac{1}{2}}(2\sigma-1)}{(\sigma-1+it)(\sigma-it)} - x^{-\frac{1}{2}}\sum_{n=1}^{\infty} \frac{x^{-2n}(2\sigma-1)}{(2n+\sigma+it)(\sigma-1-2n-it)}. \end{aligned} \tag{3.6}$$

Both sides of equation (3.6) are continuous for $x \geq 1$, so the values $x = 1$, $x = p^n$ no *longer will be excluded.*

We next proceed to bound the terms on the right hand side of equation (3.6)*. We will do this by using the following bound for* $1 < \sigma < 2$ *derived in [30]:*

$$\begin{aligned} \frac{\zeta'(1-\sigma+it)}{\zeta(1-\sigma+it)} &= -\frac{\zeta'(\sigma-it)}{\zeta(\sigma-it)} - \log\tau + O(1) \\ &= \sum_{n=1}^{\infty} \Lambda(n) n^{-\sigma+it} - \log\tau + O(1) \\ &= -\log\tau + O(1), \end{aligned} \tag{3.7}$$

where $\tau = |t| + 2$*. Where we also have,*

$$x^{-\frac{1}{2}} \sum_{n=1}^{\infty} \frac{x^{-2n}(2\sigma-1)}{(2n+\sigma+it)(\sigma-1-2n-it)} = O(x^{\frac{1}{2}}\tau^{-1}) \tag{3.8}$$

and

$$\frac{x^{\frac{1}{2}}(2\sigma-1)}{(\sigma-it)(\sigma-1+it)} = O(x^{\frac{1}{2}}\tau^{-2}). \tag{3.9}$$

Inserting equations (3.7)*,* (3.8) *and* (3.9) *into equation* (3.6)*, we obtain the desired result:*

$$\begin{aligned} (2\sigma-1)\sum_{\gamma} \frac{x^{i\gamma}}{\left(\sigma-\frac{1}{2}\right)^2 + (t-\gamma)^2} &= -x^{-\frac{1}{2}} \left(\sum_{n\le x} \Lambda(n) \left(\frac{x}{n}\right)^{1-\sigma+it} + \sum_{n>x} \Lambda(n) \left(\frac{x}{n}\right)^{\sigma+it} \right) \\ &\quad -x^{\frac{1}{2}-\sigma+it}(\log\tau + O(1)) + O(x^{\frac{1}{2}}\tau^{-1}). \quad \square \end{aligned}$$

3.1.2 Proof of Montgomery's theorem

Now, taking $\sigma = \frac{3}{2}$ on equation (4.1) we get

$$\begin{aligned} 2\sum_{\gamma} \frac{x^{i\gamma}}{1+(t-\gamma)^2} &= -x^{\frac{1}{2}} \left(\sum_{n\le x} \Lambda(n) \left(\frac{x}{n}\right)^{-\frac{1}{2}+it} + \sum_{n>x} \Lambda(n) \left(\frac{x}{n}\right)^{\frac{3}{2}+it} \right) \\ &\quad +x^{-1+it}(\log\tau + O(1)) + O(x^{\frac{1}{2}}\tau^{-1}). \end{aligned} \tag{3.10}$$

Define $L(x,t)$ and $R(x,t)$ as the left hand side and right hand side of equation (3.10) respectively.

In order to prove the second and third assertions of this theorem, Montgomery considered the integral

$$\int_0^T |L(x,t)|^2 dt = 4\int_0^T \sum_{\gamma,\gamma'} \frac{x^{i(\gamma-\gamma')}}{(1+(t-\gamma)^2)(1+(t-\gamma')^2)} dt. \tag{3.11}$$

Since the theorem involves only the zeros whose imaginary parts lie in $[0,T]$, it is convenient to consider only those zeros in the integral and find a bound for the others.

Using the fact that for $t \in [0,T]$ and assuming RH,

$$\sum_{\gamma \notin [0,T]} \frac{1}{1+(t-\gamma)^2} \ll \left(\frac{1}{t-1} + \frac{1}{T-t+1}\right) \log T \tag{3.12}$$

and

$$\sum_{\gamma} \frac{1}{1+(t-\gamma)^2} \ll \log T. \tag{3.13}$$

where both sums are over all $\gamma > 0$ [4], where $f \ll g$ means that there is a constant c such that $f < cg$. We proceed to express the integral in (3.11) as follows:

$$\begin{aligned}
\int_0^T |L(x,t)|^2 dt &= 4\int_0^T \sum_{\gamma,\gamma'} \frac{x^{i(\gamma-\gamma')}}{(1+(t-\gamma)^2)(1+(t-\gamma')^2)} dt \\
&= 4\int_0^T \sum_{\gamma,\gamma' \in [0,T]} \frac{x^{i(\gamma-\gamma')}}{(1+(t-\gamma)^2)(1+(t-\gamma')^2)} dt \\
&\quad +8\int_0^T \sum_{\gamma,\gamma' : \gamma \notin [0,T]} \frac{x^{i(\gamma-\gamma')}}{(1+(t-\gamma)^2)(1+(t-\gamma')^2)} dt.
\end{aligned}$$

Now, by using equations (3.12) and (3.13), and using the fact that $x^{i(\gamma-\gamma')}$ has modulus 1, we have that the last integral is bounded by $O(\log^3 T)$ because

$$\begin{aligned}
&\int_0^T \sum_{\gamma,\gamma' : \gamma \notin [0,T]} \frac{dt}{(1+(t-\gamma)^2)(1+(t-\gamma')^2)} \\
= &\int_0^T \left(\sum_{\gamma \notin [0,T]} \frac{1}{1+(t-\gamma)^2}\right)\left(\sum_{\gamma'} \frac{1}{1+(t-\gamma')^2}\right) dt \\
\ll &\int_0^T \left(\left(\frac{1}{t+1} + \frac{1}{T-t+1}\right)\log T\right)(\log T) dt \\
= &\ 2\log(T+1)\log^2 T = O(\log^3 T).
\end{aligned}$$

We therefore conclude that

$$\int_0^T |L(x,t)|^2 dt = 4\int_0^T \sum_{\gamma,\gamma'\in[0,T]} \frac{x^{i(\gamma-\gamma')}}{(1+(t-\gamma)^2)(1+(t-\gamma')^2)} dt + O(\log^3 T). \tag{3.14}$$

The expression on the right hand side of this equation can be replaced by the same expression but interchanging the limits of the integral to $-\infty$ and ∞; it is convenient to do this because this integral can then be evaluated by residues. We prove that this interchange is valid by using the relation

$$\sum_{\gamma\in[0,T]} \frac{1}{1+(t-\gamma)^2} \ll \frac{1}{|t-T+1|}\log T, \tag{3.15}$$

which holds for $t \in (-\infty, 0] \cup [T, \infty)$ assuming RH [4]. By using equation (3.15) we have that

$$\begin{aligned} \int_T^\infty \sum_{\gamma,\gamma'\in[0,T]} \frac{dt}{(1+(t-\gamma)^2)(1+(t-\gamma')^2)} &= \int_T^\infty \left(\sum_{\gamma\in[0,T]} \frac{1}{1+(t-\gamma)^2}\right)^2 dt \\ \ll \log^2 T \int_T^\infty \frac{dt}{(t-T+1)^2} &= \log^2 T, \end{aligned}$$

and similarly

$$\int_{-\infty}^0 \sum_{\gamma,\gamma'\in[0,T]} \frac{dt}{(1+(t-\gamma)^2)(1+(t-\gamma')^2)} \ll \log^2 T \int_{-\infty}^0 \frac{0}{(t-T+1)^2}$$

$$= \frac{\log^2 T}{T-1} = o(\log^2 T).$$

Combining these results and noting that $\log^2 T = o(\log^3 T)$, we rewrite equation (3.14) as

$$\int_0^T |L(x,t)|^2 dt = 4\int_{-\infty}^\infty \sum_{\gamma,\gamma'\in[0,T]} \frac{x^{i(\gamma-\gamma')}}{(1+(t-\gamma)^2)(1+(t-\gamma')^2)} dt + O(\log^3 T). \tag{3.16}$$

Next, we evaluate the integral on the right hand side of this equation using calculus of residues and show that the function $F(\alpha)$ (see definition 3.1), will come up, which will allow us to prove the second assertion of the theorem.

Proposition 3.3. *For $\gamma, \gamma' \in \mathbb{R}^+$,*

$$\int_{-\infty}^{\infty} \frac{dt}{(1+(t-\gamma)^2)(1+(t-\gamma')^2)} = \frac{\pi}{2} w(\gamma - \gamma'),$$

where $w(u) = \frac{4}{4+u^2}$.

Proof. *See Appendix B.3.*

Using proposition 3.3 we can rewrite equation (3.16) as

$$\int_0^T |L(x,t)|^2 dt = 2\pi \sum_{\gamma,\gamma' \in [0,T]} x^{i(\gamma-\gamma')} w(\gamma - \gamma') + O(\log^3 T).$$

Using the definition of $F(\alpha)$ and making the substitution $x = T^\alpha$ for $T \geq 2$ and $\alpha \in \mathbb{R}$ we get

$$\begin{aligned} \int_0^T |L(x,t)|^2 dt &= 2\pi \sum_{\gamma,\gamma' \in [0,T]} T^{i\alpha(\gamma-\gamma')} w(\gamma - \gamma') + O(\log^3 T) \\ &= F(\alpha) T \log T + O(\log^3 T). \end{aligned} \tag{3.17}$$

Since $|L(T^\alpha, t)|^2 \geq 0$ for every $\alpha \in \mathbb{R}$

$$\Rightarrow F(\alpha) \geq \frac{-O(\log^3 T)}{T \log T} = -O\left(\frac{\log^2 T}{T}\right).$$

Since $\frac{\log^2 T}{T}$ tends to zero for large T, we conclude that for every $\epsilon > 0$ there is a T_ϵ such that $F(\alpha) \geq -\epsilon$ for all α. This proves the second assertion of the theorem.

In order to prove the third assertion, we will now consider the integral $\int_0^T |R(x,t)|^2 dt$, where $R(x,t)$ was defined as the right hand side of equation (3.10), i.e.

$$\begin{aligned} R(x,t) &= -x^{\frac{1}{2}} \left(\sum_{n \leq x} \Lambda(n) \left(\frac{x}{n}\right)^{-\frac{1}{2}+it} + \sum_{n>x} \Lambda(n) \left(\frac{x}{n}\right)^{\frac{3}{2}+it} \right) \\ &\quad + x^{-1+it}(\log \tau + O(1)) + O(x^{\frac{1}{2}} \tau^{-1}), \end{aligned}$$

and proceed to show that for $T \geq 2$ and $0 \leq \alpha \leq 1 - \epsilon$,

$$\int_0^T |R(T^\alpha, t)|^2 dt = ((1+o(1)) T^{-2\alpha} \log T + \alpha + o(1)) T \log T. \tag{3.18}$$

Then, by equating this expression with the expression found for $\int_0^T |L(T^\alpha, t)|^2 dt$ we will prove the third assertion of the theorem.

In order to prove equation (3.18) we will consider the integrals M_1, M_2, M_3 and M_4 defined for $T \geq 2$, $x \geq 2$, where

$$M_1 := \int_0^T \left| -x^{-\frac{1}{2}} \left(\sum_{n \leq x} \Lambda(n) \left(\frac{x}{n}\right)^{-\frac{1}{2}+it} + \sum_{n > x} \Lambda(n) \left(\frac{x}{n}\right)^{\frac{3}{2}+it} \right) \right|^2 dt,$$

$$\begin{aligned} M_2 &:= \int_0^T |x^{-1+it} \log \tau|^2 dt = \frac{1}{x^2} \int_0^T |\log(|t|+2)|^2 dt = \frac{1}{x^2} \int_2^{T+2} \log^2 t dt \\ &= \frac{t}{x^2}(2 - 2\log t + \log^2 t) \bigg|_2^{T+2} = \frac{T}{x^2}(\log^2 T + O(\log T)), \end{aligned}$$

$$M_3 := \int_0^T |x^{-1+it} O(1)|^2 dt = O\left(\frac{1}{x^2}\right) \int_0^T dt = O\left(\frac{T}{x^2}\right)$$

and

$$\begin{aligned} M_4 &:= \int_0^T |O(x^{\frac{1}{2}} \tau^{-1})|^2 dt = O(x) \int_0^T (t+2)^{-2} dt \\ &= O(x) \left(\frac{1}{2} - \frac{1}{T+2}\right) = O(x). \end{aligned}$$

Its proof is omitted here, but it can be shown that $M_1 = T(\log x + O(1)) + O(x \log x)$ [28].

Using the bounds for M_1, M_2, M_3 and M_4 we will deduce a bound for $\int_0^T |R(x,t)|^2 dt$. In order to do so we will use the following proposition.

Proposition 3.4. *Suppose that*

$$\int_0^T |f_n(t)|^2 dt \leq A_n,$$

for $n \in \{1, \dots, m\}$. *Where* $A_1 \geq A_2 \geq \cdots \geq A_m$. *Then*

$$\int_0^T \left| \sum_{n=1}^m f_n(t) \right|^2 dt \leq A_1 + O((A_1 A_2)^{\frac{1}{2}}).$$

Proof. *By the Cauchy-Schwarz inequality we have that*

$$\int_0^T \left| \sum_{n=1}^m f_n(t) \right|^2 dt \leq \int_0^T \left(\sum_{n=1}^m |f_n(t)| \right)^2 dt$$

$$= \int_0^T \sum_{n,n'=1}^m |f_n(t)||f_{n'}(t)|dt = \sum_{n,n'=1}^m \int_0^T |f_n(t)||f_{n'}(t)|dt \leq \sum_{n,n'=1}^m (A_n A_{n'})^{\frac{1}{2}}.$$

Note that all terms in this sum are bounded by $(A_1A_2)^{\frac{1}{2}}$, *except for* $(A_1A_1)^{\frac{1}{2}} = A_1$. *We conclude that*

$$\int_0^T \left| \sum_{n=1}^m f_n(t) \right|^2 \leq A_1 + O((A_1A_2)^{\frac{1}{2}}). \quad \square$$

We will apply this proposition to M_1, M_2, M_3 and M_4 defined above, to find an expression for $\int_0^T |R(x,t)|^2 dt$, which will allow us to prove the third and final assertion of Montgomery's theorem.

Recall that the third assertion of the theorem assumes α to lie in $[0, 1-\epsilon]$ for arbitrary $\epsilon > 0$. Recall also that we made the substitution $x = T^\alpha$ when we were finding an expression for $\int_0^T |L(x,t)|^2 dt$. Therefore, $1 \leq x \leq \frac{T}{\log T}$.

We consider three cases:

1. $1 \leq x \leq \log^{\frac{3}{4}} T$.
2. $\log^{\frac{3}{4}} T < x \leq \log^{\frac{3}{4}}$.
3. $\log^{\frac{3}{4}} T < x \leq \frac{T}{\log T}$.

For case 1 we have that $M_2 = \frac{T}{x^2}(\log^2 T + O(\log T)) \geq \frac{T}{\log^{\frac{3}{2}} T}(\log^2 T + O(\log T))$, where $\frac{T \log^2 T}{\log^{\frac{3}{2}} T}$ is the dominant term. Hence $M_2 > O(T \log^{\frac{1}{2}} T)$. Looking at M_1, M_3 and M_4 we see that

$$\begin{aligned} M_1 &= T(\log x + O(1)) + O(x \log x) \\ &\leq T \log(\log^{\frac{3}{4}}) + O(T) + O(\log^{\frac{3}{4}} T \cdot \log(\log^{\frac{3}{4}} T)), \end{aligned}$$

where all three terms are $o(T \log^{\frac{1}{2}} T)$, and therefore $M_1 = o(M_2)$. Similarly for M_3 and M_4 we see that

$$M_3 = O\left(\frac{T}{x^2}\right) \leq O\left(\frac{T}{1}\right) = o(T \log^{\frac{1}{2}} T) = o(M_2),$$

$$M_4 = O(x) \leq O(\log^{\frac{3}{4}} T) = o(T \log^{\frac{1}{2}} T) = o(M_2).$$

By proposition 3.4, we have in this case that

$$\begin{aligned}
\int_0^T |R(x,t)|^2 dt &= M_2 + O((M_2 M_1)^{\frac{1}{2}}) \\
&= \frac{T}{x^2}(\log^2 T + O(\log T)) + o(M_2) \\
&= (1 + O(\log^{-1} T))\frac{T}{x^2}\log^2 T \\
&= (1 + o(1))\frac{T}{x^2}\log^2 T.
\end{aligned}$$

In a similar fashion for case 2, we have that all four terms are $o(T \log T)$. So we have

$$\begin{aligned}
\int_0^T |R(x,t)|^2 dt &= M_1 + O((M_1 M_2)^{\frac{1}{2}}) \\
&= o(T \log T),
\end{aligned}$$

and similarly for case 3, we have that $M_1 = T(\log x + O(1)) + O(x \log x)$ dominates all other terms, so therefore

$$\begin{aligned}
\int_0^T |R(x,t)|^2 dt &= M_1 + O((M_1 M_2)^{\frac{1}{2}}). \\
&= (1 + o(1)) T \log x
\end{aligned}$$

Combining these three results we find that

$$\int_0^T |R(x,t)|^2 dt = (1 + o(1))\frac{T}{x^2}\log^2 T + o(T \log T) + (1 + o(1)) T \log x,$$

for all $1 \leq x \leq \frac{T}{\log T}$. If we now make the substitution $x = T^{\alpha}$ for any $\alpha \in [0, 1-\epsilon]$ for arbitrary $\epsilon > 0$, we find the proof for equation (3.18):

$$\begin{aligned}
\int_0^T |R(T^{\alpha},t)|^2 dt &= (1 + o(1))\frac{T}{T^{2\alpha}}\log^2 T + o(T \log T) + (1 + o(1) T \log T^{\alpha}) \\
&= ((1 + o(1)) T^{-2\alpha} \log T + \alpha + o(1)) T \log T. \qquad (3.19)
\end{aligned}$$

Recalling that $L(x,t) = R(x,t)$, we can combine equations (3.17) and (3.19) to get

$$F(\alpha)T\log T + O(\log^3 T) = (1 + o(1)T^{-2\alpha}\log T + \alpha + o(1))T\log T,$$

which implies

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

This proves the third and final assertion of Montgomery's theorem.

3.1.3 Corollaries from Montgomery's theorem

Here we will prove an essential corollary from Montgomery's theorem which will allow us to understand the Pair Correlation Conjecture. As a matter of fact, Montgomery proves three corollaries in his paper [4], which are all important on their own. However, we will only prove the one that is important to us and state the other two.

Corollary 3.1. *Assume RH. If $0 < \alpha < 1$ is fixed then, as $T \to \infty$,*

i) $\sum_{\gamma,\gamma' \in [0,T]} \left(\frac{sin(\alpha(\gamma-\gamma')\log T)}{\alpha(\gamma-\gamma')\log T}\right) w(\gamma-\gamma') \sim \left(\frac{1}{2\alpha} + \frac{\alpha}{2}\right)\frac{T}{2\pi}\log T.$

ii) $\sum_{\gamma,\gamma' \in [0,T]} \left(\frac{sin\left(\left(\frac{\alpha}{2}\right)(\gamma-\gamma')\log T\right)}{\left(\frac{\alpha}{2}\right)(\gamma-\gamma')\log T}\right) w(\gamma-\gamma') \sim \left(\frac{1}{\alpha} + \frac{\alpha}{3}\right)\frac{T}{2\pi}\log T.$

Corollary 3.2. *Assume RH. As T tends to infinity*

$$\sum_{\substack{\gamma\in[0,T] \\ p \text{ simple}}} 1 \geq \left(\frac{2}{3} + o(1)\right)\frac{T}{2\pi}\log T,$$

where the sum is over all simple zeros of $\zeta(s)$ whose imaginary part lies in $[0,T]$.

Corollary 3.3. *Assume RH. We can compute a constant λ so that* $\liminf(\gamma_{n+1} - \gamma_n)\left(\log\frac{\gamma_n}{2\pi}\right) \leq \lambda < 1$.

We will prove corollary 1. But first note that corollary 3.2 is important because what it means is that, under RH, more than two thirds of the nontrivial zeros are simple. It is still an open problem that all of them are simple. Corollary 3.3 has some repercussions in algebraic number theory.

Before proving corollary 3.1 we prove the following relation.

Proposition 3.5. *For a kernel $\hat{r}(\alpha)$,*

$$\sum_{\gamma,\gamma' \in [0,T]} r\left((\gamma - \gamma')\frac{\log T}{2\pi}\right) w(\gamma - \gamma') = \frac{T}{2\pi}\log T \int_{-\infty}^{\infty} F(\alpha)\hat{r}(\alpha),$$

where $\hat{r}$ is the Fourier transform of r, i.e.

$$\begin{aligned} \hat{r}(\alpha) &= \int_{-\infty}^{\infty} r(u)e^{-2\pi i\alpha u}du, \\ r(u) &= \int_{-\infty}^{\infty} \hat{r}(\alpha)e^{2\pi i\alpha u}d\alpha. \end{aligned}$$

Proof. *From the definition of $F(\alpha)$ we have*

$$\begin{aligned} & \frac{T}{2\pi}\log T \int_{-\infty}^{\infty} F(\alpha)\hat{r}(\alpha)d\alpha \\ = & \int_{-\infty}^{\infty} \sum_{\gamma,\gamma' \in [0,T]} T^{i\alpha(\gamma-\gamma')} w(\gamma - \gamma')\hat{r}(\alpha)d\alpha \\ = & \sum_{\gamma,\gamma' \in [0,T]} w(\gamma - \gamma') \int_{-\infty}^{\infty} T^{i\alpha(\gamma-\gamma')}\hat{r}(\alpha)d\alpha \\ = & \sum_{\gamma,\gamma' \in [0,T]} w(\gamma - \gamma') \int_{-\infty}^{\infty} e^{2\pi i\alpha\left(\frac{(\gamma-\gamma')\log T}{2\pi}\right)}d\alpha \\ = & \sum_{\gamma,\gamma' \in [0,T]} r\left(\frac{(\gamma - \gamma')\log T}{2\pi}\right) w(\gamma - \gamma'). \quad \square \end{aligned}$$

Numeral (i) in the corollary will be proved by considering the kernel $r_1(u) := \frac{\sin(2\pi\alpha u)}{2\pi\alpha u}$ for $0 < \alpha < 1$ in conjunction with Proposition 3.5. First notice that

$$r_1(u) = \frac{\sin(2\pi\alpha u)}{2\pi\alpha u} = \frac{e^{2\pi i\alpha u} - e^{2\pi i\alpha u}}{4\pi i\alpha u} = \frac{1}{2\alpha}\int_{-\infty}^{\infty} e^{2\pi yu}dy = \int_{-\infty}^{\infty} \frac{1}{2\alpha}\chi_\alpha e^{2\pi iyu}dy,$$

and therefore we conclude that $\hat{r}_1(y) = \frac{1}{2\alpha}\chi_\alpha(y)$. Where χ_α denotes the characteristic function of the interval $[-\infty, \infty]$, i.e. $\chi_\alpha(y) = 1$ if $y \in [-\infty, \infty]$ and $\chi_\alpha(y) = 0$ otherwise.

Now, considering $r_1(u)$ and using proposition 3.5 we get

$$\begin{aligned}
&\sum_{\gamma,\gamma'\in[0,T]}\left(\frac{\sin(\alpha(\gamma-\gamma')\log T)}{\alpha(\gamma-\gamma')\log T}\right)w(\gamma-\gamma') \\
=\ & \sum_{\gamma,\gamma'\in[0,T]}\left(\frac{\sin\left(2\pi\alpha\left((\gamma-\gamma')\frac{\log T}{2\pi}\right)\right)}{2\pi\alpha\left((\gamma-\gamma')\frac{\log T}{2\pi}\right)}\right)w(\gamma-\gamma') \\
=\ & \frac{T}{2\pi}\log T\int_{-\infty}^{\infty}F(u)\hat{r}_1(u)du \\
=\ & \left(\frac{T}{2\pi}\log T\right)\frac{1}{2\alpha}\int_{-\infty}^{\infty}F(u)du \\
=\ & \left(\frac{T}{2\pi}\log T\right)\frac{1}{\alpha}\int_{0}^{\infty}F(u)du \quad \text{(since F(u) is even)} \\
=\ & \left(\frac{T}{2\pi}\log T\right)\frac{1}{\alpha}\int_{0}^{\infty}((1+o(1))T^{-2u}\log T+u+o(1))du.
\end{aligned}$$

Recall that we are considering the limit $T\to\infty$. Therefore, the $o(1)$ terms vanish, yielding

$$\begin{aligned}
\sum_{\gamma,\gamma'\in[0,T]}\left(\frac{\sin(\alpha(\gamma-\gamma')\log T)}{\alpha(\gamma-\gamma')\log T}\right)w(\gamma-\gamma') &= \left(\frac{T}{2\pi}\log T\right)\left(\frac{1}{\alpha}\cdot\left(\frac{-e^{-2u\log T}}{2}+\frac{u^2}{2}\bigg|_0^{\alpha}\right)\right. \\
&= \frac{T}{2\pi}\log T\left(\frac{1}{2\alpha}+\frac{\alpha}{2}\right).
\end{aligned}$$

This proves numeral (i) of Corollary 3.1. For numeral (ii) we will consider the kernel $r_2(u) := \left(\frac{\pi\alpha u}{\pi\alpha u}\right)^2$, for $0<\alpha<1$. In a similar fashion as for $r_1(u)$ it can be shown that $\hat{r}_2(y)=\frac{1}{\alpha^2}(\alpha-|y|)\chi_\alpha(y)$. In this case, using proposition 3.5 again, we have that

$$\sum_{\gamma,\gamma'\in[0,T]}\left(\frac{\sin\left(\left(\frac{\alpha}{2}\right)(\gamma-\gamma')\log T\right)}{\left(\frac{\alpha}{2}\right)(\gamma-\gamma')\log T}\right)^2 w(\gamma-\gamma')=\frac{T}{2\pi}\log T\int_{-\infty}^{\infty}F(u)\hat{r}_2(u)du,$$

where

$$\begin{aligned}
\int_{-\infty}^{\infty} F(u)\hat{r}_2(u)du &= \frac{1}{\alpha^2}\int_{-\alpha}^{\alpha} F(u)(\alpha-|u|)du \\
&= \frac{2}{\alpha}\int_0^{\alpha} F(u)du - \frac{2}{\alpha^2}\int_0^{\alpha} uF(u)du \\
&= \frac{2}{\alpha}\int_0^{\alpha}((1+o(1))T^{-2u}\log T + u + o(1))du \\
&\quad -\frac{2}{\alpha^2}\int_0^{\alpha} u((1+o(1))T^{-2u}\log T + u + o(1))du.
\end{aligned}$$

The first integral tends to $\frac{1}{2}+\frac{\alpha^2}{2}$, as $T\to\infty$, as before. For the second integral we only consider the terms $uT^{-2u}\log T + u^2$ since the other ones vanish. This is easily evaluated by integrating by parts and is equal to $\frac{\alpha^3}{3}$ as $T\to\infty$. Combining these results, we have that

$$\begin{aligned}
\int_{-\infty}^{\infty} F(u)\hat{r}_2(u)du &= \frac{2}{\alpha}\left(\frac{1}{2}+\frac{\alpha^2}{2}\right) - \frac{2}{\alpha^2}\left(\frac{\alpha^3}{3}\right) \\
&= \frac{1}{\alpha}+\alpha-\frac{2\alpha}{3} \\
&= \frac{1}{\alpha}+\frac{\alpha}{3},
\end{aligned}$$

therefore

$$\sum_{\gamma,\gamma'\in[0,T]} \left(\frac{\sin\left(\left(\frac{\alpha}{2}\right)(\gamma-\gamma')\log T\right)}{\left(\frac{\alpha}{2}\right)(\gamma-\gamma')\log T}\right)^2 w(\gamma-\gamma') = \left(\frac{1}{\alpha}+\frac{\alpha}{3}\right)\frac{T}{2\pi}\log T$$

as $T\to\infty$. This proves corollary 1.

