Delft University of Technology
Bachelor Thesis
Applied Mathematics - Applied Physics

The Hilbert-Pólya Conjecture and the Prolate Spheroidal Operator

---

Nino Corak
September 27, 2023

Committee:
J.M.A.M. van Neerven (supervisor)
O. El Gawhary (supervisor)
E. Emsiz
F. Bociort

Contents

1 Introduction

One of the most longstanding and important open problems in mathematics is the *Riemann hypothesis*. Simply stated, it concerns the locations of the zeroes of a certain complex function $\zeta(z)$, called the Riemann zeta function. There is a certain sense in which these zeroes determine the distribution of prime numbers amongst the natural numbers. It is this fact which yields the Riemann hypothesis its importance, primarily in the field of number theory.

Although the Riemann hypothesis is a statement made in the context of analytic number theory, the Riemann zeta function itself and its generalisations make many appearances outside number theory. This should not be too surprising, as it is after all just a complex function which is relatively easy to define and which happens to be related to the distribution of prime numbers through analytic number theory. However, these appearances outside number theory suggest several ways of proving the Riemann hypothesis. Among these are possible proof strategies which arise from physics or from physical interpretations of the zeroes, making the study of the Riemann hypothesis in this fashion an interesting border case between mathematics and physics.

A suggestion which has been raised within this line of thinking is that the non-trivial zeroes of the Riemann zeta function, when properly rotated and shifted, might constitute the spectrum of a certain self-adjoint operator, which could represent an observable of some quantum system. This has come to be known as the *Hilbert-Pólya conjecture*, which was independently suggested by Hilbert and Pólya in the early 20th century, even though they themselves did not work on the Riemann hypothesis. Throughout the second half of the 20th century, indications supporting the conjecture arose, both mathematical and physical. However, it was only until the end of the 20th century that concrete results were obtained when Alain Connes conjectured a trace formula equivalent with the Riemann hypothesis.

Since the publication of Connes' trace formula, little progress has been made in the direction of proving the Hilbert-Pólya conjecture, and this program is now seen by some as a dead end, with Connes' reformulation of the Riemann hypothesis being no easier to prove than the hypothesis itself. However, a recent article [Connes and Moscovici, 2022] could potentially breath new life into the conjecture. In Connes' original work, the differential operator

$$W = -\frac{d}{dx}\left((\lambda^2 - x^2)\frac{d}{dx}\right) + (2\pi\lambda x)^2$$

with parameter λ plays an important, though auxiliary role in the derivation of his trace formula. It is called the *prolate spheroidal operator* and its eigenfunctions on the interval $(-\lambda, \lambda)$, known as prolate spheroidal wave functions, have important applications in signal analysis. Connes has now discovered that the eigenvalues of this operator, when defined on the larger domain $(-\infty, \infty)$ and extended to a uniquely defined self-adjoint operator, are asymptotically similar to the squares of the Riemann zeta zeroes. Taking an appropriate square root of this operator yields a concrete instance of an operator which approximately solves the Hilbert-Pólya conjecture. This unexpected discovery seems to indicate that the relationship between the prolate spheroidal operator and the Riemann zeta function is deeper than it appears to be. Explaining this relationship could form an exciting area of research. The goal of this thesis, however, will not be to contribute to this research, but to provide mathematical and physical context to Connes and Moscovici's article and to explain in more detail its reasoning.

1.1 Outline

Starting with physics, in Section 2 we give a short introduction to the Riemann hypothesis and present the physical indications of a Hilbert-Pólya proof of the Riemann hypothesis. The first of these, the pair correlation conjecture, is the conjecture by Montgomery and subsequent numerical corroboration by Odlyzko that the Riemann zeta zeroes share statistics with random matrix models, used for example in the modelling of nuclei. The second was the analogy between Riemann zeta zeroes and the energy values of a chaotic quantum system made by Berry. In addition, Berry and Keating proposed a classical system of which a quantisation may have the Riemann zeta zeroes as spectrum.

Section 3 provides details which were left out in [Connes and Moscovici, 2022]. We cover all parts of the article expect for Sections 3 and 6. The first subsection presents the theory of self-adjoint extensions, which is the most important tool used in the article. The next four subsections detail the construction of the specific self-adjoint prolate spheroidal operator that Connes and Moscovici consider. Its spectrum is consequently analysed, using a non-rigorous application of Weyl's law. Using the constructed operator, the final subsection indicates how one may construct from it a Dirac operator whose spectrum is asymptotically similar to the Riemann zeta zeroes.