3.1.4 Montgomery conjectures

In this section we will finally study the correlation of the zeros of $\zeta(s)$. Before getting to the Pair Correlation conjecture, however, we need to consider another conjecture concerning the behaviour of $F(\alpha)$ for $\alpha\geq 1$. Note that the third assertion of Montgomery's theorem only considers values of α for $0\leq\alpha<1$. The Pair Correlation Conjecture will be an immediate consequence of this conjecture, which is:

Conjecture 1 (Strong Pair Correlation Conjecture (SPC))**.** *Assume RH; then,* $F(\alpha) = 1+o(1)$ *for* $\alpha\geq 1$*, uniformly in bounded intervals.*

This conjecture emerges from trying to understand the behaviour of $F(\alpha)$ for arbitrary α. As Montgomery notes, observe that the third assertion of Montgomery's theorem cannot hold uniformly for $0 \leq \alpha \leq C$ if C is large. Because suppose it does, then by numeral (ii) in Corollary 3.1, it will imply that

$$\sum_{\gamma,\gamma'\in[0,T]} \left(\frac{\sin\left(\left(\frac{\alpha}{2}\right)(\gamma-\gamma')\log T\right)}{\left(\frac{\alpha}{2}\right)(\gamma-\gamma')\log T} \right)^2 w(\gamma-\gamma') \sim \left(\frac{1}{\alpha}+\frac{\alpha}{3}\right)\frac{T}{2\pi}\log T,$$

for $0 < \alpha \leq C$. If we write this equation as $G(\alpha) \sim H(\alpha)$, then, using the fact that $|\sin 2x| \leq 2|\sin x|$, which follows easily from the trigonometric identity $\sin 2x = 2\sin x\cos x$, we will have that $G(2\alpha) \leq G(\alpha)$ for all α. However, since $\frac{1}{2\alpha}+\frac{2\alpha}{3} > \frac{3}{2}\left(\frac{1}{\alpha}+\frac{\alpha}{3}\right)$ for $\alpha \geq 2$, we would have that $H(2\alpha) > \frac{3}{2}H(\alpha)$ for $\alpha > 2$. This leads to a contradiction. Therefore $F(\alpha)$ must have changes in its behaviour when $\alpha \geq 1$.

Montgomery gives two arguments in favor of SPC. One involves some modifications in the proof of his theorem and the other one involves some heuristic arguments related to algebraic number theory. We will only discuss the first one, since the second argument is beyond the scope of this work. Recall that we made the substitution $x = T^\alpha$ when we proved Montgomery's theorem. If $\alpha > 1$, this will imply that $x > T$. We will study how this affects the bounds of the integrals M_1, M_2, M_3 and M_4 defined previously. Recall that

$$M_1 = T(\log x + O(1)) + O(x\log x),$$

so if $x > T$, the second term is no longer dominated by the first term. Additionally, for

$$M_4 = \int_0^T |O(x^{\frac{1}{2}}\tau^{-1})|^2 dt,$$

the bound $\int_0^T x\tau^{-2}dt \leq x$ presents some issues. Is easy to see that the bounds for M_2 and M_3 are still valid. So we must reconsider the first and fourth term of $R(x,t)$, if $T > 0$. Recall that M_1 was the square integral of the first term of $R(x,t)$, etc. The term $O(x^{\frac{1}{2}}\tau^{-1})$ came from the term $\frac{-x^{\frac{1}{2}(2\sigma-1)}}{(\sigma-1+it)(\sigma-it)}$, in equation (3.9) from proposition 3.2, taking $\sigma = \frac{3}{2}$. So, in order to bound the square integral involving the first and fourth term we must consider the integral

$$\begin{aligned} M_5 \;&:= \int_0^T \left| x^{-\frac{1}{2}} \left(\sum_{n \le x} \Lambda(n) \left(\frac{x}{n}\right)^{-\frac{1}{2}+it} + \sum_{n > x} \Lambda(n) \left(\frac{x}{n}\right)^{\frac{3}{2}+it} \right) - \frac{2x^{\frac{1}{2}}}{\left(\frac{1}{2}+it\right)\left(\frac{3}{2}-it\right)} \right|^2 dt \\ &= \int_0^T \left| \frac{1}{x} \sum_{n \le x} \Lambda(n) n^{\frac{1}{2}-it} + x \sum_{n > x} \Lambda(n) n^{-\frac{3}{2}-it} - \frac{2x^{\frac{1}{2}}}{\left(\frac{1}{2}+it\right)\left(\frac{3}{2}-it\right)} \right|^2 dt. \end{aligned}$$

(By factoring out the term x^{it} whose module is 1)

Montgomery then suggested that if the Hardy-Littlewood 2-tuple conjecture regarding the distribution of twin primes was assumed, then M_5 could be found to be $\sim T \log T$. So recalling that $M_2 = \frac{T}{x^2}(\log^2 T + O(\log T))$, $M_3 = O\left(\frac{T}{x^2}\right)$ and making the substitution $x = T^\alpha$ for $\alpha \ge 1$, we would have

$$M_2 = T^{1-2\alpha}(\log^2 T + O(\log T))$$

and

$$M_3 = O(T^{-1}),$$

from which follows that $M_3 \le M_2 \le M_5$. This, in conjunction with Proposition 3.4, lead us to

$$\begin{aligned} \int_0^T |R(T^\alpha, t)|^2 dt \;&=\; M_5 + O((M_2 M_5)^{\frac{1}{2}}) \\ &=\; T \log T (1 + o(1)). \end{aligned}$$

Recalling that $\int_0^T |L(T^\alpha, t)|^2 dt = \int_0^T |R(T^\alpha, t)|^2 dt$, and looking at equation (3.17), which was valid for arbitrary α, we get

$$F(\alpha) T \log T + O(\log^3 T) = T \log T (1 + o(1)),$$

which implies

$$\begin{aligned} F(\alpha) \;&=\; 1 + o(1) + O\left(\frac{\log^2 T}{T}\right) \\ &=\; 1 + o(1), \end{aligned}$$

for $\alpha \ge 1$ as $T \to \infty$.

We now state the most important contribution of Montgomery's paper; the Pair

Correlation Conjecture. Which is an immediate consequence of SPC.

Conjecture 2 (Pair Correlation Conjecture)**.** *Assume RH. For* $0 < \alpha < \beta < \infty$*; as* T *tends to infinity*

$$\sum_{\substack{\gamma,\gamma' \in [0,T] \\ \frac{2\pi\alpha}{\log T} \le \gamma-\gamma' \le \frac{2\pi\beta}{\log T}}} 1 \sim \frac{T}{2\pi}\log T \int_\alpha^\beta 1 - \left(\frac{\sin \pi u}{\pi u}\right)^2 du,$$

Before showing that SPC implies PCC, we first show that $F(\alpha)$ behaves as $\alpha+\delta(\alpha)$ for $0 \le \alpha < 1$, as $T \to \infty$. Recall that by Montgomery's theorem

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

So, in order to prove the above statement it will suffice to show that $T^{-2\alpha}\log T$ behaves like the Dirac delta function $\delta(\alpha)$ in this limit.

First, we have that $\lim_{T\to\infty} T^{-2|\alpha|}\log T = 0$, for all values of α, except $\alpha = 0$, in which case $\lim_{T\to\infty} T^{-2|\alpha|}\log T = \infty$. Note that $F(\alpha)$ is even, so there in problem in writing $T^{-2|\alpha|}\log T$ instead of $T^{-2\alpha}\log T$. Now, since $\delta(u)$ is completely determined by

$$\delta(u) = \begin{cases} 0 & \text{for } u \neq 0 \\ \infty & \text{for } u = 0 \end{cases}, \quad \int_a^b \delta(u)du = \begin{cases} 1 & \text{for } 0 \in (a,b) \\ o & \text{otherwise} \end{cases},$$

it suffices to show that

$$\int_a^b T^{-2|\alpha}\log T d\alpha = \begin{cases} 1 & \text{for } 0 \in (a,b) \\ 0 & otherwise \end{cases}$$

as $T \to \infty$. This follows from the fact that if $a < 0 < b$, then

$$\begin{aligned} \int_a^b T^{-2|\alpha}\log T d\alpha &= \int_0^a T^{-2\alpha}\log T d\alpha + \int_0^b T^{-2\alpha}\log T d\alpha \\ &= \frac{-e^{-2\alpha\log T}}{2}\bigg|_0^a - \frac{e^{-2\alpha\log T}}{2}\bigg|_0^b \\ &= 1, \end{aligned}$$

and if $0 < a < b$ or $a < b < 0$, then $\int_a^b T^{-2\alpha}\log T d\alpha = \pm\frac{-e^{-2\alpha\log T}}{2}\Big|_b^a = 0$, as $T \to \infty$.

Therefore, in the limit $T \to \infty$,

$$F(\alpha) = |\alpha| + \delta(\alpha), \text{ for } |\alpha| < 1. \tag{3.20}$$

Recalling the kernel used for proving numeral (ii) in Corollary 3.1, and its Fourier transform, for $a = 1$; namely,

$$r_2(u) = \left(\frac{\sin \pi u}{\pi u}\right)^2, \quad \hat{r}_2(\alpha) = (1 - |\alpha|)\chi_1(\alpha),$$

we have that

$$F(\alpha) = (1 - \hat{r}_2(\alpha)) + \delta(\alpha),$$

for all α if we assume SPC. Noting that 1 is the Fourier transform of $\delta(u)$, we get

$$\hat{F}(u) = 1 - \left(\frac{\sin \pi u}{\pi u}\right)^2 \delta(u), \text{ for all } u.$$

Then, by Proposition 3.5, we have as $T \to \infty$,

$$\begin{aligned}
&\sum_{\gamma,\gamma' \in [0,T]} r\left((\gamma - \gamma')\frac{\log T}{2\pi}\right) w(\gamma - \gamma') \\
= \;& \frac{T}{2\pi} \log T \int_{-\infty}^{\infty} F(\alpha)\hat{r}(\alpha) d\alpha \\
= \;& \frac{T}{2\pi} \log T \int_{-\infty}^{\infty} \hat{F}(\alpha) r(\alpha) d\alpha \\
= \;& \frac{T}{2\pi} \log T \int_{-\infty}^{\infty} \left(1 - \left(\frac{\sin \pi\alpha}{\pi\alpha}\right)^2 + \delta(\alpha)\right) r(\alpha) d\alpha,
\end{aligned} \tag{3.21}$$

for some kernel r, where the left hand side of equation (3.21) can be written as

$$\begin{aligned}
& r(0) \sum_{\substack{\gamma,\gamma' \in [0,T] \\ \gamma = \gamma'}} 1 + \sum_{\substack{\gamma,\gamma' \in [0,T] \\ \gamma \neq \gamma'}} r\left((\gamma - \gamma')\frac{\log T}{2\pi}\right) w(\gamma - \gamma') \\
\sim \;& r(0)\frac{T}{2\pi} \log T + \sum_{\substack{\gamma,\gamma' \in [0,T] \\ \gamma \neq \gamma'}} r\left((\gamma - \gamma')\frac{\log T}{2\pi}\right) w(\gamma - \gamma'),
\end{aligned}$$

using the fact that $\sum_{\gamma \in [0,T]} 1 \sim \frac{T}{2\pi} \log T$ derived in the following chapter. Therefore, by integrating the $\delta(\alpha)r(\alpha)$ term on the right hand side of (3.21) we get

$$\begin{aligned} & r(0)\frac{T}{2\pi}\log T + \sum_{\substack{\gamma,\gamma'\in[0,T]\\ \gamma\neq\gamma'}} r\left((\gamma-\gamma')\frac{\log T}{2\pi}\right) w(\gamma-\gamma') \\ = \; & r(0)\frac{T}{2\pi}\log T + \int_{-\infty}^{\infty}\left(1-\left(\frac{\sin\pi\alpha}{\pi\alpha}\right)^2\right) r(\alpha)d\alpha, \end{aligned}$$

which implies that

$$\sum_{\substack{\gamma,\gamma'\in[0,T]\\ \gamma\neq\gamma'}} r\left((\gamma-\gamma')\frac{\log T}{2\pi}\right) w(\gamma-\gamma') = \int_{-\infty}^{\infty}\left(1-\left(\frac{\sin\pi\alpha}{\pi\alpha}\right)^2\right) r(\alpha)d\alpha,$$

as $T\to\infty$.

If we consider the kernel $r(u)=\chi_{[\alpha,\beta]}(u)$ for $0<\alpha<\beta<\infty$ in the above formula, where $\chi_{[\alpha,\beta]}$ is the characteristic function of the interval $[\alpha,\beta]$, we get

$$\sum_{\substack{\gamma,\gamma'\in[0,T]\\ \alpha\leq(\gamma-\gamma')\frac{\log T}{2\pi}\beta}} 1\cdot w(\gamma-\gamma') = \frac{T}{2\pi}\log T\int_{\alpha}^{\beta}\left(1-\left(\frac{\sin\pi u}{\pi u}\right)^2\right)du,$$

as $T\to\infty$. Now, for $\frac{(\gamma-\gamma')\log T}{2\pi}$ to lie inside $[\alpha,\beta]$ as $T\to\infty$ is necessary that $(\gamma-\gamma')\to 0$. This implies that $w(\gamma-\gamma')\to w(0)=1$. Recalling that $w(0)=\frac{1}{1+u^2}$. Therefore, we get

$$\sum_{\substack{\gamma,\gamma'\in[0,T]\\ \alpha\leq(\gamma-\gamma')\frac{\log T}{2\pi}\beta}} 1 = \frac{T}{2\pi}\log T\int_{\alpha}^{\beta}\left(1-\left(\frac{\sin\pi u}{\pi u}\right)^2\right)du,$$

which proves that SPC implies PCC. This conjecture is of great importance because as we will see in the next section, the $\left(1-\left(\frac{\sin\pi u}{\pi u}\right)^2\right)$ factor in the integral is the pair correlation function of eigenvalues of the Gaussian Unitary Ensemble of random matrices.

3.2 Gaussian Unitary Ensemble and its eigenvalue statistics

This section will be devoted to the Gaussian Unitary Ensemble (GUE), which is one of the most studied ensembles in random matrix theory. We will prove a similar result to the Pair Correlation conjecture, but this time concerning the distribution of pairs of eigenvalues from matrices of the GUE. We will follow Mehta's approach in order to derive these results [31].

3.2.1 Basic properties from the GUE

In this section we will give a brief summary about some of the most important properties from the GUE.

Definition 3.3. *The Gaussian unitary ensemble is defined as the set of $N \times N$ Hermitian matrices $M = (a_{ij})$ that satisfy the following properties:*

i) The diagonal elements $(a_{ii})_{i=1}^{N}$, as well as the real and the imaginary parts of the non-diagonal elements $(a_{ij})_{i \geq j}$ are independent random variables. Therefore the distribution function $P(H)$ satisfies

$$P(H) = \prod_{1 \leq i \leq j \leq N} f_{ij}(Re(a_{ij})) \prod_{1 \leq i < j \leq N} g_{ij}(Im(a_{ij}))$$

where f_{ij}, g_{ij} are the respective probability distribution functions .

ii) $P(H)dH$ is invariant under unitary transformations i.e. $P(H)dH = P(H')dH'$ if $H' = U^{-1}HU$ for a given unitary matrix U.

It can be shown that this is equivalent to the fact that a_{ii} are Gaussian random variables with mean 0 and variance 1, for $1 \leq i \leq N$, whereas $Re(a_{ij})$ and $Im(a_{ij})$ are Gaussian random variables with mean 0 and variance 2, for $1 \leq i < j \leq N$ [31] i.e.

$$f_{ii}(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}}, 1 \leq i \leq N, -\infty < x < \infty, \tag{3.22}$$

and,

$$f_{ij}(x) = g_{ij}(x) = \frac{1}{\sqrt{4\pi}} e^{-\frac{x^2}{4}}, 1 \leq i < j \leq N, -\infty < x < \infty. \tag{3.23}$$

It can be proved too that the joint probability density function of the eigenvalues of an $N \times N$ matrix from the GUE is equal to:

$$P_N(X_1, \dots, X_N) = C_N e^{\sum_{j=1}^{N} X_j^2} \prod_{1 \leq i < j \leq N} |X_j - X_i|^2, \tag{3.24}$$

where $C_N = (2^{-\frac{N}{2}(N-1)} \pi^{\frac{N}{2}} \prod_{j=1}^{N} j!)^{-1}$.

The n-point correlation function for $n \in 1, \dots, N$ of the GUE is defined as:

$$R_n(X_1, \dots, X_n) := \frac{N!}{(N-n)!} \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} P_N(X_1, \dots, X_N) d_{X_{n+1}} \dots d_{X_N}, \tag{3.25}$$

which is the probability density of finding eigenvalues around each of the points $X_1, \dots, X_n$, while the positions of the other eigenvalues remain unobserved.

We will prove in the next couple of sections the following theorem, which will immediately give a connection between Montgomery conjecture and Random matrices from the GUE.

Theorem 3.2. *The pair correlation function $R_2(x_1, x_2)$ from the GUE only depends on $u := |x - y|$ in the asymptotic limit and satisfies:*

$$\lim_{N \to \infty} R_2(u) = \frac{2N}{\pi^2} \left(1 - \left(\frac{\sin(\pi E)}{\pi E} \right)^2 \right), \tag{3.26}$$

where $E := \frac{(2N)^{\frac{1}{2}}}{\pi} u$.

The oscillator wave functions are essential in the proof of this theorem. So, we will talk about them in the next section before proceeding to its proof.

3.2.2 Hermite polynomials and the oscillator wave functions

In this section we will define the Hermite polynomials and the oscillator wave functions, and show some of their basic properties which will be very useful in the proof of theorem 3.2. The Hermite polynomials are defined for $n \in \mathbb{N}$ as:

$$H_n(x) := (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}, \tag{3.27}$$

It can be proved that H_n is an n-th degree polynomial given by

$$H_n(x) = n! \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^{\kappa} \frac{(2x)^{n-2\kappa}}{\kappa!(n-2\kappa)!}, \tag{3.28}$$

which also satisfy the equation

$$H_n'(x) = 2nH_{n-1}(x). \tag{3.29}$$

For $n \in \mathbb{N}$ the oscillator wave functions $\phi_n(x)$ are defined as:

$$\phi_n(x) := C_n e^{-\frac{x^2}{2}} H_n(x), \tag{3.30}$$

where $C_n = (\sqrt{\pi} 2^n n!)^{-\frac{1}{2}}$ [32].

The oscillator wave functions are very important in quantum mechanics since ϕ_n turns out to be the eigenfunction of the quantum mechanical harmonic oscillator in the n-th energy level, $E_n = \hbar\omega(n + \frac{1}{2})$ [33]; the harmonic oscillator constitutes the basis from which many theories are explained and is also the primordial example for many concepts in quantum physics. It can be shown that the oscillator wave functions $\{\phi_n(x)\}_{n=0}^{\infty}$ form an orthonormal family in $L^2(\mathbb{R}, dx)$, i.e.

$$\int_{-\infty}^{\infty} \phi_n(x)\phi_m(x)dx = \begin{cases} 1 & \text{if } n = m \\ 0 & \text{if } n = 1 \end{cases}. \tag{3.31}$$

The following theorem will be important because in the next section we are going to need a relation for some sums of products of oscillator wave functions, in order to prove some results regarding the correlation functions of the GUE.

Theorem 3.3. *(Christoffel-Darboux formula) If $\{P_n(x)\}_{n=0}^{\infty}$ is an orthogonal family of polynomials with respect to a weighting function $\omega(x)$ on $(a, b) \subseteq \mathbb{R}$ i.e.,*

$$(P_n, P_m) := \int_a^b P_n(x)P_m(x)\omega(x)dx = \begin{cases} b_n \neq 0 & \textit{if } n = m \\ 0 & \textit{if } n \neq m \end{cases}. \tag{3.32}$$

Assuming P_n to be an n-th degree polynomial. Let a_n be the coefficient of x^n in

$P_n(x)$ and let $b_n := (P_n, P_n)$ as above. Then:

$$\sum_{n=0}^{N} b_n^{-1} P_n(x) P_n(y) = \frac{a_N}{a_{N+1} b_N} \frac{P_{N+1}(x)P_N(y) - P_N(x)P_{N+1}(y)}{x-y}.$$

for $x \neq y$, and

$$\sum_{n=0}^{N} b_n^{-1} (P_n(x))^2 = \frac{a_N}{a_{N+1} b_N} (P'_{N+1}(x)P_N(x) - P'_N(x)P_{N+1}(x)).$$

Proof. See [32]. □

In our case the Hermite polynomials $\{H_n(x)\}_{n=0}^{\infty}$ are an orthogonal family of polynomials with respect to the weight function $\omega(x) := e^{x^2}$ on $(-\infty, \infty)$, where $(P_n, P_n) = b_n = \sqrt{\pi} 2^n n!$ and the leading coefficient in P_n is $a_n = 2^n$ (see equation (3.28)). Hence, from the Christoffel-Darboux formula we have

$$\sum_{n=0}^{N} (\sqrt{\pi} 2^n n!)^{-1} H_n(x) H_n(y) = \frac{2^N}{2^{N+1}(\sqrt{\pi} 2^N N!)} \frac{H_{N+1}(x)H_N(y) - H_N(x)H_{N+1}(y)}{x-y},$$

for $x \neq y$.

If we multiply this expression on both sides by $e^{-\frac{x^2}{2}}$ and $e^{-\frac{y^2}{2}}$ and rearrange some terms we obtain

$$\sum_{n=0}^{N} (\sqrt{\pi} 2^n n!)^{-1} H_n(x) e^{-\frac{x^2}{2}} H_n(y) e^{-\frac{y^2}{2}} = \frac{e^{-\frac{x^2}{2}} e^{-\frac{y^2}{2}}}{2(\sqrt{\pi} 2^N N!)} \frac{H_{N+1}(x)H_N(y) - H_N(x)H_{N+1}(y)}{x-y}.$$

Since $\phi_n(x) = (\sqrt{\pi} 2^n n!)^{-\frac{1}{2}} e^{-\frac{x^2}{2}} H_n(x)$, the above expression is equivalent to

$$\sum_{n=0}^{N} \phi_n(x) \phi_n(y) = \left(\frac{N+1}{2}\right)^{\frac{1}{2}} \frac{\phi_{N+1}(x)\phi_N(y) - \phi_N(x)\phi_{N+1}(y)}{x-y}.$$

From the Christoffel-Darboux formula we also have

$$\sum_{n=0}^{N} (\sqrt{\pi} 2^n n!)^{-1} (H_n(x))^2 = \frac{2^N}{2^{N+1}(\sqrt{\pi} 2^N N!)} (H_N(x) H'_{N+1}(x) - H'_N(x) H_{N+1}(x)).$$

If we multiply both sides by e^{-x^2} we get

$$\sum_{n=0}^{N}(\phi_n(x))^2 = \frac{e^{-x^2}}{2(\sqrt{\pi}2^N N!)}(H_N(x)H'_{N+1}(x) - H'_N(x)H_{N+1}(x)).$$

Using equation (3.29), i.e. $H'_n(x) = 2nH_{n-1}(x)$ for $n > 0$, this equation can be simplified further to give

$$\begin{aligned}\sum_{n=0}^{N}(\phi_n(x))^2 &= \frac{e^{-x^2}}{2(\sqrt{\pi}2^N N!)}(H_N(x)(2N+2)H_N(x) - 2NH_{N-1}(x)H_{N+1}(x)) \\ &= (N+1)(\phi_N(x))^2 - (N(N+1))^{\frac{1}{2}}\phi_{N-1}(x)\phi_{N+1}(x).\end{aligned}$$

We summarize these results in the following proposition, with the summation only going up to $N-1$, which will be more practical to prove the upcoming results.

Proposition 3.6. *For $N > 0$ we have the following relations:*

i) $\sum_{n=0}^{N-1}\phi_n(x)\phi_n(y) = \left(\frac{N}{2}\right)^{\frac{1}{2}}\frac{\phi_N(x)\phi_{N-1}(y)-\phi_{N-1}(x)\phi_N(y)}{x-y}$.

ii) $\sum_{n=0}^{N-1}(\phi_n(x))^2 = N(\phi_N(x))^2 - (N(N+1))^{\frac{1}{2}}\phi_{N-1}(x)\phi_{N+1}(x)$.

3.2.3 Pair correlation function for the eigenvalues of the GUE

In order to prove the formula for the pair correlation function, we will first need to prove the following two propositions:

Proposition 3.7. *If $X_1, X_2, \ldots, X_N$ are real variables and $f : \mathbb{R}^2 \to \mathbb{R}$ is a real-valued function. And M_N is an $N \times N$ matrix such that $M_{ij} = f(x_i, x_j)$ $1 \leq i, j \leq N$ which satisfy the following two conditions:*

i) $\int_{-\infty}^{\infty} f(x,x)dx$ *exists and is equal to a finite constant c.*

ii) $\int_{-\infty}^{\infty} f(x,y)f(y,z)dy = f(x,z)$.

Then the following relation holds:

$$\int_{-\infty}^{\infty}|M_N|d_{X_N} = (C-N-1)|M_{N-1}|, \tag{3.33}$$

where $|\cdot|$ is the determinant and M_{N-1} is the $N-1 \times N-1$ matrix obtained by deleting the last column and last row of M_N.

Proof. *We have that* $|M_{N-1}| = (-1)^{N-1}(f(X_N, X_1)|M_N^{(N,1)}| - f(X_N, X_2)|M_N^{(N,2)}| + \cdots + (-1)^{N-1}f(X_N, X_N)|M_N^{(N,N)}|)$ *where we define* $M_N^{(i,j)}$ *to be the* $N-1 \times N-1$ *matrix obtained by removing the i-th row and the j-th column of* M_N*. Now, only the last columns of* $M_N^{(N,m)} 1 \leq m \leq N-1$ *matrices contain the variable* X_N*. All these last columns are equal to:*

$$\begin{pmatrix} f(X1, X_N) \\ f(X_2, X_N) \\ \vdots \\ f(X_{N-1}, X_N) \end{pmatrix}.$$

And so, using the second property from the hypothesis we have:

$$\begin{aligned}
&\int_{-\infty}^{\infty} f(X_N, X_1)|M_N^{(N,1)}| \\
= &\int_{-\infty}^{\infty} f(X_N, X_1) \begin{pmatrix} f(X_1, X_2) & f(X_1, X_3) & \cdots & f(X_1, X_N) \\ f(X_2, X_2) & f(X_2, X_3) & & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ f(X_{N-1,X_2}) & \cdots & \cdots & f(X_{N-1}, X_1) \end{pmatrix} dx \\
= &\begin{pmatrix} f(X_1, X_2) & f(X_1, X_3) & \cdots & (f(X_1, X_N) \cdot f(X_N, X_1)) \\ f(X_2, X_2) & f(X_2, X_3) & & (f(X_2, X_N) \cdot f(X_N, X_1)) \\ \vdots & \vdots & \ddots & \vdots \\ f(X_{N-1,X_2}) & \cdots & \cdots & (f(X_{N-1}, X_1) \cdot f(X_N, X_1)) \end{pmatrix} dx
\end{aligned}$$

$$\begin{aligned}
= &\begin{pmatrix} f(X_1, X_2) & f(X_1, X_3) & \cdots & (f(X_1, X_{N-1}) & f(X_1, X_1)) \\ f(X_2, X_2) & f(X_2, X_3) & \cdots & (f(X_2, X_{N-1}) & f(X_2, X_1)) \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ f(X_{N-1,X_2}) & \cdots & \cdots & (f(X_{N-1}, X_{N-1}) & f(X_{N-1}, X_1)) \end{pmatrix} dx \\
= &(-1)^{N-2}|M_N^{(N,N)} = (-1)^{N-2}|M_{N-1}|.
\end{aligned}$$

Analogously we have:

$$\int_{-\infty}^{\infty} f(X_N, X_j)|M_N^{(N,j)}|d_{X_N} = (-1)^{N-j-1}|M_{N-1}|,$$

for $1 \leq j \leq N-1$. Therefore:

$$
\begin{aligned}
\int_{-\infty}^{\infty} |M_N| d_{X_N} &= \underbrace{-|M_{N-1}| - \cdots - |M_{N-1}|}_{N+1 \text{ times}} + \int_{-\infty}^{\infty} f(X_N, X_N)|M_{N-1}| d_{X_N} \\
&= (C - N + 1)|M_{N-1}| \qquad . \quad \square
\end{aligned}
$$

Proposition 3.8. *Let $M = (M_{ij})$ be the $N \times N$ matrix such that $M_{ij} = \phi_{i-1}(X_j)$ for $1 \leq i, j \leq N$ where $\phi_n(x)$ is the oscillator wave function. Then $P_N(X_1, \ldots, X_N) = \frac{1}{N!}|M|^2$ where*

$$P_N(X_1, \ldots, X_N) = C_N e^{-\sum_{j=1}^{N} X_j^2} \times \prod_{1 \leq i < j \leq N} |X_j - X_i|^2$$

is the joint probability density function of the eigenvalues of an $N \times N$ matrix from the GUE

Proof. *First consider the Vandermonde determinant:*

$$\prod_{1 \leq i < j \leq N} (X_j - X_i) = \begin{pmatrix} 1 & \cdots & 1 \\ X_1 & \cdots & X_N \\ \vdots & & \vdots \\ X_1^{N-1} & \cdots & X_N^{N-1}. \end{pmatrix} \tag{3.34}$$

Now, since for every $n \in \mathbb{N}$ the Hermite polynomial $H_n(x)$ is a polynomial in x of degree n, given by

$$H_n(x) = n! \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^{\kappa} \frac{(2x)^{n-2\kappa}}{\kappa!(n-2\kappa)!}, \tag{3.35}$$

we can take a suitable linear combination of the first $N-2$ rows of the matrix 3.34 and add them to the last row in order to convert it into $(H_{N-1}(X_1), \ldots, H_{N-1}(X_N))$. This can be done successively up to the first row. Therefore, we obtain:

$$\prod_{1 \leq i < j \leq N} |X_j - X_i| = C_0 \begin{pmatrix} H_0(X_1) & \cdots & H_0(X_N) \\ \vdots & & \vdots \\ H_{N-1}(X_1) & \cdots & H_{N-1}(X_N), \end{pmatrix} \tag{3.36}$$

where C_0 is a constant.

Now, multiply each i-th row by $(\sqrt{\pi} 2^{i-1} (i-1)!)^{\frac{1}{2}}$ and each j-th column by $e^{-\frac{x^2}{2}}$. We *obtain:*

$$e^{-\sum_{j=1}^{N}\frac{X_j^2}{2}}\prod_{1\leq i<j\leq N}|X_j-X_i| = C_1\det\left((\phi_{i-1}(X_j))_{1\leq i,j\leq N}\right) = C_1|M|, \tag{3.37}$$

where C_1 is a constant. Therefore, we obtain:

$$P_N(X_1,\ldots,X_N) = C_N e^{-\sum_{j=1}^{N}X_j^2}\prod_{1\leq i<j\leq N}|X_j-X_i|^2 = K|M|^2, \tag{3.38}$$

where K is a constant that we will determine.

We now define $K_N(x,y)$ for a fixed $N\in\mathbb{N}$ by:

$$K_N(x,y) := \sum_{n=0}^{N-1}\phi_n(x)\phi_n(y), \tag{3.39}$$

and define K_m for $m\in\{1,\ldots,N\}$ as the $m\times m$ matrix with elements:

$$(K_m)_{ij} := (K_N(x_i,x_j)), 1\leq i,j\leq m. \tag{3.40}$$

Let us then verify that K_N satisfies the condition of proposition 3.7:

i) We have

$$\int_{-\infty}^{\infty}K_N(x,x)dx = \int_{-\infty}^{\infty}\sum_{i=0}^{N-1}(\phi_i(x))^2dx = \sum_{i=0}^{N-1}\int_{-\infty}^{\infty}(\phi_i(x))^2dx = N,$$

by the orthornormality of $(\phi_n)_{n\in\mathbb{N}}$

ii)

$$\begin{aligned}
& \int_{-\infty}^{\infty} K_N(x,y)K_N(y,z)dy \\
= \;& \int_{-\infty}^{\infty} \left(\sum_{i=0}^{N-1} \phi_i(x)\phi_i(y)\right)\left(\sum_{j=0}^{N-1} \phi_j(y)\phi_j(z)\right) dy \\
= \;& \sum_{i=0}^{N-1}\sum_{j=0}^{N-1} \int_{-\infty}^{\infty} \phi_i(x)\phi_i(y)\phi_j(y)\phi_j(z)dy \\
= \;& \sum_{i=0}^{N-1}\sum_{j=0}^{N-1} \phi_i(x)\phi_j(z) \int_{-\infty}^{\infty} \phi_i(y)\phi_j(y)dy \\
= \;& \sum_{i=0}^{N-1}\sum_{j=0}^{N-1} \phi_i(x)\phi_j(z)\delta_{ij} \\
= \;& \sum_{i=0}^{N-1} \phi_i(x)\phi_i(z) \\
= \;& K_N(x,z).
\end{aligned}$$

Hence, we can apply Proposition 3.7 to K_N. We have

$$\begin{aligned}
& \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} |K_N| dx_N \dots dx_1 \\
= \;& (N-N+1) \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} |K_{N-1}| dx_{N-1} \dots dx_1 \\
& \vdots \\
= \;& (N-1)! \int_{-\infty}^{\infty} |K_1| dx_1 \\
= \;& (N-1)! \int_{-\infty}^{\infty} \sum_{n=0}^{N-1} (\phi_n(x_1))^2 dx_1 \\
= \;& N!.
\end{aligned}$$

Now, by noting that $K_N = M^T M$ we have that $|M|^2 = |K_N|$, and so

$$\begin{aligned}
& \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} P_N(x_1,\dots,x_N) dx_1 \dots dx_N = 1 \\
\iff \;& \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} K|M|^2 dx_1 \dots dx_N = 1
\end{aligned}$$

$$\iff K = (N!)^{-1}.$$

This proves the desired result $\square$

Now, using the last propositions note that the n-point correlation function is equal to:

$$\begin{aligned}
R_n(X_1, \ldots, X_n) &= \frac{1}{(N-n)!}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} P_N(X_1, \ldots, X_N) d_{X_{n+1}} \ldots d_{X_N} \\
&= \frac{1}{(N-n)!}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} |K_N| d_{X_N} \ldots d_{X_{n+1}} \\
&\vdots \\
&= \frac{1 \cdot 2 \cdot \cdots \cdot (N-(n-1))}{(N-n)!}\int_{-\infty}^{\infty} |K_{n+1}| dX_{n+1} \\
&= |K_n|,
\end{aligned}$$

where $|\cdot|$ denotes the determinant. We now have all the tools to prove the 2-point correlation formula, and also the famous Wigner Semicircle Law.

Theorem 3.4 (Wigner's Semicircle law)**.** *The probability density $R_1(x)$ of the eigenvalues from a matrix of the GUE is equal to*

$$R_1(x) = \begin{cases} \frac{1}{\pi}\sqrt{2N - x^2} & \text{if } |x| < \sqrt{2N} \\ 0 & \text{otherwise} \end{cases},$$

as $N \to \infty$.

Proof. *We will prove this result using the WKB approximation(see appendix D). Since the oscillator wave function $\phi_n(x)$ is the wave function of the quantum harmonic oscillator with energy $E_n = \hbar\omega\left(n + \frac{1}{2}\right)$, it satisfies the Schrödinger equation*

$$\phi_n''(x) = -(2E_n - x^2)\phi_n(x), \tag{3.41}$$

where for simplicity we have taken $\hbar = 1, m = 1$. For $|x| < (2E_n)^{\frac{1}{2}}$ which corresponds to the classically allowed region the solutions of equation (3.41) *show an oscillatory behaviour, whereas outside this region a very rapid exponential decay takes place. Using the WKB approximation and knowing that $\phi_n(x)$ is an even or odd function if and only* *if n is an even or odd number respectively, we can approximate $\phi_n(x)$ by*

$$\begin{aligned} \phi_n(x) &= \sqrt{\frac{2}{\pi}}\left(\frac{1}{2(E_n - V(x))}\right)^{\frac{1}{4}} \cos\left(\int_0^x \sqrt{2(E_n - V(x'))}dx' - \frac{n\pi}{2}\right) \\ &= \sqrt{\frac{2}{\pi}}(2n+1-x^2)^{-\frac{1}{4}} \cos\left(\int_0^x \sqrt{2n+1-x'^2}dx' - \frac{n\pi}{2}\right). \end{aligned}$$

Therefore, we have that

$$\begin{aligned} |\phi_n(x)|^2 &= \frac{2}{\pi}\frac{1}{\sqrt{2n+1-x^2}} \cos^2\left(\int_0^x \sqrt{2n+1-x'^2}dx' - \frac{n\pi}{2}\right) \\ &= \frac{2}{\pi}\frac{1}{\sqrt{2n+1-x^2}} \left(\frac{1+(-1)^n \cos\left(2\int_0^x \sqrt{2n+1-x'^2}dx'\right)}{2}\right) \\ &= \frac{1}{\pi\sqrt{2n+1-x^2}} \left(1+(-1)^n \cos\left(2\int_0^x \sqrt{2n+1-x'^2}dx'\right)\right), \end{aligned} \tag{3.42}$$

Where in the second step we have used the trigonometric identities $\cos^2 = \frac{1}{2}(1+\cos(2x))$ *and* $\sin^2(x) = \frac{1}{2}(1-\cos(2x))$*, noting that* $\cos\left(x - \frac{n\pi}{2}\right) = \sin x$ *if n is odd.*

In the limit of large N the oscillatory terms become negligible in the sum

$$R_1(x) = K_N(x,x) = \sum_{k=0}^{N-1} |\phi_k(x)|^2,$$

due to the fact that they approximately constitute a decreasing alternating series. Hence,

$$\sum_{n=0}^{N-1} |\phi_n(x)|^2 \approx \sum_{n=0}^{N-1} \frac{1}{\pi\sqrt{2n+1-x^2}},$$

and since $\frac{1}{\sqrt{2n+1-x^2}}$ *is a decreasing function in n we can approximate the sum in the above expression by an integral in n, giving us the desired result*

$$R_1(x) = \begin{cases} \frac{1}{\pi}\sqrt{2N+1-x^2} & \textit{if } |x| < \sqrt{2N+1} \\ 0 & \textit{otherwise} \end{cases},$$

as $N \to \infty$, where in the last step we have taken into account the fact that we neglected the contributions of $\phi_n(x)$ when $2n+1 < x^2$. $\square$

We are now finally able to derive the 2-point correlation function form the GUE in the limit of large N. We will use the following asymptotic formula for the oscillator wave functions due to H. Bateman.

Theorem 3.5. *The oscillator wave functions satisfy the following asymptotic relations:*

i) $\lim_{m\to\infty}(-1)^m m^{\frac{1}{4}}\phi_{2m}(x) = \frac{1}{\sqrt{\pi}}\cos(2m^{\frac{1}{2}}x)$.

ii) $\lim_{m\to\infty}(-1)^m m^{\frac{1}{4}}\phi_{2m+1}(x) = \frac{1}{\sqrt{\pi}}\sin(2m^{\frac{1}{2}}x)$.

Proof. *See [32].*

Now, we finally prove theorem 3.2. From equation (3.41) we have that

$$\begin{aligned} R_2(x,y) &= |K_2| \\ &= \sum_{n=0}^{N-1}(\phi_n(x))^2\sum_{n=0}^{N-1}(\phi_n(y))^2 - \left(\sum_{n=0}^{N-1}\phi_n(x)\phi_n(y)\right)^2. \end{aligned} \tag{3.43}$$

From proposition 3.6 we have that

$$\sum_{n=0}^{N-1}\phi_n(x)\phi_n(y) = \left(\frac{N}{2}\right)^{\frac{1}{2}}\frac{\phi_N(x)\phi_{N-1}(y)-\phi_{N-1}(x)\phi_N(y)}{x-y}.$$

Assume without loss of generality that $N = 2m$ for some $m \in \mathbb{N}$. By theorem 3.5 we have, as $m \to \infty$,

$$\begin{aligned} \sum_{n=0}^{2m-1}\phi_n(x)\phi_n(y) &= m^{\frac{1}{2}}\frac{\phi_{2m}(x)\phi_{2m-1}(y)-\phi_{2m-1}(x)\phi_{2m}(y)}{x-y} \\ &= -\frac{1}{\pi}\frac{\cos(2m^{\frac{1}{2}}x)\sin(2m^{\frac{1}{2}}y)-\sin(2m^{\frac{1}{2}}x)\cos(2m^{\frac{1}{2}}y)}{x-y} \\ &= -\frac{1}{\pi}\frac{-\sin(2m^{\frac{1}{2}}(x-y))}{x-y} \\ &= \frac{\sin(2m^{\frac{1}{2}}(x-y))}{x-y}, \end{aligned} \tag{3.44}$$

where have used the trigonometric identity $\cos x\sin y - \sin x\cos y = -\sin(x-y)$. Now, on the other hand as $N \to \infty$,

$$\left(\sum_{n=0}^{N-1}(\phi_n(x))^2\right)\left(\sum_{n=0}^{N-1}(\phi_n(y))^2\right) \approx \frac{2N}{\pi^2}, \tag{3.45}$$

which follows from Wigner's semicircle law. If we make the substitutions $E_1 = (2N)^{\frac{1}{2}}\frac{x}{\pi}$ and $E_2 = (2N)^{\frac{1}{2}}\frac{y}{\pi}$ in equation (3.44) and then insert both equation (3.44) and (3.45) into equation (3.43) we get

$$R_2(x,y) \sim \frac{2N}{\pi^2}\left(1-\left(\frac{\sin(\pi(E_1-E_2))}{\pi(E_1-E_2)}\right)^2\right).$$

Since $R_2(x,y)$ depends in $|x-y|$ only, in the limit $N \to \infty$, this expression could also be written as

$$R_2(u) \sim \frac{2N}{\pi^2}\left(1-\left(\frac{\sin(\pi E)}{\pi E}\right)^2\right),$$

where $u := |x-y|$ and $E := |E_1 - E_2| = \frac{(2N)^{\frac{1}{2}}}{\pi}u$.

3.3 Numerical evidence in favor of Montgomery's conjecture

Thanks to the computer era, the hard task of computing the zeros of $\zeta(s)$ was further simplified, going from only knowing the first 1041 zeros (above the critical line, starting from the real axis) in 1936 [34] to knowing more than 10^{13} zeros today. As more and more zeros were computed, mathematicians were finally able to analyse the properties of the zeros from an statistical point of view. As a side note, it is remarkable how Riemann was able to make this conjecture about the Zeta function since he only knew three nontrivial zeros at the time.

In order to verify that the zeros of $\zeta(s)$ satisfy the pair correlation function predicted by Montgomery, Andrew Odlyzko computed millions of consecutive zeros at very large heights [12]; recall that the Montgomery Pair Correlation conjecture regards the distribution of the zeros in the asymptotic limit, so many consecutive zeros have to be calculated in order to make a reliable statistical analysis. He obtained large amounts of numerical data that heavily support the Montgomery conjecture, strongly suggesting that the search of the hypothetical Riemann Hamiltonian should be directed to similar matrices as those from the GUE.

More specifically, in 1987 he computed the $10^{12}th$ zero and its 10^5 successors to an accuracy of $\pm 10^{-8}$[12], showing how the first 10^5 zeros behave statistically as opposed to the other 10^5 zeros at larger height; in 1989 he computed the $10^{20}th$ zero and 75 million of its neighbours[13], and later refined this result in 1992 by computing 175 million of its neighbours[14]. The results were very satisfactory: The higher one goes in the critical line, the better the fit in the numerical data with the prediction from the GUE, as it can be seen from 3.1 to 3.8.

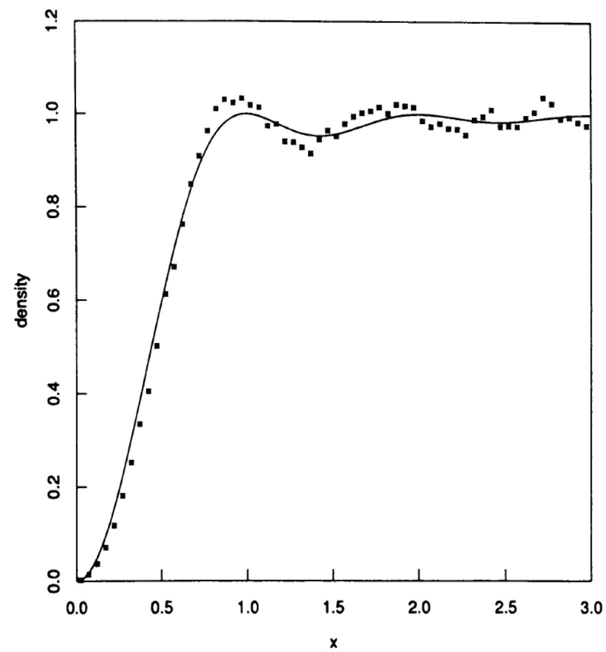

Figure 3.1: Pair correlation of zeros of the zeta function. Solid line: GUE prediction. Scatter plot: empirical data based on zeros γ_n, $1 \leq n \leq 10^5$. Taken with permission from [12].

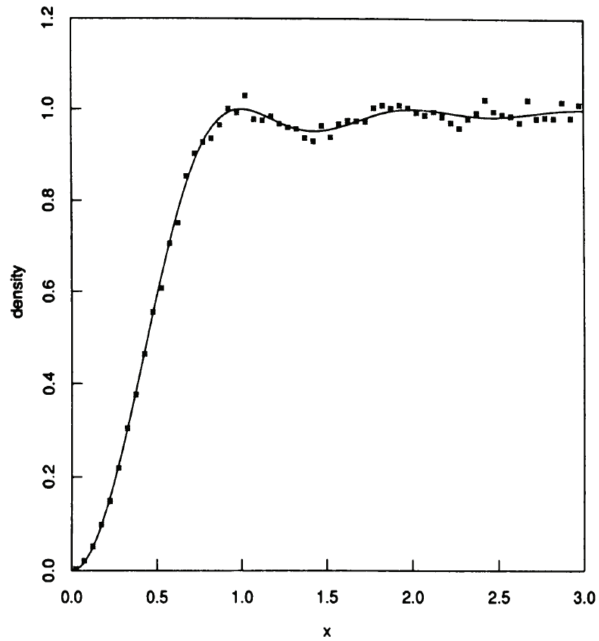

Figure 3.2: Pair correlation of zeros of the zeta function. Solid line: GUE prediction. Scatter plot: empirical data based on zeros γ_n, $10^{12}+1 \leq n \leq 10^{12}+10^5$. Taken with permission from [12].

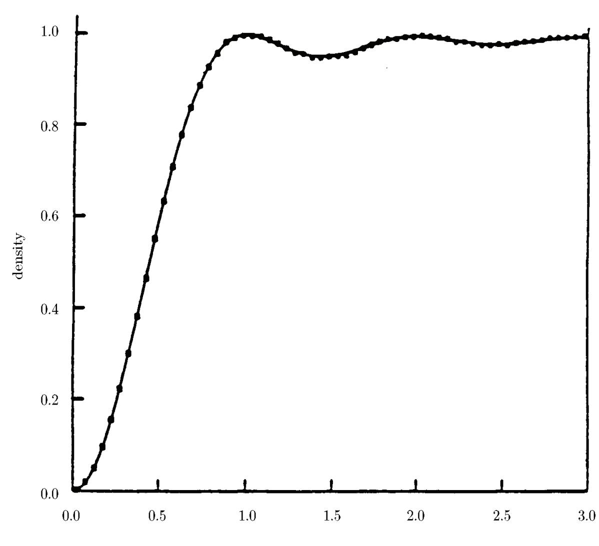

Figure 3.3: Pair correlation for zeros of zeta based on 8×10^6 zeros near the $10^{20}-th$ zero, versus the GUE conjectured density $1 - \left(\frac{\sin \pi x}{\pi x}\right)^2$. Taken with permission from [21].

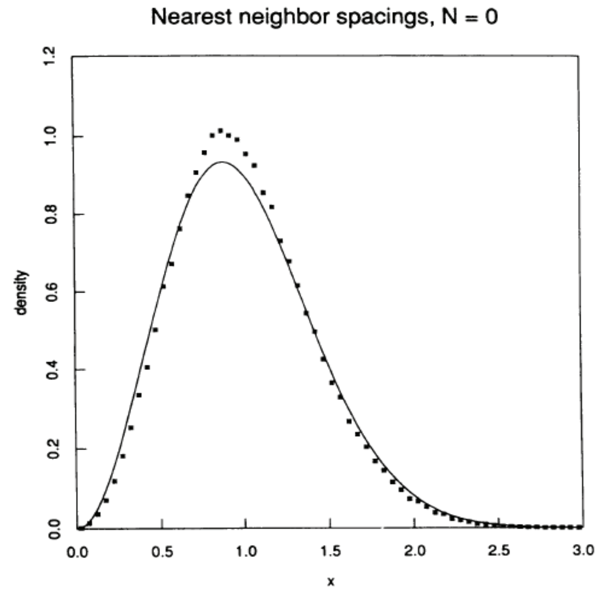

Figure 3.4: Probability density of the normalized spacing δ_n. Solid line: GUE prediction. Scatter plot: empirical data based on zeros γ_n, $1 \leq n \leq 10^5$. Taken with permission from [12].

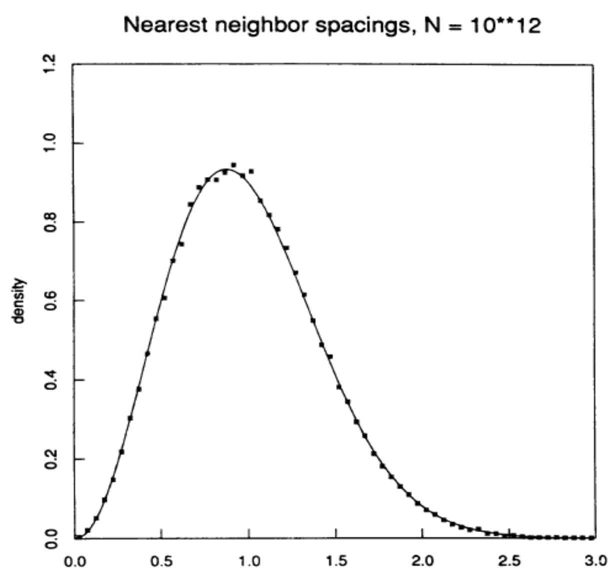

Figure 3.5: Probability density of the normalized spacings δ_n. Solid line: GUE prediction. Scatter plot: empirical data based on zeros γ_n, $10^{12} + 1 \leq n \leq 10^{12} + 10^5$. Taken with permission from [12].