1.2 Prerequisites

The most important mathematical prerequisite for this thesis is familiarity with operator theory, especially with unbounded operators and the notion of a spectrum. A classical reference for operator theory is [Akhiezer and Glazman, 1981a] and [Akhiezer and Glazman, 1981b]. A more modern text concerning functional analysis in general is [van Neerven, 2022]. Some results on orthogonal decompositions of operators have been included in Appendix A for convenience. Also required is sufficient familiarity with measure-theoretic integration and differential equations. For the first topic, we recommend [Rudin, 1986], while [Braun, 1992] is a good reference for the second. Some facts about absolute continuity and distribution theory are required. Because these do not usually appear in undergraduate mathematics courses and can be tedious to find in literature, we have included two more appendices which contain the necessary results and references for further study. Finally, the reader should also have some familiarity with physics, specifically with the Hamiltonian formulation of classical mechanics and with the basics of quantum mechanics. One can consult any standard textbook on these topics, for example [Goldstein et al., 2001] and [Griffiths and Schroeter, 2018].

1.3 Conventions

Integrals. Throughout this thesis, integrals are always taken in the sense of Lebesgue, i.e. as defined in measure theory with respect to the Lebesgue measure. We will only need one-dimensional integrals. The integral of a function $f(x)$ over a set A will be denoted by

$$\int_A f(x)\,dx.$$

Furthermore, the notation

$$\int_a^b f(x)\,dx$$

will be taken to mean the integral of $f(x)$ over $[a, b]$ if $a \leq b$ or the negative of this integral if $a \geq b$.

Inner product. We use the physicist's convention for Hilbert space inner products, meaning the first argument is ant-linear, while the second is linear. For $L^2(\mathbb{R})$, this means that we choose the inner product

$$\langle \xi, \eta \rangle = \int_{\mathbb{R}} \overline{\xi(x)} \eta(x) \, dx.$$

Asymptotics. The reader should be familiar with asymptotic notation. Specifically, the notation $f(x) = g(x) + O(h(x))$ means that the difference $|f(x) - g(x)|$ is bounded by $C|h(x)|$ as $x \to \infty$ for some constant $C > 0$, and $f(x) = g(x) + o(h(x))$ means that

$$\lim_{x \to \infty} \frac{|f(x) - g(x)|}{|h(x)|} = 0.$$

Indicator functions. We denote the indicator function of the set $A \subseteq \mathbb{R}$ by $\mathbf{1}_A$, defined as

$$\mathbf{1}_A(x) = \begin{cases} 1 & x \in A \\ 0 & x \notin A. \end{cases}$$

2 The Riemann Hypothesis and Physics

We give here a short introduction to the Riemann hypothesis and its importance to number theory. The Hilbert-Pólya conjecture will also be introduced and we present physical indications for it. A fuller introduction to the Riemann hypothesis, including proofs of important theorems, may be found in [Edwards, 1974] and [Titchmarsh, 1986]. For an introduction to the techniques of complex analysis, one may consult [Stein and Shakarchi, 2003], which also includes two chapters on the Riemann zeta function.

2.1 Riemann hypothesis

The Riemann zeta function is defined for complex numbers with real part $\Re(s) > 1$ by the absolutely convergent infinite series

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

Riemann showed that this function may be analytically extended to a meromorphic function on $\mathbb{C}$, having a simple pole at $s = 1$, satisfying the functional equation

$$\zeta(s) = 2^s \pi^{s-1} \sin\left(\frac{\pi s}{2}\right) \Gamma(s-1)\zeta(s-1). \tag{2.1}$$

Here $\Gamma(s)$ is the gamma function, itself a meromorphic function on $\mathbb{C}$ and a generalisation of the factorial operation $n!$. The extended function is also called the Riemann zeta function. Even though it is named after Bernhard Riemann, it was first defined by Leonhard Euler in the 18th century for real $s > 1$ in connection with his work on prime numbers. It was Euler who discovered the important product formula

$$\zeta(s) = \prod_{p \text{ prime}} \frac{1}{1 - p^{-s}} \tag{2.2}$$

which was of central importance in Riemann's classical paper [Riemann, 1859] relating the distribution of prime numbers to the Riemann zeta function. This relation consists of a formula connecting the prime number counting function

$$\pi(x) = \text{number of primes } p \leq x.$$

to the zeroes of the Riemann zeta function. The prime number counting function $\pi(x)$ was already studied by mathematicians of the 18th century, who conjectured that $\pi(x)$ is asymptotically equal to the logarithmic integral

$$\mathrm{li}(x) = \int_0^x \frac{dt}{\log t}.$$

Riemann went a step further and gave an explicit formula for the prime number counting function. This formula reads

$$\pi(x) = \sum_{n=1}^{\infty} \frac{\mu(n)}{n} J(x^{\frac{1}{n}}),$$

in which $\mu(n)$ is the Möbius function (see [Edwards, 1974]) and the function $J(x)$ depends on the zeroes ρ of the Riemann zeta function through the formula

$$J(x) = \mathrm{li}(x) - \sum_{\rho} \mathrm{li}(x^{\rho}) + \int_{x}^{\infty} \frac{dt}{t(t^2-1)\log t} - \log 2. \tag{2.3}$$