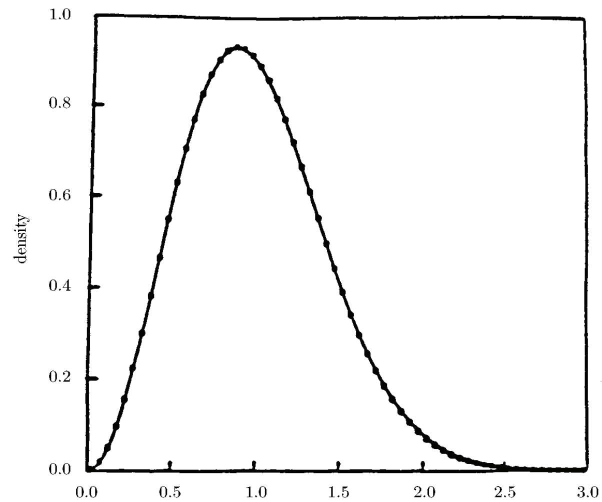

Figure 3.6: Nearest neighbor spacing among 70 million zeros beyond the $10^{20}-th$ zero of zeta, verses $\mu_1(GUE)$. Taken with permission from [21].

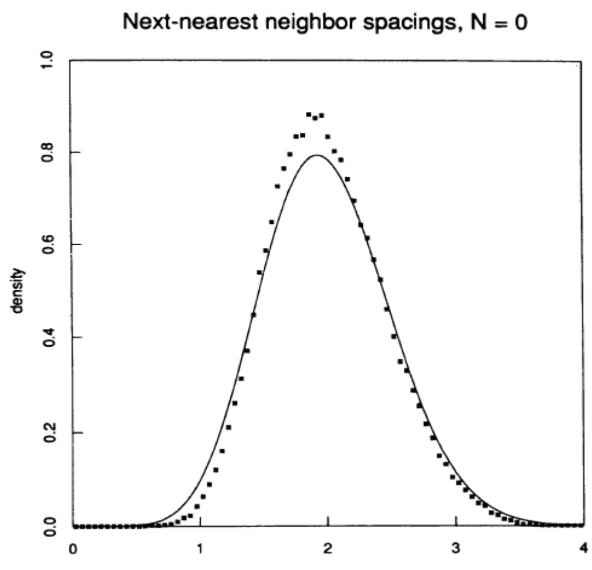

Figure 3.7: Probability density of the normalized spacings $\delta_n + \delta_{n+1}$. Solid line: GUE prediction. Scatter plot: empirical data based on zeros γ_n $1 \leq n \leq 10^5$. Taken with permission from [12].

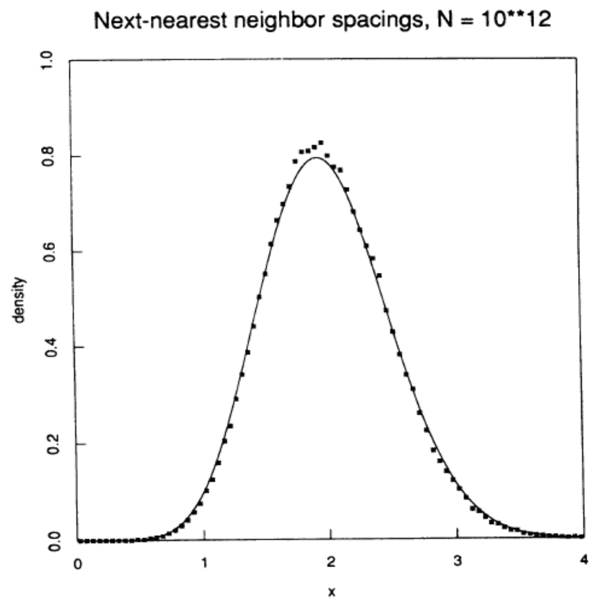

Figure 3.8: Probability density of the normalized spacings $\delta_n + \delta_{n+1}$. Solid line: GUE prediction. Scatter plot: empirical data based on zeros γ_n $10^{12} + 1 \leq n \leq 10^{12} + 10^5$. Taken with permission from [12].

The statistical similarities between the zeros and energy levels of a matrix from the GUE was the starting point that led mathematicians to benefit from the extensive research physicists had made about the GUE and the distribution of its eigenvalues [16], and to analyse from this perspective the distribution of the zeros of the Zeta function. We emphasize that the similarities not only rely on the pair correlation functions, but on the n-th correlation functions too, for $n \geq 2$ [21]. Hence, the GUE seems to be a good source of information in the study of the zeta function. The study of the behaviour and statistical properties of the zeros is no easy task. As a matter of fact, nothing about the zeta function is an easy task; not for nothing the Riemann Hypothesis is one of the seven problems of the millennium. So, having encountered in the GUE another tool for studying it is a very valuable asset.

Now, one may be tempted to say, for example, that the Montgomery Pair Correlation conjecture does not contribute much to finding a proof of the Riemann Hypothesis via a physical path, because in order to get there, the Riemann Hypothesis was assumed to be true all the way in the first place. And in order to prove the Hilbert-Polya conjecture, one simply cannot assume the Riemann Hypothesis. One has to find a Hamiltonian having the zeta function so deeply at its core, that it is deducible from it that its spectrum contains the nontrivial zeros of $\zeta(s)$ minus $\frac{1}{2}$. However, we make emphasis in the fact that while the correspondence of n-th correlation functions with the GUE has yet not given a direct insight into a possible mathematical proof or counterexample of the Riemann Hypothesis, its study has confirmed that the spectral approach of the Riemann Hypothesis is a very promising path to finally solve this old hard riddle. In particular, knowing what are the best options of physical systems to start looking at in order to find a Hamiltonian deeply connected with the zeta function i.e., the same physical systems the GUE represent: strongly chaotic systems, with no time reversal symmetries.

CHAPTER 4

Counting functions for both the nontrivial zeros and the energy levels of quantum chaotic systems

This chapter will be devoted to deriving the counting function for both the nontrivial zeros of the Riemann Zeta function above the real axis up to a given point, as well as following Gutzwiller's steps to derive the counting function of energy levels of a quantum chaotic system. We will then make some conclusions regarding their similarities.

4.1 Counting function for the nontrivial zeros

We first start with the counting function of the nontrivial zeros of the Riemann zeta function up to a certain height in the complex plane, starting from the real axis. By this we mean that we will count the number of zeros of the Riemann zeta function inside the open set $\{\sigma + it \in \mathbb{C} : 0 < \sigma < 1, 0 < t < T\}$ where we will denote the number of zeros inside this set as

$$N(T) := \#\{\sigma + it \in \mathbb{C} : 0 < \sigma < 1, 0 < t < T, \zeta(\sigma + it) = 0\}.$$

There is no loss of information regarding the zeros with negative imaginary part, since as we saw in Chapter 1, the zeros of the zeta function are symmetric with respect to the real axis. See theorem 1.6. To this end we will use the following theorem.

Theorem 4.1 (Argument Principle)**.** *Let C denote a positively oriented simple closed* *contour, and suppose that a function $f(z)$ is meromorphic inside C, and is analytic and nonzero on C. Then*

$$N - P = \frac{1}{2\pi i}\int_C \frac{f'(z)}{f(z)}dz = \frac{1}{2\pi}\Delta_c \arg f(z),$$

where z is the number of zeros and p the number of poles of $f(z)$ inside C, counting multiplicities, and $\Delta_c \arg f(z)$ denotes the change in argument of $f(z)$ as z describes C once in the positive direction.

Proof. *See [7].*

In order to calculate $N(T)$ we will apply the theorem to the Riemann xi function $\xi(s)$. The result will be the same as that to $\zeta(s)$, since as we saw in chapter 1 the zeros of $\xi(s)$ are the nontrivial zeros of $\zeta(s)$.

The contour C we will consider will be the positively oriented rectangle whose vertices are $-1, 2, 2+iT$ and $-1+iT$. We now divide C into three sub-contours; $C_1 := \{\sigma + it \in \mathbb{C} : -1 \leq \sigma \leq 2, t = 0\}$, $C_2 := \{\sigma + it \in \mathbb{C} : \sigma = 2, 0 \leq t \leq T\} \cup \{\sigma + it \in \mathbb{C} : \frac{1}{2} \leq \sigma \leq 2, t = T\}$ and $C_3 := \{\sigma + it \in \mathbb{C} : -1 \leq \sigma \leq \frac{1}{2}, t = T\} \cup \{\sigma + it \in \mathbb{C} : \sigma = -1, 0 \leq t \leq T\}$. By the argument principle we have

$$N(T) := \frac{1}{2\pi}\Delta_c \arg(\xi(s)) = \frac{1}{2\pi}(\Delta_{C_1} \arg(\xi(s)) + \Delta_{C_2} \arg(\xi(s)) + \Delta_{C_3} \arg(\xi(s))).$$

Let's proceed to calculate the argument change of $\xi(s)$ along C_1,C_2 and C_3.

First of all, since $\xi(s)$ takes real values when restricted to $0 < Re(s) < 1$, as we saw in chapter 1, we get $\Delta_{C_1} arg(\xi(s)) = 0$.

Since $\xi(s)$ satisfy the relations $\xi(s) = \xi(1-s)$ and $\xi(\bar{s}) = \overline{\xi(s)}$ for $0 < Re(s) < 1$ (See theorems 1.4 and 1.6), we have that

$$\xi(s) = \xi(1-s) = \overline{\xi(1-\bar{s})}.$$

Therefore, looking at the definitions of C_2 and C_3, we find that the argument changes of $\xi(s)$ along C_2 and C_3 are the same. Therefore,

$$N(T) = \frac{1}{\pi}\Delta_{C_2} \arg(\xi(s)). \tag{4.1}$$

From the definition of $\xi(s)$ and the Reduction formula for the Gamma function $\Gamma(s)$ (see theorem 1.4 and proposition 1.2), we have that

$$\begin{aligned}\xi(s) &= \frac{1}{2}s(s-1)\pi^{-\frac{1}{2}s}\Gamma\left(\frac{s}{2}\right)\zeta(s) \\ &= (s-1)\pi^{-\frac{1}{2}s}\Gamma\left(\frac{s}{2}+1\right)\zeta(s).\end{aligned} \tag{4.2}$$

We now calculate the argument changes along C_2 on each of the four functions in $\xi(s)$ in equation (4.2), and then add them to obtain $\Delta_{C_2} arg(\xi(s))$.

For $s-1$ we have

$$\begin{aligned}\Delta_{C_2}\arg(s-1) &= \arg\left(\frac{1}{2}+iT-1\right)-\arg(2-1) \\ &= \arg\left(-\frac{1}{2}+iT\right)-\arg(1) \\ &= \arg\left(-\frac{1}{2}+iT\right) \\ &= \frac{\pi}{2}+\arctan\left(\frac{1}{2T}\right) \\ &= \frac{\pi}{2}+O\left(\frac{1}{T}\right),\end{aligned} \tag{4.3}$$

where the last equality follows from the Taylor series for $\arctan\left(\frac{1}{2T}\right)$ for $T \geq \frac{1}{2}$, which is

$$\arctan\left(\frac{1}{2T}\right) = \sum_{n=0}^{\infty}\frac{(-1)^n}{2n+1}(2T)^{-2n-1}.$$

Now, for $\pi^{-\frac{s}{2}}$ we have:

$$\begin{aligned}\Delta_{C_2}\arg(\pi^{-\frac{s}{2}}) &= \Delta_{C_2}\arg(e^{-\frac{s}{2}\log\pi}) \\ &= \arg(e^{\left(\frac{1}{4}-\frac{iT}{2}\right)\log\pi}) \\ &= \arg(e^{-\frac{iT}{2}\log\pi}) \\ &= -\frac{T}{2}\log\pi.\end{aligned} \tag{4.4}$$

For $\Gamma\left(\frac{s}{2}+1\right)$ we will make us of the Stirling series for $\log\Gamma(s)$ [2], which is an asymptotic expression for $\log\Gamma(s)$, given by:

$$\begin{aligned}\log\Gamma(s) &= \frac{1}{2}\ln(2\pi)+\left(s-\frac{1}{2}\right)\log s - s + \frac{1}{125} - \frac{1}{360s^3} + \frac{1}{1260s^5} - \dots \\ &= \frac{1}{2}\ln 2\pi + \left(s-\frac{1}{2}\right)\log s - s + O(|s|^{-1}).\end{aligned}$$

We therefore have that

$$\begin{aligned}\Delta_{C_2}\arg\left(\Gamma\left(\frac{s}{2}+1\right)\right) &= \arg\left(\Gamma\left(\frac{5}{4}+\frac{iT}{2}\right)\right)+\arg(\Gamma(2)) \\ &= \arg\left(\Gamma\left(\frac{5}{4}+\frac{iT}{2}\right)\right) \\ &= \Im\left(\log\left(\Gamma\left(\frac{5}{4}+\frac{iT}{2}\right)\right)\right) \\ &= \Im\left(\frac{1}{2}\ln(2\pi)+\left(\frac{3}{4}+\frac{iT}{2}\right)\log\left(\frac{5}{4}+\frac{iT}{2}\right)-\frac{5}{4}-\frac{iT}{2}+O\left(\frac{1}{T}\right)\right) \\ &= \frac{T}{2}Re\left(\log\left(\frac{5}{4}+\frac{iT}{2}\right)+\frac{3}{4}\Im\left(\log\left(\frac{5}{4}+\frac{iT}{2}\right)\right)-\frac{T}{2}+O\left(\frac{1}{T}\right)\right) \\ &= \frac{T}{2}\log\left(\frac{25}{16}+\frac{T^2}{4}\right)^{\frac{1}{2}}+\frac{3}{4}\left(\frac{\pi}{2}-\arctan\left(\frac{5}{2T}\right)\right)-\frac{T}{2}+O\left(\frac{1}{T}\right) \\ &= \frac{T}{2}\log\frac{T}{2}-\frac{T}{2}+\frac{3\pi}{8}+O\left(\frac{1}{T}\right). \qquad (4.5)\end{aligned}$$

Looking at equations (4.1), (4.3), (4.4) and (4.5), we finally obtain

$$\begin{aligned}N(T) &= \frac{1}{\pi}\Delta_{C_2}\arg(\xi(s)) \\ &= \frac{1}{\pi}\left(\frac{\pi}{2}+O\left(\frac{1}{T}\right)-\frac{T}{2}\log\pi+\frac{T}{2}\log\frac{T}{2}-\frac{T}{2}+\frac{3\pi}{8}+O\left(\frac{1}{T}\right)+\Delta_{C_2}\arg(\zeta(s))\right) \\ &= \frac{T}{2\pi}\log\left(\frac{T}{2\pi}\right)-\frac{T}{2\pi}+\frac{7}{8}+O\left(\frac{1}{T}\right)+\frac{1}{\pi}\arg\left(\zeta\left(\frac{1}{2}+iT\right)\right).\end{aligned}$$

4.1.1 Smooth and oscillatory parts of $N(T)$

The counting function can be decomposed as follows:

$$N(T) = \langle N(T)\rangle + N_{fl}(T),$$

where $\langle N(T)\rangle$ and $N_{fl}(T)$ are interpreted as the smooth and fluctuating parts, respectively, of the counting function, where [6]

$$\langle N(T)\rangle = \frac{T}{2\pi}\log\left(\frac{T}{2\pi}\right) - \frac{T}{2\pi} + \frac{7}{8} + O\left(\frac{1}{T}\right) \tag{4.6}$$

and

$$N_{fl}(T) = \frac{1}{\pi} arg\left(\zeta\left(\frac{1}{2}+iT\right)\right). \tag{4.7}$$

This can be seen from the fact that $\langle N(T)\rangle$ is a smooth increasing function, while $N_{fl}(T)$ is an oscillating function taking values between -1 and 1.

It will be of great interest to calculate $N_{fl}(T)$ since this function will be later compared to the fluctuating part of the counting function for the energy levels in a quantum chaotic system.

To calculate $N_{fl}(T)$ we will use the Euler product expression for $\zeta(s)$ which, as must be noted, only coincides with the extended Riemann Zeta function for $Re(s) > 1$, since it diverges for other values. However, the following expression is formally exact [6]:

$$\begin{aligned}
N_{fl}(T) &= \frac{1}{\pi} arg\left(\zeta\left(\frac{1}{2}+iT\right)\right) \\
&= \frac{1}{\pi}\Im\left(\log\left(\zeta\left(\frac{1}{2}+iT\right)\right)\right) \\
&= \frac{1}{\pi}\Im\left(\log\left(\prod_{p \text{ prime}}\left(\frac{1}{1-p^{-\left(\frac{1}{2}+iT\right)}}\right)\right)\right) \\
&= -\frac{1}{\pi}\Im\left(\log\left(\prod_{p \text{ prime}}\left(1-p^{-\left(\frac{1}{2}+iT\right)}\right)\right)\right) \\
&= -\frac{1}{\pi}\Im\sum_{p \text{ prime}}\log\left(1-p^{-\frac{1}{2}-iT}\right) \\
&= -\frac{1}{\pi}\sum_{p \text{ prime}}\Im\left(\log\left(1-e^{\left(-\frac{1}{2}-iT\right)\ln p}\right)\right),
\end{aligned}$$

where by using the Taylor series for $\log(1+s)$, $|s| \leq 1$, $s \neq -1$, which is equal to

$\log(1+s) = \sum_{m=1}^{\infty} \frac{(-1)^{m+1}}{m} x^m$, we obtain

$$\begin{aligned} N_{fl}(T) &= -\frac{1}{\pi} \sum_{p \text{ prime}} \Im \left(\sum_{m=1}^{\infty} \frac{(-1)^{m+1}}{m} \left(-e^{\left(-\frac{1}{2}-iT\right)\ln p} \right)^m \right) \\ &= -\frac{1}{\pi} \sum_{p \text{ prime}} \sum_{m=1}^{\infty} \frac{(-1)^{2m+1} e^{-\frac{1}{2} m \ln p}}{m} \Im(-e^{-imT\ln p}) \\ &= -\frac{1}{\pi} \sum_{p \text{ prime}} \sum_{m=1}^{\infty} \frac{-e^{-\frac{1}{2} m \ln p}}{m} \sin(mT\ln p) \end{aligned}$$

$$\Rightarrow N_{fl}(T) = -\frac{1}{\pi} \sum_{p \text{ prime}} \sum_{m=1}^{\infty} \frac{-e^{-\frac{1}{2} m \ln p}}{m} \sin(mT\ln p). \tag{4.8}$$

Altough it is a divergent series, the first primes are usually used to give an excellent approximation of $N_{fl}(T)$ [6], as we can see in the next graphic due to Berry and Keating [6].

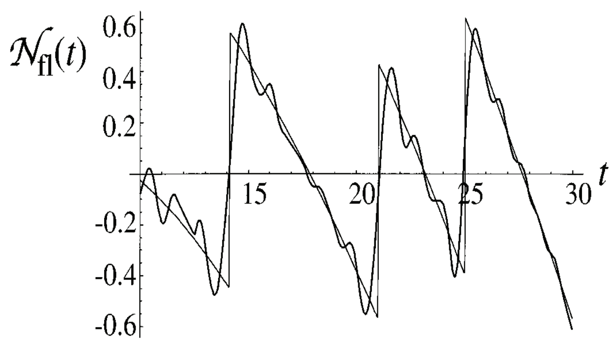

Figure 4.1: Thick line: Divergent series for the counting function fluctuations $\mathcal{N}_{fl}$ of the Riemann zeros, including all values of m and the first 50 primes p. Thin line: Exact calculation of $\mathcal{N}_{fl}$. Taken with permission from [6].

In the next section we will derive the counting function, due to Gutzwiller [5], of energy levels in a quantum chaotic system. A comparison will be made between both $\langle N(T)\rangle$ and $N_{fl}(T)$, and the corresponding smooth and fluctuating part of the energy counting function. We will also talk about what to expect from the Riemann Hamiltonian based on these similarities.

4.2 Gutzwiller Trace formula and the counting function of energy levels

Having derived to counting function for the zeros of $\zeta(s)$ in the last section we will compare it to the counting function of eigenvalues from a quantum chaotic system. In order to do so, we will show a proof of Gutzwiller Trace formula, which is a formula derived by Martin Gutzwiller that serves to calculate the density of states of a nonintegrable quantum system. Then we will proceed to derive the counting function $\mathcal{N}(E)$ for the energy levels of the system i.e.,

$$\mathcal{N}(E) = |E_n : E_n \text{ is an eigenenergy of the system and } E_n < E|.$$

To this end we will follow Stöckmann's and Gutzwiller's approach in [18] and [5] respectively. But before we can start to say anything regarding this topic, one important question need to be addressed.

4.2.1 What is quantum chaos?

Classically, we say a dynamical system is chaotic if it displays exponentially sensitive dependence on initial conditions. By this we mean the following: suppose $x(0) := (x_1(0), \ldots, x_n(0)$ is the vector which denotes the initial variables of a dynamical system in n dimensions at time $t = 0$. For example if we consider a a system of N particles in three dimensions, then this vector must have $6N$ components corresponding to both the space and momentum coordinates of each particle. Now, consider a nearby vector $y(0) := x(0) + \eta(0)$. Suppose the evolution in time of the dynamical system is given by $x(t) = F(x(0), t)$ for some function F. If in the limit of both $\|\eta(0)\| \to 0$ and large t, we have that

$$\frac{\|\eta(t)\|}{\|\eta(0)\|} \sim e^{\lambda t}, \qquad \lambda > 0,$$

then we say that the dynamical system is chaotic [35]. The lambda term λ is usually called the Lyapunov exponent. There are alternate ways of defining chaos in a dynamical system, however the essence of the definitions is always the same: sensitive dependence on the initial conditions, meaning that an small variation in initial conditions are exponentially amplified in time [5].

On the other hand, and where the problem in our discussion lies is that using the same definition of chaos for a quantum system is a nonsense. From Heisenberg"s uncertainty principle $\Delta x \Delta p \geq \frac{1}{2}\hbar$, a precise determination of the initial conditions of the system is impossible. This, together with the fact that the Schrödinger equation is a linear equation, led many physicists to question if quantum chaos is a relevant concept at all [18].

However, Bohr's Correspondence principle states that quantum mechanics reproduces classical mechanics in the semiclassical region, which is the limit of large quantum numbers, and this transition is continuous. Hence, for any classical dynamical system, including chaotic ones, there must exist a quantum system which resembles the classical one in the semiclassical limit. Therefore, as Stöckmann states *"Today the term 'quantum chaos'is generally understood to comprise all problems concerning the quantum mechanical behaviour of classically chaotic systems"*.

With this in mind we are now ready to talk about quantum chaotic systems without being ambiguous.

4.2.2 Density of states

We are interested in deriving an expression for the counting function $N(E)$ of the energies of a quantum system up to a given $E > 0$. To do this we will first consider the density of states $\rho(E)$ of the system defined as $\rho(E) = \sum_{n \in \mathbb{N}} \delta(E - E_n)$, where δ is the Dirac delta function. The counting function will be given by the relation $\rho(E) = \frac{d\mathcal{N}(E)}{dE}$, since the counting function could be viewed as a sum of unit step functions, and the derivative of a unit step function is a delta of Dirac.

First, note that the function

$$f(E) = \frac{\epsilon}{\pi} \frac{1}{E^2 + \epsilon^2},$$

for $\epsilon > 0$ behaves as the delta of Dirac in the limit $\epsilon \to 0$: For $E \neq 0$, is clear that

$$\lim_{\epsilon \to 0} \frac{\epsilon}{\pi} \frac{1}{E^2 + \epsilon^2} = 0,$$

whereas, if $E = 0$ we have that

$$\lim_{\epsilon \to 0} \frac{\epsilon}{\pi} \frac{1}{E^2 + \epsilon^2} = \infty,$$

which follows easily from L'Hôpital's rule. We only need to check that

$$\int_a^b \lim_{\epsilon\to 0}\frac{\epsilon}{\pi}\frac{1}{E^2+\epsilon^2}dE = \chi_{(a,b)}(0) = \begin{cases} 1 & \text{if } 0\in(a,b) \\ 0 & otherwise \end{cases}.$$

Now, by uniform convergence, we can interchange the limit and the integral, hence

$$\begin{aligned} \int_a^b \lim_{\epsilon\to 0}\frac{\epsilon}{\pi}\frac{1}{E^2+\epsilon^2}dE &= \lim_{\epsilon\to 0}\int_a^b \frac{\epsilon}{\pi}\frac{1}{E^2+\epsilon^2}dE \\ = \lim_{\epsilon\to 0}\frac{1}{\pi}\arctan\left(\frac{E}{\epsilon}\right)\Big|_a^b &= \chi_{(a,b)}(0). \end{aligned}$$

Therefore, we can write the density of states as

$$\begin{aligned} \rho(E) &= \sum_n \lim_{\epsilon\to 0}\frac{\epsilon}{\pi}\frac{1}{(E-E_n)^2+\epsilon^2} \\ &= -\frac{1}{\pi}\lim_{\epsilon\to 0} Im\left(\sum_n \frac{E-E_n-i\epsilon}{(E-E_n)^2+\epsilon^2}\right) \\ &= -\frac{1}{\pi}Im\left(\sum_n \frac{1}{E-E_n+i\epsilon}\right). \end{aligned}$$

For simplicity we write this last expression as

$$\rho(E) = -\frac{1}{\pi}Im\sum_n \frac{1}{E-E_n},$$

and we understand, whenever an expression like this is encountered in the next sections, that E has an infinitesimally small imaginary part.

Now, since the E_n are the eigenvalues of the Hamiltonian of the system H, we have that $E-E_n$ are the eigenvalues of $E-H$ and subsequently $\frac{1}{E-E_n}$ are the eigenvalues of $\frac{1}{E-H}$. Since the trace of an operator is equal to the sum of its eigenvalues, we deduce that

$$p(E) = -\frac{1}{\pi}Im\left(Tr\left(\frac{1}{E-H}\right)\right). \tag{4.9}$$

We can also express the density of states in terms of the quantum mechanical Green's function corresponding to the Schrödinger equation of a system.