However, not all zeroes of the Riemann zeta function enter in the formula (2.3). From the functional equation (2.1), it follows that all negative even integers are zeroes of the Riemann zeta function. These are called the trivial zeroes. It can be proven that any other zeroes must lie within the so-called critical strip $0 < \Re(s) < 1$ and that they are located symmetrically around the real axis and the so-called critical line $\Re(s) = 1/2$. These zeroes are the ones that enter into (2.3) and are called the non-trivial zeroes. Numerically, these zeroes appear to all be simple and lie on the critical line. This observation allows us to formulate the Riemann hypothesis.

Conjecture 2.1. (Riemann hypothesis) All non-trivial zeroes of the Riemann zeta function $\zeta(s)$ lie on the critical line $\Re(s) = 1/2$.

Much effort has been given to prove this conjecture, as the knowledge that all non-trivial zeroes lie on the critical line combined with the formula (2.3) gives precise information on the distribution of prime numbers and hence implies many number theoretical results. It has for example been proven by Hardy that there are infinitely many zeroes on the critical line and by Conrey that at least 40% of non-trivial zeroes lie on the critical line. To this day, no definitive proof has been found that indeed all non-trivial zeroes lie on the critical line, though many strongly suspect this to be true.

In the study of the non-trivial zeroes of the Riemann zeta function, one quantity which is of interest is the zero counting function $N(T)$, defined as the number of non-trivial zeroes with imaginary part in the interval $[0, T]$. One may derive an asymptotic formula for this counting function (see [Titchmarsh, 1986]), given by

$$N(T) = \frac{T}{2\pi}\log\left(\frac{T}{2\pi}\right) - \frac{T}{2\pi} + \frac{7}{8} + \frac{1}{\pi}\arg\left(\zeta\left(\frac{1}{2}+iT\right)\right) + O(T^{-1}). \tag{2.4}$$

Looking at this formula and ignoring the asymptotic error, it may be seen that it decomposes into a gradually increasing part

$$\langle N(T)\rangle = \frac{T}{2\pi}\log\left(\frac{T}{2\pi}\right) - \frac{T}{2\pi} + \frac{7}{8} \tag{2.5}$$

and a rapidly fluctuating term

$$N_{\mathrm{fl}}(T) = \frac{1}{\pi}\arg\left(\zeta\left(\frac{1}{2}+iT\right)\right). \tag{2.6}$$

We think of $\langle N(T)\rangle$ as the mean number of zeroes with imaginary part in $[0, T]$ and of $N_{\mathrm{fl}}(T)$ as the fluctuation around this mean. Making use of the product formula (2.2) in the fluctuating part (2.6), one obtains the formal expression

$$N_{\mathrm{fl}}(T) = -\frac{1}{\pi}\sum_{p}\sum_{m=1}^{\infty}\frac{\exp\left(-\frac{1}{2}m\log p\right)}{m}\sin\left(mT\log p\right) \tag{2.7}$$

which expresses the fluctuating part of the counting function as a series of oscillatory contributions labelled by prime powers p^m. We will return to this counting function in the next subsection, in which

we interpret its mean and fluctuating parts physically, and in Section 3 when deriving the asymptotics of the spectrum of the prolate spheroidal operator and the derived Dirac operator constructed in [Connes and Moscovici, 2022].

2.2 Hilbert-Pólya conjecture

Denote the sequence of non-trivial Riemann zeta zeroes with positive imaginary part by $\rho_n = \sigma_n + it_n$ and define the sequence

$$E_n = \frac{1}{i}\left(\rho_n - \frac{1}{2}\right) = t_n + i\left(\frac{1}{2} - \sigma_n\right).$$

The statement that all zeroes satisfy $\sigma_n = 1/2$ is obviously equivalent to all quantities E_n being real. Pictorially, this corresponds to shifting and rotating the domain of the Riemann zeta function such that the critical line becomes the real axis. A possible explanation for the reality of the E_n is that they correspond to the eigenvalues, or more generally the spectrum of some self-adjoint operator H on some Hilbert space $\mathcal{H}$. This idea was first conjectured by Hilbert and Pólya in the early 20th century[1].

Conjecture 2.2. (Hilbert-Pólya) There exists a self-adjoint operator on some Hilbert space whose spectrum coincides with the non-trivial zeroes of the Riemann zeta function, when appropriately rotated and shifted.

We call such an operator a Hilbert-Pólya operator. The obvious physical interpretation of this conjecture is that the Hilbert space $\mathcal{H}$ corresponds to some quantum system and the self-adjoint operator H to an observable of that system, the most likely candidate being the Hamiltonian. The numbers E_n are then the energies of this quantum system. However, this physical interpretation was not made by Hilbert and Pólya, as their conjecture was made during the days of the old quantum theory, before the connection between operator theory and quantum mechanics was made. Furthermore, Hilbert did not even ascribe a physical interpretation to his conjecture.

The first mathematical indication supporting the Hilbert-Pólya conjecture was the Selberg trace formula, which we do not discuss in this thesis. More important to the current section are the physical motivations, which will now be presented. The main line of thinking in physical interpretations of the Riemann hypothesis is that the non-trivial zeroes correspond to the energy levels of some quantum system. Recall that the possible energy values of a quantum system are not continuous, but form a discrete set of energy levels. These often cannot be computed exactly, hence physicists resort to calculating derived properties of the energy spectrum, such as the number of energy levels with values in an interval $[0, E]$, which may be easier. This is similar to the situation with the Riemann hypothesis, in which the Riemann zeta zeroes themselves are intractable, but something like the counting function $N(T)$ is more manageable. If it is possible to show that these 'statistics' derived from the Riemann zeta zeroes satisfy the same patterns as those derived from physical systems, then this could be seen as an indication that a Hilbert-Pólya operator exists.

2.2.1 Pair correlation conjecture

The first such statistic was discovered by Montgomery and Dyson in 1973, and its physical interpretation came from the theory of random matrices. We do not discuss the theory of random matrices in

[1] According to a correspondence between Pólya and Odlyzko, Pólya conjectured it in the years 1912 - 1914. The attribution to Hilbert, who apparently informally conjectured it in the years 1904 - 1909, is due to Hellinger.

detail. The reader may consult [Mehta, 1967], [Kota, 2012] and [Weidenmüller and Mitchell, 2009] for better introductions. The use of random matrices in physics first arose in the study of nuclear energy levels. Before the quantum field theory of the strong interaction was laid out, the precise nature of the interactions within a nucleus were unknown. Hence, physicists had to resort to approximate models of the nucleus for the calculation of nuclear energy levels. According to quantum theory, these energy levels should be given by the eigenvalues, or spectrum, of some Hamiltonian on a Hilbert space. But, because the nuclear Hamiltonian was unknown, Eugene Wigner proposed to replace it with a statistical ensemble of Hamiltonians which do not have any specific properties other than generic properties, for example dictated by symmetry considerations.

For each physical system that is to be modelled using random matrices, one needs to choose an appropriate ensemble of random matrices. It was shown by Dyson that there are three important ensembles which generally occur in the modelling of physical systems. These are the Gaussian orthogonal ensemble GOE(n), the Gaussian unitary ensemble GUE(n) and the Gaussian symplectic ensemble GSE(n) of $n \times n$ matrices. The assumption that large nuclei are described by Gaussian distributions is justified by the central limit theorem. These ensembles are defined by what kind matrices they consist of and under what kind of transformations their distributions are invariant (see Table 1).

Table 1: Three main types of random matrix ensembles

Ensemble	Matrix Type	Invariant under
GOE(n)	Real symmetric	Orthogonal conjugation
GUE(n)	Complex Hermitian	Unitary conjugation
GSE(n)	Quaternionic Hermitian	Conjugation by symplectic matrices

For example, the joint probability distribution of the Gaussian unitary distribution, which will be the only ensemble of concern here, may be expressed in terms of the eigenvalues $\lambda_1, \dots, \lambda_n$ of the matrix (see [Mehta, 1967]), giving

$$P(\lambda_1, \dots, \lambda_n) = C \exp\left(-\frac{1}{2}\sum_{i=1}^{n} \lambda_i^2\right) \prod_{\substack{i,j=1 \\ i<j}}^{n} |\lambda_i - \lambda_j|^2, \tag{2.8}$$

in which C is a normalisation constant. An important statistic which can be derived from this distribution is the k-point correlation function. This is essentially a marginal distribution, defined by

$$R_k(\lambda_1, \dots, \lambda_k) = \frac{n!}{(n-k)!} \int P(\lambda_1, \dots, \lambda_n)\, d\lambda_{n+1} \dots d\lambda_n. \tag{2.9}$$