It is given by

$$G(q_A, q_B, E) = \sum \frac{\psi_n^*(q_A)\psi_n(q_B)}{E - E_n},$$

where the $\psi_n(q)$ are the eigenfunctions of the Hamiltonian corresponding to the eigenvalue E_n where

$$\begin{aligned}
\sum_n \frac{\psi_n^*(q_A)\psi_n(q_B)}{E - E_n} &= \sum_n \langle \psi_n(q)|q_A\rangle \frac{1}{E - E_n} \langle q_B|\psi_n(q)\rangle \\
&= \int\int \sum_n \langle q_A|q\rangle \langle q|\psi_n\rangle \frac{1}{E - E_n} \langle \psi_n|q'\rangle \langle q'|q_B\rangle \, dqdq' \\
&= \int\int \langle q_A|q\rangle \langle q| \sum_n |\psi_n\rangle \langle \psi_n| \frac{1}{E - H} |q'\rangle \langle q'|q_B\rangle \, dqdq' \\
&= \langle q_A| \frac{1}{E - H} |q_B\rangle \,,
\end{aligned}$$

because of the completeness of $|q\rangle$ and $|\psi_n\rangle$. And then by the equation (4.9) we have

$$p(E) = -\frac{1}{\pi} Im \left(\int G(q, q, E) dq \right).$$

So now we will look for an expression for the trace of the Green function.

4.2.3 Quantum mechanical propagator and Feynman path integral

In this section we will find a relation between the Green function and the quantum mechanical propagator and derive an expression for it in the semiclassical limit by means of the Feynman path integral. This expression will be valid for infinitesimally small times, but then we will show that is also valid for arbitrary times.

In quantum physics, the propagator $K(q_A, q_B, t)$ is a function that gives the probability density $|K(q_A, q_B, t)|^2$, for a particle to reach the position q_B at a time t after starting in a position q_A at time $t = 0$, $K(q_A, q_B, t)$ is zero for $t < 0$, and for $t \geq 0$ is given by $K(q_A, q_B, t) = \langle q_B|U(t)|q_A\rangle$ where $U(t) = e^{-\frac{i}{\hbar}Ht}$ is the time-evolution operator.

First, lets note that the time Fourier transform of the propagator is equal to the Green function. We have

$$\int_{-\infty}^{\infty} K(q_A, q_B, t) e^{\frac{i}{\hbar}Et} dt = \int_0^{\infty} \langle q_B| \, e^{-\frac{iHt}{\hbar}} \, |q_A\rangle \, e^{\frac{i}{\hbar}Et} dt$$

$$= \int_0^\infty \int \delta(q_B - q) e^{-\frac{-iHt}{\hbar}} \delta(q_A - q) dq (e^{\frac{i}{\hbar}Et}) dt,$$

By Fubini's theorem [9], the integrals can be interchanged, yielding

$$\begin{aligned} \int_{-\infty}^\infty K(q_A, q_B, t) e^{\frac{i}{\hbar}Et} &= \int \int_0^\infty \delta(q_B - q) e^{-\frac{-iHt}{\hbar}} \delta(q_A - q) e^{\frac{i}{\hbar}Et} dt dq \\ &= \int \delta(q_B - q) \int_0^\infty e^{-\frac{-i}{\hbar}(E-H)t} dt \delta(q_A - q) dq. \end{aligned}$$

Recalling that we have assumed that E has a small imaginary part, we deduce that the inside integral converges. Hence,

$$\begin{aligned} \int_{-\infty}^\infty K(q_A, q_B, t) e^{\frac{i}{\hbar}Et} &= \int \delta(q_B - q) \left(\frac{-\hbar}{i} \frac{1}{E - H} \right) \delta(q_A - q) dq \\ &= \frac{-\hbar}{i} G(q_A, q_B, E). \end{aligned}$$

Therefore,

$$G(q_A, q_B, E) = \frac{-i}{\hbar} \int_0^\infty K(q_A, q_B, t) e^{2\pi i \frac{E}{\hbar} t} dt.$$

Now, by diving the time t into N smaller intervals of length $\tau = \frac{t}{N}$, and by noting that the time-evolution operator satisfies the relation $U(t) = (e^{-i\frac{H\tau}{\hbar}})^N = (U(\tau))^N$, we see that the propagator can be written as:

$$K(q_A, q_B, t) = \int \langle q_B | U(\tau) | q_{N-1} \rangle \ldots \langle q_1 | U(\tau) | q_A \rangle \, dq_1 \ldots dq_{N-1}. \tag{4.10}$$

We will now look for an expression for $\langle q_B | U(\tau) | q_C \rangle$ in the limit for large values of N, and hence very small τ.

For this we will consider the Hamiltonian to be $H = \frac{p^2}{2m_e} + V(q)$. Using the Baker-Campbell-Haussdorff formula for two operators X and Y [33]:

$$e^X e^Y = e^{X + Y + \frac{1}{2}[X,Y] + \frac{1}{12}[X,[X,Y]] - \frac{1}{12}[Y,[X,Y]] + \ldots}, \tag{4.11}$$

we have, in the limit of very small τ, that

$$U(\tau) = e^{-\frac{i\tau}{\hbar}(\frac{p^2}{2m} + V(q))} \approx e^{\frac{-i\tau}{\hbar}\frac{p^2}{2m}} e^{\frac{-i\tau}{\hbar}V(q)}.$$

Thus,

$$\langle q_B|U(\tau)|q_C\rangle \approx \langle q_B|e^{-\frac{i\tau}{\hbar}\frac{p^2}{2m}}|q_C\rangle\, e^{-\frac{i\tau}{\hbar}V(q_A)},$$

Where

$$\begin{aligned}
\langle q_B|e^{-\frac{i\tau}{\hbar}\frac{p^2}{2m}}|q_C\rangle &= \int \delta(q_B-q)e^{-\frac{i\tau p^2}{2m\hbar}}\delta(q_C-q)dq \\
&= \int \delta(q_B-q)e^{-\frac{i\tau p^2}{2m\hbar}}\left(\int \frac{1}{(2\pi\hbar)^d}e^{\frac{i}{\hbar}(q_C-q)p}dp\right)dq \\
&= \left(\frac{1}{2\pi\hbar}\right)^d \int e^{-\frac{i\tau p^2}{2m\hbar}}e^{\frac{i}{\hbar}(q_C-q_B)p}dp \\
&= \left(\frac{1}{2\pi\hbar}\right)^d e^{\frac{i}{\hbar}(q_C-q_B)p}\int e^{\frac{i}{\hbar}(i(\frac{\tau}{2m})^{\frac{1}{2}})p+\frac{q_C-q_B}{i}(\frac{m}{2\tau})^{\frac{1}{2}}} \\
&= \left(\frac{1}{2\pi\hbar}\right)^d\left(\frac{1}{i}\left(\frac{2m}{\tau}\right)^{\frac{1}{2}}\right)^d e^{\frac{im}{2\tau\hbar}(q_C-q_B)^2}\int e^{\frac{i}{\hbar}x^2}dx,
\end{aligned}$$

where in the second step we replaced $|q_C\rangle$ by its Fourier representation $|q_C\rangle = \delta(q_C - q) = \frac{1}{(2\pi\hbar)^d}\int e^{\frac{i}{\hbar}(q_C-q)p}dp$, where d is the dimension of the system; and in the last step we used the change of variables: $x = i\sqrt{\frac{\tau}{2m}}p + \frac{q_C-q_B}{i}\sqrt{\frac{m}{2\tau}})$. Now, the last integral is in d components from $-\infty$ to ∞, and therefore is a product of d Fresnel integrals (See appendix B.1). Therefore, we have:

$$\begin{aligned}
\langle q_B|e^{-\frac{i\tau}{\hbar}\frac{p^2}{2m}}|q_C\rangle &= \left(\frac{1}{2\pi\hbar}\right)^d\left(\frac{1}{i}\sqrt{\frac{2m}{\tau}}\right)^d e^{\frac{im}{2\tau\hbar}(q_C-q_B)^2}(\sqrt{i\hbar\pi})^d \\
&= \left(\frac{m}{2\pi i\hbar\tau}\right)^{\frac{d}{2}} e^{\frac{im}{2\hbar\tau}(q_C-q_B)^2}.
\end{aligned}$$

Hence, the propagator can be written as:

$$\begin{aligned}
\langle q_B|U(\tau)|q_C\rangle &\approx \left(\frac{m}{2\pi i\hbar\tau}\right)^{\frac{1}{2}} e^{\frac{im}{2\hbar\tau}(q_C-q_B)^2}e^{-\frac{i\tau}{\hbar}V(q_C)} \\
&\approx \left(\frac{m}{2\pi i\hbar\tau}\right)^{\frac{1}{2}} e^{\frac{i}{\hbar}\left(\frac{m}{2\tau}(q_C-q_B)^2-\tau V\left(\frac{q_B+q_C}{2}\right)\right)}. \qquad (4.12)
\end{aligned}$$

Using the Baker-Campbell-Haussdorff formula again and substituting $V(q_C)$ by $V\left(\frac{q_B+q_C}{2}\right)$ assuming the potential is "smooth enough ". In [5] it is discussed that this substitution is essential especially when the Hamiltonian contains a vector potential term.

We now define $W_{BC}(\tau)$ as:

$$\begin{aligned} W_{BC}(\tau) &= W(q_C, q_B, \tau) \\ &= \frac{m}{2\tau}(q_C - q_B)^2 - \tau V\left(\frac{q_C + q_B}{2}\right). \end{aligned}$$

This function has a classical interpretation: For very small τ we can write $\frac{q_A - q_B}{C}$ as $\dot{q_A}$ or $-\dot{q_B}$. Hence, it follows that

$$\begin{aligned} W_{BC}(\tau) &= \tau\left(\frac{m}{2}(\dot{q_C})^2 - V\left(\frac{q_B + q_C}{2}\right)\right) \\ &= \int_0^\tau L(q, \dot{q})dt, \end{aligned}$$

where $L(q, \dot{q}) = \frac{m}{2}\dot{q}^2 - V(q)$ is the classical Lagrangian. Therefore $W_{BC}(\tau)$ can be seen as Hamilton's principal function (see appendix A.3).

Furthermore, we have:

$$\begin{aligned} \frac{\partial^2 W_{BC}(\tau)}{\partial q_{C_i}\partial q_{B_j}} &= \frac{\partial^2}{\partial q_{C_i}\partial q_{B_j}}\left(\frac{m}{2\tau}\sum_{n=1}^{d}(q_{C_n} - q_{B_n})^2 - \tau V\left(\frac{q_C + q_B}{2}\right)\right) \\ &= \frac{m}{\tau}\frac{\partial}{\partial q_{B_j}}(q_{C_i} - q_{B_i}) - \tau\frac{\partial^2}{\partial q_{C-i}\partial q_{B_j}}V\left(\frac{q_C + q_B}{2}\right) \\ &= -\frac{m}{\tau}\delta_{ij} - \tau\frac{\partial^2}{\partial q_{C_i}\partial q_{B_j}}V\left(\frac{q_C + q_B}{2}\right), \end{aligned} \tag{4.13}$$

Where

$$\delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}.$$

In the limit of very small τ the second term in (3.7) vanishes. Therefore:

$$\frac{\partial^2 W_{BC}(\tau)}{\partial q_{C_i}\partial q_{B_j}} \approx \begin{cases} \frac{m}{\tau} & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}.$$

We now define the Van Vleck determinant D_{BC} as the $d\times d$ matrix $D_{BC} := \left(-\frac{\partial^2 W_{BC}(\tau)}{\partial q_{C_i}\partial q_{B_j}}\right)_{1\leq i,j\leq d}$.

By all of the above we can write equation (4.12) as:

$$\langle q_B|U(\tau)|q_C\rangle = \left(\frac{1}{2\pi i\hbar}\right)^{\frac{d}{2}} |D_{BC}|^{\frac{1}{2}} e^{\frac{i}{\hbar}W_{BC}(\tau)}. \tag{4.14}$$

Inserting this expression in equation (4.10) in the limit $N \to \infty$ we arrive at the Feynman path integral formulation for the quantum mechanical propagator,

$$\begin{aligned} K(q_A, q_B, t) &= \lim_{N\to\infty} \left(\frac{1}{2\pi\hbar i}\right)^{\frac{Nd}{2}} \int \prod_{i=0}^{N-1} |D_{i,i+1}|^{\frac{1}{2}} e^{\frac{i}{\hbar}\sum_{i=0}^{N-1} W_{i,i+1}} \\ &= \int \mathcal{D}(q) e^{\frac{i}{\hbar}\int_0^t L(q,\dot{q})dt}, \end{aligned}$$

where $q_0 = q_A$ and $q_N = q_B$ $\square$.

4.2.4 The propagator in the semiclassical limit

In this section we will show that equation (4.14) is still valid for an arbitrary time τ in the semiclassical limit. So now, instead of considering $K(q_A, q_B, \tau)$ we will consider $K(q_A, q_B, 2\tau)$ and show that equation (4.14) still applies.

We start by writing $K(q_A, q_B, 2\tau)$ as:

$$\begin{aligned} K(q_A, q_B, 2\tau) &= \int \langle q_B|U(\tau)|q_C\rangle \langle q_C|U(\tau)|q_A\rangle \, dq_C \\ &= \left(\frac{1}{2\pi\hbar i}\right)^{d} \int |D_{BC}|^{\frac{1}{2}} |D_{CA}|^{\frac{1}{2}} e^{\frac{i}{\hbar}(W_{BC}(\tau)+W_{CA}(\tau))} dq_C. \end{aligned}$$

This integral will be calculated by using the stationary phase approximation (see Appendix B.2). In this case the phase $\Phi(q_C)$ of the exponential function and its derivatives are given by:

$$\begin{aligned} \Phi(q_C) &= \frac{1}{\hbar}(W_{BC}(\tau) + W_{CA}(\tau)) \\ \Phi'(q_C) &= \frac{1}{\hbar}\left(\frac{\partial W_{BC}(\tau)}{\partial q_C} + \frac{\partial W_{CA}(\tau)}{\partial q_C}\right) \\ \Phi''(q_C) &= \frac{1}{\hbar}\left(\frac{\partial^2 W_{BC}(\tau)}{\partial q_C^2} + \frac{\partial^2 W_{CA}(\tau)}{\partial q_C^2}\right). \end{aligned}$$

Keeping in mind that we are integrating over the d components of q_C and therefore the second and third equation are a vector equation and a matrix equation respectively, where $\Phi''(q_C) = \frac{\partial^2\Phi(q_C)}{\partial q_C^2}$ is the Hessian matrix:

$$Hess(\Phi(q_C)) = \begin{pmatrix} \frac{\partial^2\Phi(q)}{\partial q_1^2} & \cdots & \frac{\partial^2\Phi(q)}{\partial q_1 \partial q_d} \\ \vdots & \ddots & \vdots \\ \frac{\partial^2\Phi(q)}{\partial q_d \partial q_1} & \cdots & \frac{\partial^2\Phi(q)}{\partial q_d^2} \end{pmatrix}_{q=q_C}, \tag{4.15}$$

Where the stationary point q_C is given by equation (A.9):

$$\frac{\partial W_{BC}}{\partial q_C} + \frac{\partial W_{CA}}{\partial q_C} = -P_C^{(BC)} + P_C^{(CA)} = 0, \tag{4.16}$$

where $P_C^{(CA)}$ is the momentum at the end of the (4.16) trajectory from q_A to q_C, and $P_C^{(BC)}$ is the momentum at the beginning of the trajectory from q_C to q_B. This condition implies that both momenta are equal. Therefore the impulse on the trajectory from q_A to q_B must be continuous at q_C, which means that the trajectory from q_A to q_B via q_C is classically allowed. And since we will only consider classical trajectories, it means that we can also consider the classical interpretation of the W function i.e., Hamilton's principal function. Using equation (A.8) we have:

$$\begin{aligned} W_{BC}(\tau) + W_{CA}(\tau) &= \int_{q_A}^{q_C} p dq - E\tau + \int_{q_C}^{q_B} p dq - E\tau \\ &= \int_{q_A}^{q_B} p dq - 2E\tau \\ &= W_{BA}(2\tau). \end{aligned} \tag{4.17}$$

The stationary phase approximation (see Appendix B.2) now yields:

$$K(q_A, q_B, 2\tau) = \left(\frac{1}{2\pi i\hbar}\right)^{\frac{d}{2}} \left(\frac{\left|\frac{-\partial^2 W_{BC}}{\partial q_B \partial q_C}\right| \left|\frac{-\partial^2 W_{CA}}{\partial q_C \partial q_A}\right|}{\left|\frac{\partial^2 W_{BC}}{\partial q_C^2} + \frac{\partial^2 W_{CA}}{\partial q_C^2}\right|}\right)^{\frac{1}{2}} e^{\frac{i}{\hbar} W_{BA}(2\tau)}. \tag{4.18}$$

We will now proceed to simplify the prefactor in order to find the desired result. We start by differentiating the stationary point condition, equation (4.16), with respect to q_C while keeping the starting point q_A fixed, and then multiply both sides of the equation by $\frac{\partial^2 W_{BA}}{\partial q_B \partial q_A}$:

$$\begin{aligned} 0 &= \frac{-\partial^2 W_{BA}}{\partial q_B \partial q_A}\left(\frac{\partial}{\partial q_C}\left(\frac{\partial W_{BC}}{\partial q_C}+\frac{\partial W_{CA}}{\partial q_C}\right)\right) \\ &= \frac{-\partial^2 W_{BA}}{\partial q_B \partial q_A}\left(\frac{\partial^2 W_{BC}}{\partial q_C^2}+\frac{\partial^2 W_{BC}}{\partial q_C \partial q_B}\cdot\frac{\partial q_B}{\partial q_C}+\frac{\partial^2 W_{CA}}{\partial q_C^2}\right). \end{aligned}$$

Therefore,

$$\frac{-\partial^2 W_{BA}}{\partial q_B \partial q_A}\left(\frac{\partial^2 W_{BC}}{\partial {q_C}^2}+\frac{\partial^2 W_{CA}}{\partial {q_C}^2}\right)=\frac{\partial^2 W_{BA}}{\partial q_B \partial q_A}\cdot\frac{\partial^2 W_{BC}}{\partial q_C \partial q_B}\cdot\frac{\partial q_B}{\partial q_C}.$$

We insert two minus signs on the right hand side of the equation, and take the determinant on both sides:

$$\begin{aligned} \left|\frac{-\partial^2 W_{BA}}{\partial q_B \partial q_A}\right|\left|\frac{\partial^2 W_{BC}}{\partial q_C^2}\right| &= \left|\frac{-\partial^2 W_{BC}}{\partial q_C \partial q_B}\right|\left|\frac{-\partial^2 W_{BA}}{\partial q_B \partial q_A}\cdot\frac{\partial q_B}{\partial q_C}\right| \\ &= \left|\frac{-\partial^2 W_{BC}}{\partial q_B \partial q_C}\right|\left|\frac{-\partial^2 W_{BA}}{\partial q_C \partial q_A}\right| \\ &= \left|\frac{-\partial^2 W_{BC}}{\partial q_B \partial q_C}\right|\left|\frac{-\partial^2 W_{CA}}{\partial q_C \partial q_A}\right|. \end{aligned}$$

In the last equality we have used the fact that $\frac{\partial W_{BA}}{\partial q_A}=\frac{\partial W_{CA}}{\partial q_A}$ which follows from equation (4.17). By the above equations we find the relation:

$$\left|\frac{\partial^2 W_{BC}}{\partial q_C^2}+\frac{\partial^2 W_{CA}}{\partial q_C^2}\right|=\frac{\left|\frac{-\partial^2 W_{BC}}{\partial q_B \partial q_C}\right|\left|\frac{-\partial^2 W_{CA}}{\partial q_C \partial q_A}\right|}{\left|\frac{-\partial^2 W_{BA}}{\partial q_B \partial q_A}\right|}. \tag{4.19}$$

Inserting this expression in equation (4.18) we find the desired result:

$$\begin{aligned} K(q_A, q_B, 2\tau) &= \left(\frac{1}{2\pi i\hbar}\right)^{\frac{d}{2}}\left|\frac{-\partial^2 W_{BA}}{\partial q_B \partial q_A}\right|^{\frac{1}{2}} e^{\frac{i}{\hbar}W_{BA}(2\tau)} \\ &= \left(\frac{1}{2\pi i\hbar}\right)^{\frac{d}{2}}|D_{BA}|^{\frac{1}{2}}\, e^{\frac{i}{\hbar}W_{BA}(2\tau)}. \end{aligned}$$

Nowhere in this section have we assumed that τ is small. Therefore, we can conclude that in the semiclassical limit i.e., in the limit $\hbar \to 0$, the above expression holds for arbitrarily large values of τ. However, there are two issues in the derivation of the last equation. First of all, we have only considered the stationary point q_C, i.e. we have only considered one possible classically allowed path. Because of this, when performing the stationary phase approximation we have to sum over all the classically allowed paths, because all those paths will contribute to the approximation of the integral. The second issue concerns the points along the trajectories in which the determinant of $\frac{\partial^2 W_{BA}}{\partial q_B \partial q_A}$ becomes singular. These points are called conjugate points. When such thing happens the stationary phase approximation breaks down. Gutzwiller addresses this issue [5], and finds that the formula is still valid if one adds a phase of $-\frac{\nu\pi}{2}$ to the exponential, where ν denotes the number of conjugate points along the trajectory.

This leads us to the final result for the semiclassical propagator:

$$K(q_A, q_B, t) = \left(\frac{1}{2\pi\hbar i}\right)^{\frac{d}{2}} \sum_r |D_{BA,r}|^{\frac{1}{2}} \exp\left(\frac{i}{\hbar} W_{BA,r}(t) - \frac{i\pi\nu_r}{2}\right),$$

where the summation is over all classically allowed trajectories from q_A to q_B.

4.2.5 The Green function in the semiclassical limit

In this section we will obtain an expression for the Green function in the semiclassical limit, which will help us in obtaining an expression for the density of states.

Recall that the relation between the Green function and the propagator was given by:

$$G(q_A, q_B, E) = -\frac{i}{\hbar} \int_0^\infty K(q_A, q_B, t) e^{\frac{iEt}{\hbar}} dt. \tag{4.20}$$

Inserting equation (4.18) into (4.20) we obtain:

$$\begin{aligned} G(q_A, q_B, E) &= -\frac{i}{\hbar} \int_0^\infty \left(\frac{1}{2\pi\hbar i}\right)^{\frac{d}{2}} \sum_r |D_{BA,r}|^{\frac{1}{2}} \exp\left(\frac{i}{\hbar} W_{BA,r}(t) - \frac{i\pi\nu_r}{2} + \frac{iEt}{\hbar}\right) dt \\ &= -\frac{i}{\hbar} \left(\frac{1}{2\pi\hbar i}\right)^{\frac{d}{2}} \sum_r e^{\frac{-i\pi\nu_r}{2}} \int_0^\infty |D_{BA,r}|^{\frac{1}{2}} \exp\frac{i}{\hbar}(W_{BA,r}(t) - Et) dt. \end{aligned}$$

This integral will be evaluated by means of the one-dimensional stationary phase approximation, where the phase of the exponential and its corresponding derivatives are given by:

$$\begin{aligned}\Phi(t) &= \frac{1}{\hbar}(W_{BA,r}(t) + Et) \\ \frac{d\Phi}{dt} &= \frac{1}{\hbar}\left(\frac{\partial W_{BA,r}}{\partial t} + E\right) \\ \frac{d^2\Phi}{dt^2} &= \frac{1}{\hbar}\frac{\partial^2 W_{BA,r}}{\partial t^2}.\end{aligned}$$

The stationary phase time t_o is given by the relation:

$$\left.\frac{\partial W_{BA,r}}{\partial t}\right|_{t=to} = -E \tag{4.21}$$

This implies that the time t_o is a function of q_A, q_B and E. Now, using equation ((A.9)) and noting that the phase at time t_o, $\Phi(t_o) = \frac{1}{\hbar}(W_{BA,r}(t_o) + Et_o)$ can be written as $\frac{1}{\hbar}S_r(q_A, q_B, E)$, see equation ((A.10)), we get the following expression for the Green function:

$$\begin{aligned}G(q_A, q_B, E) &= -\frac{i}{\hbar}\left(\frac{1}{2\pi i\hbar}\right)^{\frac{d}{2}}\sqrt{2\pi\hbar}\sum_r e^{\frac{-i\pi\nu_r}{2}}\left(\frac{|D_{BA,r}|}{\left|\frac{\partial^2 W_{BA,r}}{\partial t^2}\right|}\right)^{\frac{1}{2}} \\ &\quad\times\exp\left(\frac{i}{\hbar}S_r(q_A, q_B, E) + \frac{i\pi}{4}sgn\left(\frac{\partial^2 W_{BA,r}}{\partial t^2}\right)\right),\end{aligned} \tag{4.22}$$

where $sgn(x)$ denotes the sign function. The argument of the exponential depends now on the action and not on the principal function, and because of this we will now express the term $\frac{|D_{BA,r}|}{\left|\frac{\partial^2 W_{BA,r}}{\partial t^2}\right|}$ in terms of the action as well. But first we will find the sign of $\frac{\partial^2 W_{BA,r}}{\partial t^2}$ in the exponential.

If we differentiate equation (4.21) with respect to E, we obtain:

$$\frac{\partial^2 W_{BA,r}}{\partial t^2}\frac{\partial t_o}{\partial E} = -1,$$

Hence,

$$\frac{\partial^2 W_{BA,r}}{\partial t^2} = \left(\frac{\partial t_o}{\partial E}\right)^{-1}$$

where t_o can be expressed as the partial derivative of the action with respect to E,

$t_o = \frac{\partial S}{\partial E}$, see equation (A.11), and hence:

$$\frac{\partial^2 W_{BA,r}}{\partial t^2} = -\left(\frac{\partial^2 S}{\partial E^2}\right)^1. \tag{4.23}$$

Now, since we are considering the Hamiltonian $H = \frac{p^2}{2m} + V(q)$ and the trajectory to be classical we can write the momentum as $p = \sqrt{2m(E-V)}$. And since the differential dq points in the same direction as p, the inner product $p \cdot dq$ will always be positive. Hence, we can write the action as:

$$S(q_A, q_B, E) = \int_{q_A}^{q_B} p \cdot dq = \int_{q_A}^{q_B} \sqrt{2m(E-V)}|dq|. \tag{4.24}$$

Now, differentiating equation (4.24) two times with respect to E we obtain:

$$\begin{aligned} \frac{\partial^2 S}{\partial E^2} &= \frac{\partial}{\partial E}\left(\int_{q_A}^{q_B} \frac{1}{2}\sqrt{2m}(E-V)^{\frac{-1}{2}}|dq|\right) \\ &= -\frac{\sqrt{2m}}{4}\int_{q_A}^{q_B}(E-V)^{\frac{-3}{2}}|dq|, \end{aligned}$$

which is negative, since the integral is positive.

Therefore, by using equation (4.23), we find that $\frac{\partial^2 W_{BA,r}}{\partial t^2}$ is positive, which implies that:

$$\frac{i\pi}{4} sgn\left(\frac{\partial W_{BA,r}}{\partial t^2}\right) = \frac{i\pi}{4} sgn\left(-\left(\frac{\partial^2 S}{\partial E^2}\right)^{-1}\right) = \frac{i\pi}{4}. \tag{4.25}$$

Now, in order to write the determinant prefactor in equation (4.25) in terms of the action we will start by considering the phase at time t_o multiplied by $\hbar$, $\hbar\Phi(t_o) = W_{BA,r}(t_o) + Et_o = S_r(q_A, q_B, E)$. And now, differentiating this expression with respect to q_A and keeping in mind that we will then evaluate the resulting expression at $t = t_o$ we obtain:

$$\begin{aligned} \frac{\partial S_r}{\partial q_A} &= \frac{\partial W_{BA,r}}{\partial q_A} + \frac{\partial W_{BA,r}}{\partial t} \cdot \frac{\partial t_o}{\partial q_A} + E\frac{\partial t_o}{\partial q_A} \\ &= \frac{\partial W_{BA,r}}{\partial q_A} + \left(-E\frac{\partial t_o}{\partial q_A}\right) + E\frac{\partial t_o}{\partial q_A} \qquad (4.26) \\ &= \frac{\partial W_{BA,r}}{\partial q_A}. \qquad (4.27) \end{aligned}$$

Now, differentiating equation (4.26) with respect to q_B yields:

$$\begin{aligned} \frac{\partial^2 S_r}{\partial q_A \partial q_B} &= \frac{\partial^2 W_{BA,r}}{\partial q_A \partial q_B} + \frac{\partial^2 W_{BA,r}}{\partial q_A \partial t}\frac{\partial t_o}{\partial q_B} \\ &= \frac{\partial^2 W_{BA,r}}{\partial q_A \partial q_B} + \frac{\partial^2 W_{BA,r}}{\partial q_A \partial t}\frac{\partial^2 S_r}{\partial q_B \partial E}. \end{aligned} \tag{4.28}$$

On the other hand, by differentiating equation (4.21) with respect to q_A, we obtain

$$\frac{\partial^2 W_{BA,r}}{\partial q_A \partial t} + \frac{\partial^2 W_{BA,r}}{\partial t^2}\frac{\partial t_o}{\partial q_A} = 0,$$

which implies that

$$\begin{aligned} \frac{\partial^2 W_{BA,r}}{\partial q_A \partial t} &= \frac{\partial^2 W_{BA,r}}{\partial t^2}\frac{\partial t_o}{\partial q_A} \\ &= \left(\frac{\partial^2 S}{\partial E^2}\right)^{-1}\frac{\partial t_o}{\partial q_A} \quad \text{(using equation (4.21))} \\ &= \left(\frac{\partial^2 S}{\partial E^2}\right)^{-1}\frac{\partial^2 S}{\partial q_A \partial E} \quad \left(\text{since } t_o = \frac{\partial S}{\partial E}\right). \end{aligned} \tag{4.29}$$

Inserting equation (4.29) into (4.28) and rearranging terms we obtain:

$$\frac{\partial^2 W_{BA,r}}{\partial q_A \partial q_B} = \frac{\partial^2 S_r}{\partial q_A \partial q_B} - \left(\frac{\partial^2 S}{\partial E^2}\right)^{-1}\frac{\partial^2 S}{\partial q_A \partial E}\frac{\partial^2 S}{\partial q_B \partial E}.$$

On the other hand, since $D_{BA,r}$ is a $d \times d$ matrix which is equal to $\left|-\frac{\partial^2 W_{BA}}{\partial q_B \partial q_A}\right|$ and since $\frac{\partial^2 W_{BA,r}}{\partial t^2} = \left(-\frac{\partial^2 S_r}{\partial E^2}\right)^{-1}$ is a scalar quantity, we have that:

$$\begin{aligned} \frac{|D_{BA,r}|}{\left|\frac{\partial^2 W_{BA,r}}{\partial t^2}\right|} &= (-1)^{d+1}\frac{\partial^2 S_r}{\partial E^2}\cdot\left|\frac{\partial^2 W_{BA,r}}{\partial q_A \partial q_B}\right| \\ &= (-1)^{d+1}\frac{\partial^2 S_r}{\partial E^2}\left|\frac{\partial^2 S_r}{\partial q_A \partial q_B} - \frac{\partial^2 S_r}{\partial q_A \partial E}\cdot\frac{\partial^2 S_r}{\partial q_B \partial E}\Big/\frac{\partial^2 S_r}{\partial E^2}\right|. \end{aligned} \tag{4.30}$$

By using the relation for determinants, $\begin{pmatrix} A & B \\ C & D \end{pmatrix} = |A - BD^{-1}C||D|$ where A is a $N \times N$ matrix, B an $N \times M$ matrix, C an $M \times N$ matrix and D a nonsingular $M \times M$ matrix, which can be proved by simply taking the determinant at both sides of the relation

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} 1 & 0 \\ -D^{-1}C & 1 \end{pmatrix} = \begin{pmatrix} A - BD^{-1}C & B \\ 0 & D \end{pmatrix},$$

we find that equation (4.30) can be simplified to:

$$\frac{|D_{BA,r}|}{\left|\frac{\partial^2 W_{BA,r}}{\partial t^2}\right|} = (-1)^{d+1} \begin{pmatrix} \frac{\partial^2 S_r}{\partial q_A \partial q_B} & \frac{\partial^2 S_r}{\partial q_A \partial E} \\ \frac{\partial^2 S_r}{\partial q_B \partial E} & \frac{\partial^2 S_r}{\partial E^2} \end{pmatrix} = \begin{pmatrix} \frac{-\partial^2 S_r}{\partial q_A \partial q_B} & \frac{-\partial^2 S_r}{\partial q_A \partial E} \\ \frac{-\partial^2 S_r}{\partial q_B \partial E} & \frac{-\partial^2 S_r}{\partial E^2} \end{pmatrix}. \tag{4.31}$$

Whence follows by defining $\Delta_{BA,r} = \frac{|D_{BA,r}|}{|\partial^2 W_{BA,r}|}$ and by inserting equations (4.25) and (4.31) into equation (4.25), that the semiclassical Green function can be written as:

$$G(q_A, q_B, E) = -\frac{i}{\hbar}\left(\frac{1}{2\pi i \hbar}\right)^{\frac{(d-1)}{2}} \sum_r |\Delta_{BA,r}|^{\frac{1}{2}} e^{\frac{i}{\hbar}S_r(q_A,q_B,E) - \frac{i\pi\nu_r}{2}}. \tag{4.32}$$

4.2.6 Gutzwiller Trace formula

Using the expression for the Green function derived in the last section we can now calculate the density of states given by:

$$\begin{aligned} \rho(E) &= \sum_n \delta(E - E_n) \\ &= -\frac{1}{\pi} Im\left(\int G(q,q,E)dq\right), \end{aligned}$$

as we saw in a previous section.

We will now derive a semiclassical approximation for the trace $\int G(q,q,E)dq$.

Inserting equation (4.32) into this expression we obtain the following integral:

$$\int G(q,q,E)dq = -\frac{i}{\hbar}\left(\frac{1}{2\pi i \hbar}\right)^{\frac{(d-1)}{2}} \sum_r e^{-\frac{i\pi\nu_r}{2}} \int |\Delta_r|^{\frac{1}{2}} e^{\frac{i}{\hbar}S_r(q,q,E)} dq, \tag{4.33}$$

which we will evaluate by using once again the stationary phase approximation, where the phases of the exponential and its corresponding derivatives are given by:

$$\begin{aligned}
\Phi(q) &= \frac{1}{\hbar} S_r(q,q,E) \\
\Phi'(q) &= \frac{1}{\hbar}\left(\frac{\partial S_r}{\partial q_A}+\frac{\partial S_r}{\partial q_B}\right)\Bigg|_{q_A=q_B=q} \\
\Phi''(q) &= \frac{1}{\hbar}\left(\frac{\partial^2 S_r}{\partial q_A^2}+2\frac{\partial^2 S_r}{\partial q_A \partial q_B}+\frac{\partial^2 S_r}{\partial q_B^2}\right)\Bigg|_{q_A=q_B=q},
\end{aligned}$$

where the stationary point is given by the relation

$$\left(\frac{\partial S_r}{\partial q_A}+\frac{\partial S_r}{\partial q_B}\right)\Bigg|_{q_A=q_B=q} = -P_A|_{q_A=q}+P_B|_{q_B=q}=0,$$

which implies $(q_A, P_A) = (q_B, P_B)$. What this means is that the starting position and momentum must be the same as the end position and impulse. Hence, combined with the fact from previous sections that we were considering classical trajectories, we find that for finding the trace of the Green function we will only consider classical periodic orbits.

We now introduce a coordinate system in which $q_\parallel$ is the coordinate parallel to the trajectory and the rest of the $(d-1)$ coordinates $q_{\perp i}$, $i \in 1,\ldots,d-1$, are perpendicular to it. Now, the power series of the action $S(q,q,E)$ in terms of the perpendicular coordinates up to the quadratic terms is given by:

$$\begin{aligned}
S_r(q,q,E) &\approx S_r(q_\parallel,q_\parallel,E)+\frac{1}{2}\sum_{i,j} q_{\perp i}\left(\frac{\partial^2 S_r}{\partial q_{A\perp i}\partial q_{A\perp j}}+2\frac{\partial^2 S_r}{\partial q_{A\perp i}\partial q_{B\perp j}}+\frac{\partial^2 S_r}{\partial q_{B\perp i}\partial q_{B\perp j}}\right) q_{\perp j} \\
&= S_r(q_\parallel,q_\parallel,E)+\frac{1}{2} q_\perp^\top \left(\frac{\partial^2 S_r}{\partial q_{A\perp}\partial q_{A\perp}}+2\frac{\partial^2 S_r}{\partial q_{A\perp}\partial q_{B\perp}}+\frac{\partial^2 S_r}{\partial q_{B\perp}\partial q_{B\perp}}\right) q_\perp. \quad (4.34)
\end{aligned}$$

Since $S_r(q_\parallel, q_\parallel, E)$ is calculated from the action integral over a closed orbit, we have $S_r(q_\parallel, q_\parallel, E) = \oint P dq$ which is independent of $q_\parallel$. Therefore we can write the action as $S_r(q_\parallel, q_\parallel, E) = S_r(E)$.

On the other hand consider the determinant $|\Delta_r|$, which now can be written as:

$$|\Delta_r| = (-1)^{d+1}\begin{pmatrix} \frac{\partial^2 S_r}{\partial q_{A\parallel}\partial q_{B\parallel}} & \frac{\partial^2 S_r}{\partial q_{A\parallel}\partial q_{B\perp}} & \frac{\partial^2 S_r}{\partial q_{A\parallel}\partial q_E} \\ \frac{\partial^2 S_r}{\partial q_{A\perp}\partial q_{B\parallel}} & \frac{\partial^2 S_r}{\partial q_{A\perp}\partial q_{B\perp}} & \frac{\partial^2 S_r}{\partial q_{A\perp}\partial E} \\ \frac{\partial^2 S_r}{\partial q_{B\parallel}\partial q_E} & \frac{\partial^2 S_r}{\partial q_{B\perp}\partial E} & \frac{\partial^2 S_r}{\partial E^2} \end{pmatrix}. \quad (4.35)$$

As we shall see the second derivatives of the action which involve the parallel coordinates $q_{A\parallel}, q_{B\parallel}$ can be explicitly calculated, which will considerably simplify equation (4.35).

First, consider the Hamilton-Jacobi equation (see (A.13)) $E = H\left(\frac{\partial S_r}{\partial q_B}, q_B\right)$, and differentiate both sides with respect to E to get:

$$1 = \frac{\partial H}{\partial\left(\frac{\partial S_r}{\partial q_B}\right)} \cdot \frac{\partial^2 S_r}{\partial q_B \partial E} = \frac{\partial H}{\partial P_B}\frac{\partial^2 S_r}{\partial q_B \partial E} = \dot{q_B}\frac{\partial^2 S_r}{\partial q_B \partial E}. \tag{4.36}$$

Where we have used Hamilton's equations of motion (see equation (A.6)) and the equations for the partial derivatives of the action (see equation (A.12)).

Furthermore, since the position only varies along the trajectory, we have that $\dot{q_{B\perp}} = 0$, and thus equation (4.36) can be written as $\dot{q_{B\parallel}}\frac{\partial^2 S_r}{\partial q_{B\parallel}\partial E} = 1$, which implies that:

$$\frac{\partial^2 S_r}{\partial q_{B\parallel}\partial E} = \frac{1}{\dot{q_{B\parallel}}}. \tag{4.37}$$

Let's consider again the Hamilton-Jacobi equation $E = H\left(\frac{\partial S_r}{\partial q_B}, q_B\right)$, but this time differentiate both sides with respect to an arbitrary component q_{A_i} of q_A. We get:

$$\begin{aligned}\frac{\partial E}{\partial q_{A_i}} = 0 = \frac{\partial}{\partial q_{A_i}} H\left(\frac{\partial S_r}{\partial q_B}, q_B\right) &= \frac{\partial^2 S_r}{\partial q_{A_i}\partial q_B} \cdot \frac{\partial H}{\partial\left(\frac{\partial S_r}{\partial q_B}\right)} \\ = \frac{\partial^2 S_r}{\partial q_{A_i}\partial q_B}\frac{\partial H}{\partial P_B} = \frac{\partial^2 S_r}{\partial q_{A_i}\partial q_B}\dot{q_B} &= \frac{\partial^2 S_r}{\partial q_{A_i}\partial q_{B\parallel}}\dot{q_{B\parallel}},\end{aligned}$$

which implies that:

$$\frac{\partial^2 S_r}{\partial q_{A_i}\partial q_{B\parallel}} = 0. \tag{4.38}$$

Analogously, considering the Hamiltonian-Jacobi equation for q_A, $E = H\left(-\frac{\partial S_r}{\partial q_A}, q_A\right)$, and differentiating both sides with respect to E, keeping in mind once again the Hamilton's equation of motion, and the relations for the partial derivatives of the action, we get:

$$\begin{aligned}1 = \frac{\partial H}{\partial\left(-\frac{\partial S_r}{\partial q_A}\right)} \cdot \frac{-\partial^2 S_r}{\partial q_A \partial E} &= \frac{\partial H}{\partial P_A} \cdot \frac{-\partial^2 S_r}{\partial q_A \partial E} \\ -\dot{q_A}\frac{\partial^2 S_r}{\partial q_A \partial E} &= -\dot{q_{A\parallel}}\frac{\partial^2 S_r}{\partial q_{A\parallel}\partial E},\end{aligned}$$

using the fact that $\dot{q_{A\perp}}$ is zero. From this equation we find:

$$\frac{\partial^2 S_r}{\partial q_{A\|}\partial E} = -\frac{1}{\dot{q_{A\|}}}. \tag{4.39}$$

And finally, differentiating $E = H\left(-\frac{\partial S_r}{\partial q_A}, q_A\right)$ with respect to an arbitrary component q_{B_i} of q_B, we find:

$$\begin{aligned}\frac{\partial E}{\partial q_{B_i}} = 0 = \frac{\partial}{\partial q_{B_i}} H\left(\frac{\partial S_r}{\partial q_A}, q_A\right) &= \frac{\partial^2 S_r}{\partial q_A \partial q_{B_i}} \cdot \frac{\partial H}{\partial\left(\frac{-\partial S_r}{\partial q_A}\right)} \\ = \frac{-\partial^2 S_r}{\partial q_A \partial q_{B_i}} \frac{\partial H}{\partial P_A} = \frac{\partial^2 S_r}{\partial q_A \partial q_{B_i}} \dot{q_A} &= \frac{-\partial^2 S_r}{\partial q_{A\|} \partial q_{B_i}} \dot{q_{A\|}}.\end{aligned}$$

This leads us to:

$$\frac{\partial^2 S_r}{\partial q_{A\|}\partial q_{B_i}} = 0. \tag{4.40}$$

Now, inserting equations (4.37), (4.38), (4.39) and (4.40) into equation (4.35), we can simplify the determinant $|\Delta_r|$:

$$\begin{aligned}|\Delta_r| &= (-1)^{d+1} \begin{pmatrix} 0 & 0 & -\frac{1}{\dot{q_{A\|}}} \\ 0 & \frac{\partial^2 S_r}{\partial q_{A\perp}\partial q_{B\perp}} & \frac{\partial^2 S_r}{\partial q_{A\perp}\partial E} \\ \frac{1}{\dot{q_{B\|}}} & \frac{\partial^2 S_r}{\partial q_{B\perp}\partial E} & \frac{\partial^2 S_r}{\partial E^2} \end{pmatrix} \\ &= (-1)^{d+1} \frac{1}{\dot{q_{B\|}}} \cdot \frac{1}{\dot{q_{A\|}}} \left| \frac{\partial^2 S_r}{\partial q_{A\perp}\partial q_{B\perp}} \right|.\end{aligned}$$

Now, recalling that this expression must be evaluated at the stationary point $q = q_A = q_B$, and by noticing that $\frac{\partial^2 S_r}{\partial q_{A\perp}\partial q_{B\perp}}$ is a $d-1 \times d-1$ matrix, we find that this last expression can be written as:

$$|\Delta_r| = \frac{1}{|\dot{q_\|}|^2} \left| -\frac{\partial^2 S_r}{\partial q_{A\perp}\partial q_{B\perp}} \right| = \frac{|D_r|}{\frac{\partial^2 W}{\partial t^2}},$$

where we found in previous sections that $|D_r|$ was approximately $\frac{m}{\tau}$ which is a positive quantity. By equation (4.25), $\frac{\partial^2 W}{\partial t^2}$ is also positive. Hence $\left| -\frac{\partial^2 S_r}{\partial q_{A\perp}\partial q_{B\perp}} \right|$ must be positive too. Therefore

$$|\Delta_r| = \frac{1}{|\dot{q_\|}|^2} \left|\left| \frac{\partial^2 S_r}{\partial q_{A\perp}\partial q_{B\perp}} \right|\right|. \tag{4.41}$$

Inserting equations (4.34) and (4.41) into the integral over the Green function, equation

(4.33) we get:

$$\begin{aligned}
&\int G(q,q,E)dq \\
= \quad & -\frac{i}{\hbar}\left(\frac{1}{2\pi i\hbar}\right)^{\frac{(d-1)}{2}} \sum_r e^{-\frac{i\pi\nu_r}{2}} \int \frac{1}{|\dot{q}_\parallel|} \left|\left|\frac{\partial^2 S_r}{\partial q_{A\perp}\partial q_{B\perp}}\right|\right| \\
&\exp\left(\frac{i}{\hbar}\left(S_r(E)+\frac{1}{2}q_\perp^\top\left(\frac{\partial^2 S_r}{\partial q_{A\perp}\partial q_{A\perp}}+2\frac{\partial^2 S_r}{\partial q_{A\perp}\partial q_{B\perp}}+\frac{\partial^2 S_r}{\partial q_{B\perp}\partial q_{B\perp}}\right)q_\perp\right)\right) \\
&dq_\parallel dq_{\perp_1},\ldots,dq_{\perp_{d-1}},
\end{aligned} \tag{4.42}$$

where the integrals over the perpendicular components are Fresnel integrals which can be evaluated as in Appendix B.2 to yield:

$$\begin{aligned}
&\int \left|\left|\frac{\partial^2 S_r}{\partial q_{A\perp}\partial q_{B\perp}}\right|\right|^{\frac{1}{2}} \\
&\exp\left(\frac{i}{\hbar}\left(\frac{1}{2}q_\perp^\top\left(\frac{\partial^2 S_r}{\partial q_{A\perp}\partial q_{A\perp}}+2\frac{\partial^2 S_r}{\partial q_{A\perp}\partial q_{B\perp}}+\frac{\partial^2 S_r}{\partial q_{B\perp}\partial q_{B\perp}}\right)q_\perp\right)\right)dq_\perp \\
= \quad & \left|\left|\frac{\partial^2 S_r}{\partial q_{A\perp}\partial q_{B\perp}}\right|\right|^{\frac{1}{2}} \frac{(2\pi i\hbar)^{\frac{d-1}{2}}}{\sqrt{\left|\frac{\partial^2 S_r}{\partial q_{A\perp}\partial q_{A\perp}}+2\frac{\partial^2 S_r}{\partial q_{A\perp}\partial q_{B\perp}}+\frac{\partial^2 S_r}{\partial q_{B\perp}\partial q_{B\perp}}\right|}}.
\end{aligned} \tag{4.43}$$

Since the determinant of a matrix is equal to the product of its eigenvalues, we can write:

$$\begin{aligned}
&\left|\frac{\partial^2 S_r}{\partial q_{A\perp}\partial q_{A\perp}}+2\frac{\partial^2 S_r}{\partial q_{A\perp}\partial q_{B\perp}}+\frac{\partial^2 S_r}{\partial q_{B\perp}\partial q_{B\perp}}\right| \\
= \quad & (-1)^{-\alpha_r}\left|\frac{\partial^2 S_r}{\partial q_{A\perp}\partial q_{A\perp}}+2\frac{\partial^2 S_r}{\partial q_{A\perp}\partial q_{B\perp}}+\frac{\partial^2 S_r}{\partial q_{B\perp}\partial q_{B\perp}}\right|,
\end{aligned}$$

where α_r is the number of negative eigenvalues of this matrix in question. And now, inserting equation (4.43) into equation (4.42) and using equation (C.3) for the Monodromy matrix M_r (see Appendix C). The integral over the Green function simplifies to:

$$\int G(q,q,E)dq = -\frac{i}{\hbar}\sum_r e^{\frac{-i\pi(\nu_r+\alpha_r)}{2}} \int \frac{1}{|\dot{q}_\parallel|}||M_r-1||^{-\frac{1}{2}} e^{\frac{i}{\hbar}S_r(E)}dq_\parallel,$$

where only $\frac{1}{|\dot{q}_\parallel|}$ depends on $q_\parallel$ inside the integral. And so, we can replace $\dot{q}_\parallel = \frac{dq_\parallel}{dt}$ to get:

$$\begin{aligned}\int G(q,q,E)dq &= -\frac{i}{\hbar}\sum_r e^{\frac{-i\pi(\nu_r+\alpha_r)}{2}}||M_r-1||^{-\frac{1}{2}}e^{\frac{i}{\hbar}S_r(E)}\oint dt \\ &= -\frac{i}{\hbar}\sum_r \frac{(T_p)_r}{||M_r-1||^{\frac{1}{2}}}e^{\left(\frac{i}{\hbar}S_r(E)-\frac{i\mu_r\pi}{2}\right)},\end{aligned}$$

where T_p is the period of the primitive orbit; which is the time needed for one passage. And where $\mu_r = \nu_r + \alpha_r$ is called the Maslov index.

Therefore the density of states can now be written as:

$$\begin{aligned}\rho(E) &= -\frac{1}{\pi}Im\left(\int G(q,q,E)dq\right) \\ &= \frac{1}{\pi\hbar}\sum_r \frac{(T_p)_r}{||M_r-1||^{\frac{1}{2}}}\cos\left(\frac{S_r(E)}{\hbar}-\frac{\mu_r\pi}{2}\right).\end{aligned} \tag{4.44}$$

This equation is known as the Gutzwiller Trace formula. It has to be noted that Gutzwiller himself found a problem with respect to the derivation of such a formula. The problem relies on the difficulty of finding all classical trajectories from the starting point q_A to the end point q_B in the semiclassical Green function, for a chaotic system. The progress on that matter seems to be quite slow [36]. The Trace formula, however, has been tested in particular problems such as the Anisotropic Kepler problem, and has proved to be quite a good approximation [5].

4.2.7 Smooth and oscillatory parts of the Gutzwiller Trace Formula

As we pointed earlier, we are interested in comparing the smooth part and fluctuating part of the counting function for the nontrivial zeros of the zeta function with the smooth part and fluctuating part of the counting function for energy levels in a quantum chaotic system. Therefore, it is convenient to split the Gutzwiller Trace formula into a smooth and a fluctuating part. We begin by noticing that in the Gutzwiller Trace formula the orbits of length zero are included too. If we look at equation (4.33) we notice that the determinant $|\Delta_r|$ becomes singular for these orbits. Therefore, the stationary phase approximation we have been performing does not hold up for these orbits. So in this case we have to go back to the equation for the propagator (4.12), valid for infinitesimally small times, which correspond to the limit $|q_A - q_B| \longrightarrow 0$,

$$K_0(q_A, q_B, t) = \left(\frac{m}{2\pi\hbar i t}\right)^{\frac{d}{2}} \exp\left(\frac{i}{\hbar}\left(\frac{m}{2t}(q_B - q_A)^2 - tV\left(\frac{q_A + q_B}{2}\right)\right)\right),$$

where we have written a subscript $'0'$ to denote that we will only consider the direct path from q_A to q_B. Recalling the quantum mechanical Green function was the Fourier transform of the propagator we get

$$\begin{aligned} G_0(q_A, q_B, E) &= -\frac{i}{\hbar}\int_0^\infty K_0(q_A, q_B, t)dt \\ &= -\frac{i}{\hbar}\left(\frac{m}{2\pi\hbar i}\right)^{\frac{d}{2}} \int_0^\infty t^{-\frac{d}{2}} \exp\left(\frac{i}{\hbar}\left(\frac{m}{2t}(q_B - q_A)^2\right.\right. \\ &\quad \left.\left. +tV\left(\frac{q_A + q_B}{2}\right) + Et\right)\right)dt. \end{aligned} \tag{4.45}$$

To evaluate this integral, first let's consider the following integral in d dimensions

$$\begin{aligned} &\int \exp\left(\frac{i}{\hbar}\left(p(q_B - q_A) - \frac{p^2}{2m}t\right)\right) dp \\ = &\int \exp\left(\frac{i}{\hbar}\left(i\left(\frac{t}{2m}\right)^{\frac{1}{2}} p + \frac{1}{2i}\left(\frac{t}{2m}\right)^{-\frac{1}{2}}(q_B - q_A)\right)^2 + \frac{m}{2t}(q_B - q_A)^2\right) dp \\ = &\exp\left(\frac{i}{\hbar}(q_B - q_A)^2\right)\left(-i\left(\frac{2m}{t}\right)^{\frac{1}{2}}\right)^d \int e^{\frac{i}{\hbar}x^2} dx, \end{aligned}$$

where we made the change of variables $x = i\left(\frac{t}{2m}\right)^{\frac{1}{2}} p + \frac{1}{2i}\left(\frac{t}{2m}\right)^{-\frac{1}{2}}(q_B - q_A)$. Noting that the integral on the right of this expression is a Fresnel integral in d dimensions, see appendix B, we get

$$\begin{aligned} \int e^{\frac{i}{\hbar}\left(p(q_B - q_A) - \frac{p^2}{2m}t\right)} dp &= \exp\frac{im}{2\hbar t}(q_B - q_A)^2 \left(-i\left(\frac{2m}{t}\right)^{\frac{1}{2}}\right)^d (\pi\hbar)^{\frac{d}{2}} e^{\frac{i\pi d}{4}} \\ &= \exp\frac{im}{2\hbar t}(q_B - q_A)^2 \left(\frac{2m\pi\hbar}{it}\right)^{\frac{d}{2}} \\ \Rightarrow e^{\frac{im}{2\hbar t}(q_B - q_A)^2} &= \left(\frac{it}{2m\pi\hbar}\right)^{\frac{d}{2}} \int \exp\left(\frac{i}{\hbar}\left(p(q_B - q_A) - \frac{p^2}{2m}t\right)\right) dp. \end{aligned} \tag{4.46}$$

Inserting this expression into equation (4.45) we get

$$\begin{aligned} G_0(q_A, q_B, E) &= -\frac{i}{\hbar}\left(\frac{1}{2\pi\hbar}\right)^d \int\int_0^\infty \exp\left(\frac{i}{\hbar}\left(p(q_B - q_A)\right.\right. \\ &\quad \left.\left. + \left(E - V\left(\frac{q_A + q_B}{2}\right) - \frac{p^2}{2m}\right)\right)\right) dt dp. \end{aligned} \tag{4.47}$$

Recall that in the beginning we assumed E to have an infinitesimally small imaginary part. This then means that the integral with respect to t converges, resulting in the following equation:

$$\begin{aligned} G_0(q_A, q_B, E) &= -\frac{i}{\hbar}\left(\frac{1}{2\pi\hbar}\right)^d \int \frac{i\hbar e^{\frac{i}{\hbar}p(q_B - q_A)}}{E - \frac{p^2}{2m} - V\left(\frac{q_A+q_B}{2}\right)} dp \\ &= -\frac{i}{\hbar}\left(\frac{1}{2\pi\hbar}\right)^d \int \frac{e^{\frac{i}{\hbar}p(q_B - q_A)}}{E - \frac{p^2}{2m} - V\left(\frac{q_A+q_B}{2}\right)} dp. \end{aligned}$$

Recalling that we must perform the limit $|q_B - q_A| \to 0$, looking at equation (4.9) for the density of states, and taking $H(p, q) = \frac{p^2}{2m} + V(q)$, we obtain

$$\begin{aligned} \rho_0 &= -\frac{1}{\pi} Im\left(\int G_0(q, q, E) dq\right) \\ &= -\frac{1}{\pi} Im\left(\frac{1}{2\pi\hbar}\right)^d \int\int \frac{1}{E - H(p, q)} dp dq \\ &= -\frac{1}{\pi}\left(\frac{1}{2\pi\hbar}\right)^d \int\int \lim_{\epsilon\to 0} Im \frac{1}{E - H(p, q) + i\epsilon} dp dq \\ &= -\frac{1}{\pi}\left(\frac{1}{2\pi\hbar}\right)^d \int\int \lim_{\epsilon\to 0} Im \frac{E - H(p, q) - i\epsilon}{(E - H(p, q))^2 + \epsilon^2} dp dq \\ &= -\frac{1}{\pi}\left(\frac{1}{2\pi\hbar}\right)^d \int\int \lim_{\epsilon\to 0} \frac{-\epsilon}{(E - H(p, q))^2 + \epsilon^2} dp dq \\ &= \left(\frac{1}{2\pi\hbar}\right)^d \int\int \lim_{\epsilon\to 0} \frac{\epsilon}{\pi} \frac{1}{(E - H(p, q))^2 + \epsilon^2} dp dq \\ &= \left(\frac{1}{2\pi\hbar}\right)^d \int \delta(E - H(p, q)) dp dq, \end{aligned} \tag{4.48}$$

where in the last equality we have used the fact that the function in the integrand behaves as a delta of Dirac, as we proved at the very beginning of our derivation of the density of states. Looking at equation (4.48) we can interpret that $\rho_0(E)$ corresponds precisely to the subset of the phase space corresponding to a classical particle whose energy is E. We can consider $\rho_0(E)$ as the smooth part of $\rho(E)$ since it corresponds to the classical part of the system. Hence $\rho_{fl}(E)$ will correspond to its quantum fluctuations. We conclude that for a quantum chaotic system:

$$\rho(E) = \rho_0(E) + \rho_{fl}(E),$$

$$\rho_0(E) = \left(\frac{1}{2\pi\hbar}\right)^d \int \delta(E - H(p,q))dpdq,$$

$$\rho_{fl}(E) = \frac{1}{\pi\hbar}\sum_{r'} \frac{(T_p)_{r'}}{||M_r - 1||^{\frac{1}{2}}} \cos\left(\frac{1}{\hbar}S_{r'}(E) - \frac{\mu_r \pi}{2}\right).$$

where the summation in the last expression is over the classical orbits r' whose length is greater than zero. This expression is more conveniently written as

$$\rho_{fl}(E) = \frac{1}{\pi\hbar}\sum_{\ell}\sum_{m=1}^{\infty} \frac{(T_p)_{\ell}}{||M_\ell^m - 1||^{\frac{1}{2}}} \cos\left(\frac{m}{\hbar}S_{\ell}(E) - \frac{1}{2}m\pi\mu_\ell\right),$$

where the first summation is over the classical periodic orbits, which are only traversed once, and the second summation corresponds to their repetitions. Recalling that the density of states $\rho(E)$ is related to the counting function $\mathcal{N}(E)$ by the relation $\rho(E) = \frac{d\mathcal{N}}{dE}$, we get the following expressions:

$$\begin{aligned} \mathcal{N}(E) &= \mathcal{N}_0(E) + \mathcal{N}_{fl}(E), \\ \mathcal{N}_0(E) &= \left(\frac{1}{2\pi\hbar}\right)^d \int\int \mathcal{U}(E - H(p,q))dpdq, \end{aligned}$$

where $\mathcal{U}(x)$ denotes the unit step function defined as

$$\mathcal{U}(x) = \begin{cases} 0 & x < 0 \\ \frac{1}{2} & x = 0 \\ 1 & x > 0. \end{cases}$$

Also, noting that the period of the orbit is related to the action by the relation $\frac{\partial S_p(E)}{\partial E} = T_p$, we get

$$\mathcal{N}_{fl}(E) = \frac{1}{\pi}\sum_{\ell}\sum_{m} \frac{\sin\left(\frac{mS_\ell(E)}{\hbar} - \frac{1}{2}m\pi\mu_\ell\right)}{m||M_\ell^m - 1||^{\frac{1}{2}}}. \tag{4.49}$$

We are now ready to make a comparison between the counting function of the zeros of $\zeta(s)$ and the counting function of the energy levels in a quantum chaotic system.

4.3 Relations between the counting functions

Before a comparison between the counting functions derived in this chapter is made, we are going to open a brief parenthesis and to discuss the Lyapunov exponent of a trajectory in a dynamical system. This will help us write equation (4.49) in a more convenient way that will make the comparison between the counting functions simpler.

The Lyapunov exponent is an indicator of how unstable a trajectory is. If it is positive, then the trajectory is said to be sensible to changes in its initial conditions. More specifically, consider two infinitesimally close points at an initial time $t = 0$ in a dynamical system, $x(0)$ and $x^{'}(0) = x(0) + \eta(0)$, with $\Delta(0) := ||\eta(0)|| \ll 1$. The Lyapunov exponent (of the trajectory of $x(t)$) is then defined as the double limit [37]:

$$\lambda = \lim_{t\to\infty} \lim_{\Delta(0)\to 0} \frac{1}{t} \ln\left(\frac{\Delta(t)}{\Delta(0)}\right). \tag{4.50}$$

The fact that the trajectory is unstable if λ is positive can be intuitively seen from the fact that $\Delta(t) \sim \Delta(0)e^{\gamma t}, \gamma > 0$, for chaotic systems. Now, Berry and Keating pointed out that the Monodromy matrix respective to a primitive periodic orbit p tarversed m times satisfy the relation[6]

$$||M_p^m - 1|| \sim e^{m\lambda_p T_p},$$

as the period mT_p of the orbit becomes large (see equation (4.49)). This can be intuitively seen from the fact that the Monodromy matrix (see Appendix C) serves to approximate the variations $\eta_\perp(t)$ in the final state $x(t)$ of the trajectory in the phase space, given some small perpendicular variations $\eta_{perp}(0)$ in the initial state of the trajectory $x(0)$, i.e. $\eta_\perp(t) \approx M\eta_\perp(0)$. Also, notice that if the system is chaotic, then $|\eta(t)| \gg |\eta(0)|$, so $||M|| \gg 1$. Therefore, one would expecte that

$$||M - 1|| \sim ||M|| \sim \frac{|\eta_\perp(t)|}{|\eta_\perp(0)|} \sim e^{\eta t}.$$

This of course does not count as a rigorous proof, but serves to give a general idea about the above approximation. For a more detailed discussion about Lyapunov exponents the reader is referred to [38].

With the above approximation in mind, Berry and Keating wrote equation (4.49) in a more convenient form [6]:

$$\mathcal{N}_{fl}(E) = \frac{1}{\pi}\sum_p \sum_{m=1}^{\infty} \frac{e^{-\frac{1}{2}m\lambda_p T_p}}{m} \sin\left(\frac{mS_p(E)}{\hbar} - \frac{1}{2}\pi m\mu_p\right),$$

where have replaced the index of the first summation by p just for convenience when we compare this fluctuating part of the counting function with the Zeta function's analogous.

Now, let's look at the two counting functions:

$$\begin{aligned} N(T) &= \langle N(T)\rangle + N_{fl}(T), \\ \langle N(T)\rangle &= \frac{T}{2\pi}\log\left(\frac{T}{2\pi}\right) - \frac{T}{2\pi} + \frac{7}{8} + O\left(\frac{1}{T}\right), \\ N_{fl}(T) &= -\frac{1}{\pi}\sum_{p \text{ prime}} \sum_{m=1}^{\infty} \frac{-e^{-\frac{1}{2}m\ln p}}{m}\sin(mT\ln p), \end{aligned}$$

for the zeros of $\zeta(s)$, and

$$\begin{aligned} \mathcal{N}(E) &= \mathcal{N}_0(E) + \mathcal{N}_{fl}(E), \\ \mathcal{N}_0(E) &= \left(\frac{1}{2\pi\hbar}\right)^d \int\int \mathcal{U}(E - H(p,q))dpdq, \\ \mathcal{N}_{fl}(E) &= \frac{1}{\pi}\sum_p \sum_{m=1}^{\infty} \frac{e^{-\frac{1}{2}m\lambda_p T_p}}{m} \sin\left(\frac{mS_p(E)}{\hbar} - \frac{1}{2}\pi m\mu_p\right), \end{aligned}$$

for the energy levels of a quantum chaotic system. Looking at the great similarities between the fluctuating parts of the counting functions, Berry and Keating conjectured that the Riemann Hamiltonian must correspond to a quantum chaotic physical system.

Let's first look at the smooth parts of the counting functions. By looking at $\mathcal{N}_0(E)$ we see that this is in fact the volume, multiplied by $(2\pi\hbar)^{-d}$, of the subset of the phase space corresponding to the classical states with an energy less than E. Note that by the Heisenberg uncertainty principle, $\Delta x_1 \ldots \Delta x_d \Delta p_1 \ldots \Delta p_n \approx (2\pi\hbar)^d$, the volume of each state in the space is $\sim 2\pi\hbar$. Therefore, $\mathcal{N}_0(E)$ can be regarded as the number of classical states of the system in the semiclassical limit, with an energy less than E. By Looking at $\langle N(T)\rangle$, we can conclude that in the search of the Riemann Hamiltonian, it will be convenient to look at quantum chaotic systems such that

$$\mathcal{N}_0(E) = \frac{E}{2\pi}\log\left(\frac{E}{2\pi}\right) - \frac{E}{2\pi} + \frac{7}{8} + O\left(\frac{1}{E}\right).$$

. In the next chapter we will talk about the Hamlitonians of the type $H = xp$, first suggested by Berry and Keating [22], which seem to satisfy this relation for $\mathcal{N}_0(E)$ as well as other necessary characteristics based on the similiraties of the fluctuating parts of the counting functions.

Now, let's look at the fluctuating parts of the counting function. By looking at both formulas, if the Riemann Hamiltonian exists, then it will be quite possible that it has the following characteristics in the semiclassical limit[6]:

i) Looking at the remarkable resemblance between the two formulas, it seems like $N_{fl}(T)$ is a periodic-orbit formula, scaled so that $\hbar = 1$, whose semiclassical limit correspond to $T \to \infty$.

ii) Its orbits are labelled by the prime numbers. This can be seen from the fact that the summations of one formula are over the primitive orbits and its repetitions(the positive integers) and in the other formula the summations are over the prime numbers and the postive integers.

iii) The Maslov phase associated with each orbit is π. This can be intuitively from the fact that the signs of the counting functions are opposite. Hence, adding a phase of π to the sine functions will change the sign of the formula. One problem, however, is that if π is the Maslov phase of an orbit, the 2π should be the Maslov phase of the same orbit traversed twice. However, Connes finds an explanation for this issue in [39]. His arguments, though, are beyond the scope of this thesis.

iv) The dimensionless action $\frac{mS_p(E)}{\hbar}$ of each orbit is given by $tm\log p$, since the action is placed in the sinusoidal function. It can be seen here that the semiclassical limit of one formula corresponds to the limit $\hbar \to 0$ and in the other one corresponds to the limit $T \to \infty$.

v) The periods of the orbits mT_p are connected with the logarithms of the primes, and are given by $m\log p$. This can be seen by looking at how the mT_p terms are placed in the formula, as well as by looking at the relations $mT_p = \frac{\partial S}{\partial E}$ and $m\log p = \frac{\partial(tm\log p)}{\partial t}$, which mean that the periods of the orbits of the Riemann

Hamiltonian are the partial derivatives of the action corresponding to the orbit, in concordance with the physical theory. One very important feature of the Riemann Hamiltonian is this one. The periods of the orbits in the system do not depend at all on the energy, but in the prime numbers.

vi) Looking at the terms in the exponentials, since $m \log p$ should be equal to mT_p, then the Lyapunov exponent of each of the orbits must be equal to 1. This would imply that the Riemann Hamiltonian would be uniformly chaotic.

vii) The Riemann Hamiltonian is a quasi one-dimensional system. There are two arguments for this. The first one is that the exponential term in $\mathcal{N}_{fl}(E)$ is an approximation, while the formula for $N_{fl}(T)$ is exact. Hence, recalling where this approximation came from, is as if the Monodromy matrix of the orbits of the system was of rank 1. The other argument is that in a generic d dimensional scaling system the number of energy levels increases as $\sim E^d$, and by looking at the counting function $N(T)$ of the nontrivial zeros of $\zeta(s)$, we see that the number of zeros up to a given T satisfy $T < N(T) \sim T \log T < T^2$[16].

viii) The Riemann dynamics has a classical counterpart. The absence of an analogue of $\hbar$ in the equation for $N_{fl}(T)$ seems to indicate that there is a scaling of the dynamics i.e., the trajectories are the same for all energy scales.

ix) The dynamics of the Riemann system does not possess time-reversal symmetry, because if it did, then the degeneracy of the actions between each orbit and it time-reversed analogue would led both terms to contribute coherently to the counting function $N(T)$, so the prefactor in $N(T)$ would be $\frac{2}{\pi}$ instead of $\frac{1}{\pi}$.

Note that this approach of the problem also agrees with what random matrix predicts i.e., that the Riemann Hamiltonian can be modeled by matrices similar to those from the GUE, and therefore is a chaotic system with no time-reversal symmetry.

This list of requirements for the Riemann Hamiltonian were a big step in the search of a suitable dynamical system[16]. There are very important aspects of it. Perhaps, the most important question that arises is: How to construct a Hamiltonian that distinguishes composite numbers from primes?, in such a way that every primitive orbit of the dynamical system is labelled by one, and also in a way that the periods of the primitive orbits are independent of the energy and depend only on the logarithms of primes. If this is answered, it will not only shed light into the Hilbert-Polya conjecture, but it will also give a connection between two fields of science which until now appeared to be completely unrelated: Quantum chaos and number theory.

CHAPTER 5

Conclusions and final thoughts

As we saw in the previous chapters, the resemblance between the n-th correlation functions from both the nontrivial zeros of $\zeta(s)$ and the eigenvalues from the GUE, added to the similarities between the fluctuating part of the counting functions of both the zeros and the energy levels of quantum chaotic systems, seem to indicate that the Riemann Hamiltonian represents a strongly chaotic system, with particular characteristics such as lack of time reversal symmetry, having level repulsion in its energy levels, having its periodic classical orbits characterized by a prime number, etc.

For instance, the similarities in the statistical properties of the zeros and the eigenvalues of matrices from the GUE, could lead mathematicians to study the distribution of the zeros of the zeta function from a different point of view; through random matrix theory extensively studied by physicists. This might give great benefits to those who study the zeta function, taking into account how hard it is to study the properties and behaviour of the zeros. Reciprocally, physicists might get some benefits from it too. Maybe the Zeta function could also be a valuable tool to study matrix ensembles, such as the GUE. Also, the similarities between the counting functions could led number theory and quantum chaos to benefit from each other.

The mutual benefits in both cases, though, are for now quite unbalanced. In the first case the statistical properties from the GUE are more accessible to that of the zeros. In the second case the formula for the fluctuations in the counting function of the nontrivial zeros would facilitate extensevely the calculations required to handle its quantum chaotic counterpart. However, as Keating states [40], to look what the Riemann Hamiltonian might be based on the similiraties of the counting functions is an extremely hard problem to pursue. So rather, in what these similiraties come more useful is that the relationship between the fluctuating functions could serve to understand the complex mathematical structure from the Gutzwiller Trace formula. There are several advantages to it. For instance, $\mathcal{N}_f l(T)$ offers a lot of mathematical simplicity; it is an exact formula rather than an asymptotic approximation, and what is more important, the tremendous task concerning the calculations of the periodic classical orbits is overly simplified by translating it to calculations with prime numbers.

Nevertheless, motivated by the characteristics listed in the previous section of how the Riemann Hamiltonian should be, Berry and Keating propose a Hamiltonian related in the classical limit to a Hamiltonian of the form $H = xp$[6], where x and p are the position and momentum of a particle moving in one dimension. There were various reasons for this formulation such as:

i) The system is one-dimensional.

ii) From the Hamilton equations of motion $\dot{x} = \frac{\partial H}{\partial p} = x$, $-\dot{p} = \frac{H}{x} = p$, which lead to the equations $x = x(0)e^t$, $p = p(0)e^{-t}$, we can see that the system is uniformly unstable, since all trajectories tend away from the origin if $E \neq 0$.

iii) We can see from the above equations of motion that the Lyapunov exponent of th etrajectories is $\lambda_p = 1$, as required.

iv) The system has no time-reversal symmetry since, for example, the Hamiltonian is not invariant under the transformation $p \mapsto -p$.

v) After some modifications of the system, such as modified $H = xp$ to $\frac{xp+px}{2}$ to make the operator Hermitian, the resulting smooth part from the counting function is $\mathcal{N}_0(E) = \frac{E}{2\pi} \log\left(\frac{E}{2\pi}\right) - \frac{E}{2\pi} + \frac{7}{8}$, as it must be looking at the smooth part of $N(T)$

However, there were issues about this formulation; Berry and Keating could not find an association between the prime numbers and the orbits of the system, for example. But, what is important about it, is that this Hamiltonian was the basis for many suggestions of what the Riemann Hamiltonian should be[16]. As an interesting side note, recently Germán Sierra, in a paper named: The Riemann zeros as energy levels of a Dirac fermion in a potential built from the prime numbers in Rindler spacetime [27], has proposed that relativity theory must also be present, in order to encode the primes, because the properties of accelerated objects, in a Minkowski spacetime, can be used to encode arithmetic information. He proposes a Hamiltonian, whose counting function for energy levels is similar to the counting function of the zeros, which also try to attend the issue of providing periodic primitive orbits associated with the prime numbers. Hopefully, this approach proves to be useful in a future proof of the Hilbert-Polya conjecture.

As often happens with hard problems in mathematics, the quest for a solution often ends with vast amounts of new theories applicable to various fields, as well as useful new mathematical methods for the resolution of various problems. Such was the case of Fermat's Last theorem, which consisted in proving that the equation $x^n + y^n = z^n$, where x, y, z are positive integers, have no solutions for n integer, $n > 2$. It took 358 years for mathematicians to solve this. Perhaps, the most valuable thing about it, was that in the process of finding a solution, a large amount of new techniques and theories emerged [41]. So, in particular, if the Hilbert-Polya conjecture is ever proved to be true, it will mean more than just proving that the zeros of a particular function are on the line $Re(s) = \frac{1}{2}$. Its importance lies far beyond that. It will answer one of the most tantalizing questions in the history of mathematics, which will have strong consequences in many areas of mathematics; particularly giving heavy insights into how is the behaviour of the primes, which maybe were not as random as we thought. While doing so, it will make a connection between number theory and quantum mechanics, which until now seemed to be totally unrelated. New areas of physics could be explored while answering this problem.

Appendices

APPENDIX A

Classical mechanics

In this appendix we make a short review on some of the important aspects of classical mechanics. For a more detailed and extensive analysis on the subject see [42] for example.

A.1 Lagrangian Formalism

The Lagrangian formalism is a method to calculate the equations of motion of a classical physical system, which is based on variational calculus. For such a system the Lagrangian is defined as:

$$\mathcal{L}(q, \dot{q}) := T - V,$$

where T and V denote the kinetic energy and potential energy respectively, of the system. Where q denotes the position of the particle and $\dot{q} := \frac{d}{dt}q$ its speed. If the system has more particles, the above expression is generalized by summing over the Lagrangians of the particles.

By Hamilton's principle the path of a particle follows is the one that minimizes the action defined by $s := \int_{t_1}^{t_2} \mathcal{L}(q, \dot{q})dt$, i.e.

$$\delta \int_{t_1}^{t_2} \mathcal{L}(q, \dot{q})dt = 0.$$

By the Leibniz rule this expression is equal to

$$\begin{aligned} 0 = \int_{t_1}^{t_2} \mathcal{L}(q,\dot{q})dt &= \int_{t_1}^{t_2} \sum_i \left(\frac{\partial \mathcal{L}}{\partial q_i}\delta q_i + \frac{\partial \mathcal{L}}{\partial \dot{q}_i}\delta \dot{q}_i \right) dt \\ &= \int_{t_1}^{t_2} \sum_i \left(\frac{\partial \mathcal{L}}{\partial q_i}\delta q_i - \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{q}_i}\delta \dot{q}_i \right) dt + \sum_i \frac{\partial \mathcal{L}}{\partial \dot{q}_i}\delta q_i \Big|_{t_1}^{t_2} \\ &= \int_{t_1}^{t_2} \sum \left(\frac{\partial \mathcal{L}}{\partial q_i} - \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{q}_i} \right) \delta q_i dt, \end{aligned}$$

where the last term vanishes since the starting and ending points are fixed. Since the q_i are independent variables and the above integral must vanish for all possible paths, we conclude that

$$\frac{\partial \mathcal{L}}{\partial q_i} = \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{q}_i}\right), \text{ for } 1 \leq i \leq d, \tag{A.1}$$

where d denotes the dimensions of the system.

This set of d equations are known as the Euler-Lagrange equations of motion. By looking at equation (A.1), the momentum, whose coordinates are defined by $p_i := \frac{\partial \mathcal{L}}{\partial \dot{q}_i}$, satisfies the equation

$$\dot{p}_i := \frac{\partial \mathcal{L}}{\partial q_i}. \tag{A.2}$$

In accordance with the derivation of the Gutzwiller Trace formula, Stöckmann uses the analogous definition for the action

$$S := \int_{q_A}^{q_B} p dq, \tag{A.3}$$

where q_A and q_B are the starting and ending points of the trajectory.

A.2 Hamiltonian Formalism

The Hamiltonian of a physical system is defined as

$$H(q,p) := \dot{q}P - \mathcal{L}. \tag{A.4}$$

Although H is a function of q and p, while $\mathcal{L}$ is a function of q and $\dot{q}$, we can see that $\dot{q}$ can be expressed as a function of q and p by solving $p_i := \frac{\partial \mathcal{L}}{\partial \dot{q}_i}$ for $\dot{q}_i$.

Now, consider the total differential of the left hand side of (A.4) which is equal to

$$dH = \sum_i \frac{\partial H}{\partial q_i} dq_i + \frac{\partial H}{\partial p_i} dp_i, \tag{A.5}$$

while the total differential of the right hand side is equal to

$$\begin{aligned} dH &= d(\dot{q}p) - d(\mathcal{L}(q,\dot{q})) \\ &= \sum_i \dot{q}_i dp_i + p_i d\dot{q}_i - \frac{\partial \mathcal{L}}{\partial q_i} dq_i - \frac{\partial \mathcal{L}}{\partial \dot{q}_i} d\dot{q}_i \\ &= \sum_i \dot{q}_i dp_i + p_i d\dot{q}_i - \dot{p}_i dq_i - p_i d\dot{q}_i \\ &= \sum_i -\dot{p}_i dq_i + \dot{q}_i dp_i. \end{aligned}$$

Looking at equation (A.5) we conclude that

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \dot{p}_i = -\frac{\partial H}{\partial q_i} \text{ for } i \leq i \leq d. \tag{A.6}$$

Since the q_i and p_i are independent variables. These equations are known as Hamilton's equations of motion.

A.3 Hamilton Principal function and the Hamilton-Jacobi differential equations

We will assume that the Lagrangian can be written as

$$\mathcal{L}(q,\dot{q}) = T(q,\dot{q}) - V(q),$$

and assume that the kinetic energy T is an homogeneous quadratic equation in $\dot{q}$, i.e. $T(rq, r\dot{q}) = r^2 T(q,\dot{q})$. This assumption cover the most general cases since usually $T = \frac{1}{2}m\dot{q}^2$ and V almost always depends on just the position. Now, from Euler's theorem for an homogeneous function $f(x)$ we have that

$$x \cdot \nabla f(x) = nf(x),$$

therefore

$$\dot{q}p = \sum_i \dot{q}_i \frac{\partial \mathcal{L}}{\partial \dot{q}_i} = \sum_i \dot{q}_i \frac{\partial T}{\partial \dot{q}_i} = 2T(q, \dot{q}),$$

so we conclude that in this case the Hamiltonian is equivalent to the energy of the system, since

$$H(p,q) = \dot{q}p - \mathcal{L} = 2T - (T - V) = T + V.$$

We can also see that the Hamiltonian is a constant of the motion, since

$$\frac{d}{dt}H = \frac{d}{dt}(\dot{q}p) - \frac{d}{dt}\mathcal{L} = \frac{d}{dt}(\dot{q}p) - \left(\sum_i \frac{\partial \mathcal{L}}{\partial q_i}\frac{dq_i}{dt} + \frac{\partial \mathcal{L}}{\partial \dot{q}_i}\frac{d\dot{q}_i}{dt}\right)$$

$$\frac{d}{dt}(p\dot{q}) - \dot{p}\dot{q} - p\dot{q} = \frac{d}{dt}(p\dot{q}) - \frac{d}{dt}(p\dot{q}) = 0.$$

So, through this thesis we will consider the notation $E := H(p,q)$. we now define Hamilton's principal function,

$$W(q_A, q_B, t) = \int_0^t \mathcal{L}(q, \dot{q}) dt', \tag{A.7}$$

where $q_A := q(0)$ and $q_B := q(t)$. Note that this is basically the action with the starting time fixed at $t = 0$. We could rewrite this expression as

$$W(q_A, q_B, t) = \int_0^t (p\dot{q} - E)dt = \int_{q_A}^{q_B} (pdq - Et)dt. \tag{A.8}$$

This expression is easy to handle since the arguments of W are expressed explicitly. From equation (A.8) we find that

$$\frac{\partial W}{\partial q_{A_i}} = -p_{A_i}, \frac{\partial W}{\partial q_{B_i}} = p_{B_i} \text{ and } \frac{\partial W}{\partial t} = -E. \tag{A.9}$$

From equations (A.3) and (A.8) follows that

$$S(q_A, q_B, E) = W(q_A, q_B, t) + Et. \tag{A.10}$$

From the above equation we find that

$$\frac{\partial S}{\partial E} = \frac{\partial W}{\partial t}\frac{dt}{dE} + t + E\frac{dt}{dE} = t, \tag{A.11}$$

since $\frac{\partial W}{\partial t} = -E$ by equation (A.9). Hence, the relations for the partial derivatives of the action are given by

$$\frac{\partial S}{\partial q_{A_i}} = -p_{A_i}, \frac{\partial S}{\partial q_{B_i}} = p_{B_i} \text{ and } \frac{\partial S}{\partial E} = t. \tag{A.12}$$

Using all the above results we get the Hamilton-Jacobi differential equations

$$H\left(\frac{\partial S}{\partial q_B}, q_B\right) = H\left(-\frac{\partial S}{\partial q_A}, q_A\right). \tag{A.13}$$

APPENDIX B

Integral of some useful functions

In this appendix we will calculate some integrals used in this thesis

B.1 Fresnel integral

Here we will compute the general form of the Fresnel integral, and show that is equal to

$$\int_{-\infty}^{\infty} e^{iax^2} dx = \sqrt{\frac{\pi}{|a|}} e^{i\frac{\pi}{4}\mathrm{sgn}(a)}$$

, for $a \in \mathbb{R}\backslash\{0\}$. In order to do so, we first make the change of variables $y = \sqrt{|a|}e^{i\pi\left(\frac{1-sgn(a)}{4}\right)}$. From this we have

$$\int_{-\infty}^{\infty} e^{iax^2} dx = 2\int_{0}^{\infty} e^{iax^2} dx = \frac{2}{\sqrt{|a|}} e^{i\pi\left(\frac{sgn(a)-1}{4}\right)} \int_{0}^{\infty} e^{iy^2} dy \tag{B.1}$$

Now, since e^{iy^2} is an entire function, we have by the Cauchy-Goursat theorem that $\int_C e^{iy^2} dy = 0$ for any simple closed contour C [7] . In particular let C_R be the contour oriented in the positive direction consisting of $C_{R_1} := \{\sigma + it \in \mathbb{C} : 0 \leq \sigma < R, t = 0\}$, $C_{R_2} := \{s \in \mathbb{C} : |s| = R, 0 \leq arg(s) \leq \frac{\pi}{4}\}$ and $C_{R_3} := \{s \in \mathbb{C} : 0 < |s| \leq R, \arg(s) = \frac{\pi}{4}\}$, for some $R > 0$. Therefore we have

$$\begin{aligned}\oint_{C_R} e^{iy^2} dy &= \int_{C_{R_1}} e^{iy^2} dy + \int_{C_{R_2}} e^{iy^2} dy + \int_{C_{R_3}} e^{iy^2} dy \\ &= \int_0^R e^{iy^2} dy + \int_0^{\frac{\pi}{4}} e^{iR^2 e^{2i\theta}} iRe^{i\theta} d\theta - e^{i\frac{\pi}{4}} \int_0^R e^{-t^2} dt = 0. \end{aligned} \tag{B.2}$$

Now, notice that

$$\begin{aligned}
\left|\int_0^{\frac{\pi}{4}} e^{iR^2e^{2i\theta}} iRe^{i\theta}d\theta\right| &\leq \int_0^{\frac{\pi}{4}} |e^{iR^2e^{2i\theta}} iRe^{i\theta}|d\theta \\
= \int_0^{\frac{\pi}{4}} e^{-R^2\sin(2\theta)}Rd\theta &= \frac{R}{2}\int_0^{\frac{\pi}{2}} e^{-R^2\sin\theta}d\theta \\
\leq \frac{R}{2}\int_0^{\frac{\pi}{2}} e^{\frac{-2\theta R^2}{\pi}}d\theta &= -\frac{\pi}{4R}(e^{-R^2}-1),
\end{aligned} \tag{B.3}$$

where we have used the fact that $\sin\theta \geq \frac{2\theta}{\pi}$, for $0 \leq \theta \leq \frac{\pi}{2}$. Since the right hand side of equation (B.3) tends to zero as $R \to \infty$, we conclude that the second integral in equation (B.2) vanish as $R \to \infty$. Therefore,

$$\lim_{R\to\infty}\oint_{C_R} e^{iy^2}dy = \int_0^{\infty} e^{iy^2}dy - e^{\frac{i\pi}{4}}\int_0^{\infty} e^{-t^2}dt = 0,$$

where the last term is equal to $-e^{\frac{i\pi}{4}}\frac{\sqrt{\pi}}{2}$. We conclude from this and equation (B.1) that,

$$\begin{aligned}
\int_0^{\infty} e^{iy^2}dy &= \frac{\sqrt{\pi}}{2}e^{\frac{i\pi}{4}} \\
\Rightarrow \int_{-\infty}^{\infty} e^{iax^2}dx &= \frac{2}{\sqrt{|a|}}e^{i\pi\left(\frac{sgn(a)-1}{4}\right)}\frac{\sqrt{\pi}}{2}e^{\frac{i\pi}{4}} \\
&= \sqrt{\frac{\pi}{|a|}}e^{i\frac{\pi}{4}sgn(a)} \qquad \square
\end{aligned} \tag{B.4}$$

B.2 Stationary phase approximation

In this section we will give a brief explanation behind the ideas of the stationary phase approximation. For a more detailed analysis see [43]. We will try to approximate integrals of the form

$$I = \int_{-\infty}^{\infty} A(x)e^{\frac{i}{\hbar}\Phi(x)}dx,$$

in the semiclassical limit where $\hbar \to 0$. Since in this limit $\frac{1}{\hbar}\Phi(x)$ oscillates very fast, almost all contributions to the integral cancel, with the exception of the neighbourhoods of the points x_s such that $\Phi'(x_s) = 0$, which are called stationary points.

In order to calculate these contributions we expand $\Phi(x)$ in its Taylor series around the point x_s up to the quadratic term

$$\Phi(x) \approx \Phi(x_s) + \frac{(x-x_s)^2}{2}\Phi''(x_s).$$

If we assume $A(x)$ to be a smooth enough function, in which we can assume it to be nearly constant near x_s, then we can take it out of the integral and obtain

$$I \approx A(x_s)e^{\frac{i}{\hbar}\Phi(x_s)}\int_{-\infty}^{\infty} e^{\frac{i}{2\hbar}(x-x_s)^2\Phi''(x_s)}dx.$$

Note that if there are more stationary points the above expression becomes a summation over the stationary points, but we will keep the notation like this to keep it simple.

Now, notice that this integral is a Fresnel integral which we already calculate in the previous section, so we have that

$$\begin{aligned} I &\approx A(x_s)\sqrt{\frac{2\pi\hbar}{|\Phi''(x_s)|}}e^{\frac{i}{\hbar}\Phi(x_s)+\frac{i\pi}{4}sgn(\Phi''(x_s))} \\ &= A(x_s)\sqrt{\frac{2\pi\hbar}{|\Phi''(x_s)|}}e^{\frac{i}{\hbar}\Phi(x_s)}, \end{aligned} \tag{B.5}$$

taking $\sqrt{\Phi''(x_s)} = \sqrt{|\Phi''(x_s)|}e^{i\pi\left(\frac{1-sgn(\Phi''(x_s))}{4}\right)}$ and $\sqrt{i} = e^{\frac{i\pi}{4}}$. This result is called the *stationary phase approximation*; which can also be extended to $\mathbb{R}^d$, $d>1$. In this case a stationary point x_s is a point such that $\frac{\partial\Phi(x_s)}{\partial x_i} = 0$, for $i \in \{1,\ldots,d\}$. In this case the series expansion up to the quadratic term around x_s is

$$\Phi(s) \approx \Phi(x_s) + \frac{1}{2}(x-x_s)^\intercal Hess(\Phi(x_s))(x-x_s),$$

where $Hess(\Phi(x_s)) := \left(\frac{\partial\Phi(x)}{\partial x_i\partial x_j}\right)_{1\le i,j\le n}\Bigg|_{x=x_s}$ is the Hessian matrix of Φ. In this case

$$I \approx A(x_s)e^{\frac{i}{\hbar}\Phi(x_s)}\int_{\mathbb{R}^d} e^{\frac{i}{2\hbar}(x-x_s)^\top Hess(\Phi(x_s)(x-x_s)}dx_1\ldots dx_d,$$

without loss of generality we can assume $x_s = 0$; results for other x_s will be analogous by means of a simple transformation. Now, we write the term in the exponential of the integral as

$$x^\top Hess(\Phi(0))x = x_1^2\frac{\partial\Phi(0)}{\partial x_1^2} + 2\sum_{i=2}^{d} x_1x_i\frac{\partial^2\Phi(0)}{\partial x_1\partial x_i} + \sum_{\substack{i,j=2\\ i\neq j}}^{d} x_ix_j\frac{\partial^2\Phi(0)}{\partial x_i\partial x_j},$$

to be able to integrate over x_1. Define $a := \left(\frac{\partial^2\Phi(0)}{\partial x_1^2}\right)$, $b := 2\sum_{i=2}^{d} x_i\frac{\partial^2\Phi(0)}{\partial x_1\partial x_i}$. Make the changes of variables $x_1 = \frac{y_1}{\sqrt{a}} - \frac{b}{2a}$. From this we obtain a Fresnel integral for y_1

$$\begin{aligned} I &\approx A(0)e^{\frac{i}{\hbar}\Phi(0)}\int \exp\left(\frac{i}{2\hbar}\left(y_1^2 - \frac{b_1^2}{4a_1} + \sum_{\substack{i,j=2\\ i\neq j}}^{d} x_ix_j\frac{\partial^2\Phi(0)}{\partial x_i\partial x_j}\right)\right)dy_1dy_2\dots dy_d \\ &= A(0)e^{\frac{i}{\hbar}\Phi(0)}\sqrt{2\pi\hbar i}\left(\frac{\partial^2\Phi(0)}{\partial x_1^2}\right)^{-\frac{1}{2}} \\ &\quad \int \exp\left(\frac{i}{2\hbar}\left(\left(\sum_{i,j=2}^{d} x_ix_j\left(\frac{\frac{\partial^2\Phi(0)}{\partial x_1\partial x_j}\frac{\partial^2\Phi(0)}{\partial x_1\partial x_j}}{\frac{\partial^2\Phi(0)}{\partial x_1^2}}\right)\right) + x_ix_j\frac{\partial^2\Phi(0)}{\partial x_i\partial x_j}\right)\right)dx_2\dots dx_d. \end{aligned}$$

By a similar argument we could make a change of variables in order to obtain a Fresnel integral for x_2, which will result in

$$I \approx A(0)e^{\frac{i}{\hbar}\Phi(0)}(\sqrt{2\pi\hbar i})^2\left(\frac{\partial^2\Phi(0)}{\partial x_1^2}\frac{\partial^2\Phi(0)}{\partial x_2^2} - \left(\frac{\partial^2\Phi(0)}{\partial x_1\partial x_2}\right)^2\right)^{-\frac{1}{2}}\int e^{F(x_3,\dots,x_d)}dx_3,\dots,dx_d.$$

In general this process can be continued by transforming the integrals into Fresnel integrals for the x_i, resulting in the following expression

$$I \approx \frac{(2\pi i\hbar)^{\frac{d}{2}}}{\sqrt{|Hess(\Phi(0))|}}A(0)e^{\frac{i}{\hbar}\Phi(0)},$$

which by the above remarks will also be valid for arbitrary x_s, hence

$$I \approx \frac{(2\pi i\hbar)^{\frac{d}{2}}}{\sqrt{|Hess(\Phi(x_s))|}}A(x_s)e^{\frac{i}{\hbar}\Phi(x_s)} \qquad \square \tag{B.6}$$

B.3 Proof of proposition 3.3

Here we will prove that for real $\gamma, \gamma' > 0$,

$$\int_{-\infty}^{\infty} \frac{dt}{(1+(t-\gamma)^2)(1+(t-\gamma')^2)} = \frac{\pi}{2} w(\gamma - \gamma'),$$

where $w(u) = \frac{4}{4+u^2}$. In order to do so first define

$$f : \mathbb{C} \mapsto \mathbb{C},$$

$$f(z) := \frac{1}{(1+(z-\gamma)^2)(1+(z-\gamma')^2)}.$$

Now, consider the semicircular contour C_R in the upper half plane, of radius $R > 0$ and oriented in the positive direction. Hence,

$$\int_{C_R} f(z)dz = \int_{-R}^{R} \frac{1}{(1+(t-\gamma)^2)(1+(t-\gamma')^2)} dt + \int_0^{\pi} \frac{iRe^{i\theta}}{(1+(Re^{i\theta}-\gamma)^2)(1+(Re^{i\theta}-\gamma')^2)} d\theta. \tag{B.7}$$

Note that $|(1+(Re^{i\theta}-\gamma)^2)| = |(1+R^{2i\theta} - 2\gamma Re^{i\theta} + \gamma^2)| \geq |(2\gamma R - |(1+R^{2i\theta}+\gamma^2)|)| \geq |(2\gamma R - \gamma^2)|$. So, replacing the term in the second integral of equation (B.6) by $g(\theta)$, we get

$$\left| \int_0^{\pi} g(\theta) d\theta \right| \leq \int_0^{\pi} |g(\theta)| d\theta \leq \int_0^{\pi} \frac{R d\theta}{|(2\gamma R - \gamma^2)(2\gamma' R - \gamma'^2)|}$$
$$= \frac{\pi R}{|(2\gamma R - \gamma^2)(2\gamma' R - \gamma'^2)|} \longrightarrow 0, \text{ as } R \to \infty.$$

Therefore,

$$\lim_{R\to\infty} \oint_{C_R} f(z)dz = \int_{-\infty}^{\infty} \frac{1}{(1+(t-\gamma)^2)(1+(t-\gamma')^2)} dt.$$

The integral on the left of this expression is evaluated using calculus of residues, where

$$\lim_{R\to\infty} \oint_{C_R} f(z)dz = 2\pi i \sum \text{Res } f(z),$$

where the summation is over all residues of the poles of $f(z)$ inside C_R. Looking at the definition of $f(z)$ we see that its poles at $\gamma + i$ and $\gamma' + i$ are contained in C_R as

$R \to \infty$. Where

$$
\begin{aligned}
Res_{z=\gamma+i} f(z) &= \lim_{z\to\gamma+i} \frac{(z-(\gamma+i))}{(1+(z-\gamma)^2)(1+(z-\gamma')^2)} \\
&= \lim_{z\to\gamma+i} \frac{(z-(\gamma+i))}{(1+i(z-\gamma))(1-i(z-\gamma))(1-i(z-\gamma')^2)} \\
&= \lim_{z\to\gamma+i} \frac{-i}{(1-i(z-\gamma))(1-i(z-\gamma')^2)} \\
&= \frac{-i}{2((\gamma-\gamma')^2+2i(\gamma-\gamma'))},
\end{aligned}
$$

and by symmetry

$$
Res_{z=\gamma'+i} f(z) = \frac{-i}{2((\gamma'-\gamma)^2+2i(\gamma'-\gamma))}.
$$

Therefore,

$$
\begin{aligned}
&\int_{-\infty}^{\infty} \frac{1}{(1+(t-\gamma)^2)(1+(t-\gamma')^2)} dt = \lim_{R\to\infty} \oint_{C_R} f(z)dz \\
&= 2\pi i \left(\frac{-i}{2((\gamma-\gamma')^2+2i(\gamma-\gamma'))} + \frac{-i}{2((\gamma'-\gamma)^2+2i(\gamma'-\gamma))} \right) \\
&= \frac{2\pi(\gamma-\gamma')^2}{(\gamma-\gamma')^4+4(\gamma-\gamma')^2} \\
&= \frac{\pi}{2} \frac{4}{4+(\gamma-\gamma')^2} \\
&= \frac{\pi}{2} w(\gamma-\gamma').
\end{aligned}
$$

Note that in the above calculation we assumed that $\gamma \neq \gamma'$. If $\gamma = \gamma'$ then the integral is equal to

$$
\begin{aligned}
\int_{-\infty}^{\infty} \frac{1}{(1+(t-\gamma)^2)^2} dt &= \int_{-\infty}^{\infty} \frac{1}{(1+t^2)2} dt \\
&= \frac{1}{2} \left(\frac{t}{t^2+1} + \arctan(t) \right|_{-\infty}^{\infty} \\
&= \frac{\pi}{2} = \frac{\pi}{2} w(0). \qquad \square \qquad \text{(B.8)}
\end{aligned}
$$

APPENDIX C

Monodromy matrix

In this section we will give a brief discussion about the Monodromy matrix, which serves to indicate the variations on later states of a dynamical system, given a small change in the initial variables.

More specifically, consider that a trajectory, which a particle traverse, starts at a position q_A with momentum p_A and ends at a position q_B with momentum p_B. And now, consider a slight variation is made on the initial conditions; now the initial position and momentum are $q_A + \delta q_{A_\perp}$ and $p_A + \delta_{A_\perp}$ respectively. where the "$\perp$"-sign indicates the change is made perpendicular to the trajectory. The Monodromy matrix M_{BA} gives a linear approximation for obtaining the changes $\delta q_{B_\perp}$ and $\delta p_{B_\perp}$ on the final states, i.e.

$$\begin{pmatrix} \delta q_{B_\perp} \\ \delta p_{B_\perp} \end{pmatrix} = M_{BA} \begin{pmatrix} \delta q_{A_\perp} \\ \delta p_{A_\perp} \end{pmatrix}. \tag{C.1}$$

Is clear from the dimensions of $\delta q_{A_\perp}$ and $\delta p_{A_\perp}$ that M_{BA} is an $(d-1) \times (d-1)$ matrix, where d is the dimension of the system.

The relations for the partial derivatives of the action, see (A.12), can be used to calculate the components of M_{BA}. Consider the equations

$$p_A = -\frac{\partial S}{\partial q_A}, \qquad p_B = \frac{\partial S}{\partial q_B}.$$

If now q_A is replaced by $q_A + \delta q_A$, p_A by $p_A + \delta p_A$, q_B by $q_B + \delta q_B$ and p_B by $p_B + \delta p_B$, and if the right hand side from both equations is expanded up to the linear terms, we will find that

$$\begin{aligned}
\delta p_{A_\perp} &= -\frac{\partial^2 S}{\partial q_{A\perp}^2}\delta q_{A_\perp} - \frac{\partial^2 S}{\partial q_{A_\perp}\partial q_{B_\perp}} \\
\delta q_{B_\perp} &= -S_{AA}\delta q_{A\perp} - S_{AB}\delta q_{B_\perp} \\
\delta p_{B_\perp} &= S_{AB}\delta q_{A_\perp} + S_{BB}\delta q_{B_\perp},
\end{aligned}$$

which imply, by rearranging the equations, that:

$$\begin{aligned}
\delta q_{B_\perp} &= -S_{AB}^{-1}S_{AA}\delta q_{A_\perp} - S_{AB}^{-1}\delta q_{A_\perp} \\
\delta p_{B_\perp} &= S_{AB}\delta q_{A_\perp} + S_{BB}\delta q_{B_\perp}
\end{aligned}, \tag{C.2}$$

where we have introduced the notation $S_{AA} := \frac{\partial^2 S}{\partial q_{A_\perp}^2}$, $S_{AB} := \frac{\partial^2 S}{\partial q_{A_\perp}\partial q_{B_\perp}}$, etc.

Comparing equation (C.1) and (C.2), we see that the Monodromy matrix is given by

$$M_{BA} = \begin{pmatrix} -S_{AB}^{-1}S_{AA} & -S_{AB}^{-1} \\ S_{AB} - S_{BB}S_{AB}^{-1}S_{AA} & -S_{BB}S_{AB}^{-1}. \end{pmatrix}$$

In this thesis our interest is to compute an expression for the determinant of $M_{BA}-1$, which will help us to simplify the final expression for the Gutzwiller Trace formula in chapter 4. We have that:

$$\begin{aligned}
|M_{BA}-1| &= \begin{vmatrix} -S_{AB}^{-1}S_{AA} & -S_{AB}^{-1} \\ S_{AB} - S_{BB}S_{AB}^{-1}S_{AA} & -S_{BB}S_{AB}^{-1} \end{vmatrix} \\
&= \begin{vmatrix} -1 & -1 \\ S_{AB}+S_{AA} & -S_{AB}-S_{BB} \end{vmatrix} \cdot \begin{vmatrix} 1 & 0 \\ S_{AB}^{-1}S_{AA} & S_{AB}^{-1} \end{vmatrix} \\
&= \frac{|S_{AA}+2S_{AB}+S_{AA}|}{|S_{AB}|}.
\end{aligned} \tag{C.3}$$

APPENDIX D

WKB approximation

The WKB approximation named after Gregor Wentzel, Hendrik Kramers and Léon Brillouin, is a method used to approximate the solutions of a differential equation in which the term with the equation in which the term with the highest derivative is multiplied by a very small constant; $\hbar^2$ in our case of interest.

We will follow Messiah in this short review [44], which will only cover the case of the Schrödinger equation in one dimension.

Consider the wave function $\Psi(x,t) = A(x,t)e^{\frac{i}{\hbar}S(x,t)}$, satisfying the Schrödinger equation

$$\Psi'' + \frac{2m}{\hbar^2}(E - V(x))\Psi = 0.$$

This implies the equivalent equations,

$$S'^2 - 2m(E - V) = \hbar^2 \frac{A''}{A}, \tag{D.1}$$

$$2A'S' + AS'' = 0. \tag{D.2}$$

If we rearrange the last equation and integrate it we obtain

$$\frac{2A'}{A} = \frac{-S''}{S'} \Rightarrow \int \frac{2A'}{A} dx = \int \frac{-S''}{S'} dx \Rightarrow 2\ln(A) = \ln(S') + C,$$

where C is a constant,

$$\Rightarrow A = K(S')^{\frac{1}{2}},$$

with K constant.

If we insert this expression into equation (D.1) with $K = 1$, we get

$$S'^2 = 2m(E - V) + \hbar^2 \left(\frac{3}{4} \left(\frac{S''}{S'} \right)^2 - \frac{1}{2} \frac{S'''}{S'} \right). \tag{D.3}$$

This is now a third order differential equation that is equivalent to the Scrödinger equation. The WKB approximation starts by expanding S in a power series in $\hbar^2$,

$$S = S_0 + \hbar^2 S_1 + \hbar^4 S_2 + \dots,$$

and then substituting this expansion into equation (D.3), keeping only zero-order terms, in order to get

$$S'^2 \approx S'^2_0 = 2m(E - V(x)).$$

The approximate solution will depend on whether $E > V(x)$ of $E < V(x)$.

Case one: $E > V(x)$. (Classical region)

In this case, we define the wavelength

$$\lambdabar = \frac{\hbar}{\sqrt{2m(E - V(x))}}.$$

The WKB solution in this case is a linear combination of sinusoidal functions

$$\Psi(x) = \alpha\sqrt{\lambdabar}\cos\left(\int_0^x \frac{dx'}{\lambdabar} + \varphi\right) + \beta\sqrt{\lambdabar}\sin\left(\int_0^x \frac{dx'}{\lambdabar} + \gamma\right),$$

for α, β, φ and γ constants.

Case two: $E < V(x)$ (forbidden region for classical particles).

In this case we define the wavelength

$$\ell(x) = \frac{\hbar}{\sqrt{2m(V(x) - E)}}.$$

The WKB solution is now given by a linear combination of exponentials

$$\Psi(x) = \sqrt{\ell}\left(\delta \exp\left(\int_0^x \frac{dx'}{\ell}\right) + \sigma \exp\left(-\int_0^x \frac{dx'}{\ell}\right)\right),$$

for δ, σ constants.

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