Thus, $R_k(\lambda_1, \dots, \lambda_k)\, d\lambda_1 \dots d\lambda_k$ is the probability of finding an eigenvalue in each of the infinitesimal intervals $(\lambda_i, \lambda_i + d\lambda_i)$ for $i = 1, \dots, k$. The combinatorial factor in (2.9) reflects that fact that it makes no difference which eigenvalues appear in these intervals and stems from the fact that the distribution (2.8) is invariant under permutation of the eigenvalues. Of particular importance is the two-point correlation function $R_2(\lambda_1, \lambda_2)$. For the Gaussian unitary ensemble, one can show that the two-point correlation is asymptotically given by

$$1 - \left(\frac{\sin \pi(\lambda_1 - \lambda_2)}{\pi(\lambda_1 - \lambda_2)}\right)^2 \tag{2.10}$$

in the large matrix limit $n \to \infty$ under the assumption that the eigenvalues are rescaled so as to have mean spacing 1. This is a function depending only on the difference $\lambda_1 - \lambda_2$, leading us to define

$$R_2(r) = 1 - \left(\frac{\sin \pi r}{\pi r}\right)^2.$$

The corresponding form factor $K(\tau)$ is defined as the Fourier transform of this function. Using the Fourier transform convention of [Berry, 1986], opposite to the one used in this thesis (see equation (3.4)), the two-point form factor of the Gaussian unitary ensemble then becomes

$$K_{\mathrm{GUE}}(\tau) = \begin{cases} |\tau|, & |\tau| < 1 \\ 1, & |\tau| \geq 1. \end{cases}$$

This result leads to a physical interpretation of mathematical work done by Montgomery in 1973 on the Riemann zeta zeroes [Montgomery, 1973]. He investigated what is essentially the form factor of the zeroes, which according to [Berry, 1986] can be written as

$$K(\tau) = \lim_{M \to \infty} \left(\frac{1}{M} \sum_{n,m=1}^{M} \exp(2\pi i \tau (x_n - x_m)) - \frac{\sin(M\pi\tau)}{\pi\tau} \right).$$

Here, the zeroes t_n have been replaced by transformed versions x_n, so as to make the mean spacing between the zeroes equal to 1 (which was also done in computing the two-point correlation of the GUE). According to (2.5), this amounts to setting $x_n = \langle N(t_n) \rangle$. Assuming the Riemann hypothesis to be true, Montgomery proved that for $|\tau| < 1$ the form factor is given by $K(\tau) = |\tau|$. As this is essentially information about the Fourier transform of the differences $x_i - x_j$ of the zeroes, one can convolve this Fourier transform with appropriate kernels to obtain information on functions of these differences. In this manner, Montgomery proved for example that the fraction of simple Riemann zeta zeroes is at least 2/3, assuming the Riemann hypothesis is true. Montgomery also gave heuristic reasons for the equality $K(\tau) = 1$ for $|\tau| \geq 1$. This led him to the following conjecture, called the 'pair correlation conjecture'.

Conjecture 2.3. (Montgomery) The form factor of the Riemann zeta zeroes is given by

$$K(\tau) = \begin{cases} |\tau|, & |\tau| < 1 \\ 1, & |\tau| \geq 1. \end{cases}$$

The conjecture thus asserts that the Riemann zeta zeroes have the same form factor as the Gaussian unitary ensemble of random Hermitian matrices. This amounts to their two-point correlation functions being the same. Indeed, one (not completely precise) reformulation of Montgomery's conjecture states that

$$\#\left\{(n,m) \mid 1 \leq x_n, x_m \leq N, x_n - x_m \in [\alpha, \beta]\right\}$$

is asymptotically equal to

$$N \int_{\alpha}^{\beta} \left(1 - \left(\frac{\sin \pi r}{\pi r}\right)^2\right) dr \tag{2.11}$$

as $T \to \infty$ for all $0 < \alpha < \beta$. When Montgomery showed his result to Dyson, one of the pioneers of the use of random matrix theory in nuclear physics, it was he who recognised the GUE statistics

manifest in Montgomery's result. One can even go further and conjecture that the zeroes obey GUE statistics in general, for example that all k-correlation functions are identical to those of the GUE. This hypothesis was numerically tested by Odlyzko (see Fig. 1), publishing his findings in [Odlyzko, 1987]. He found that indeed many statistics of the Riemann zeta zeroes agree with those of the GUE, though in certain regimes this correspondence breaks down, as predicted by [Berry, 1986].

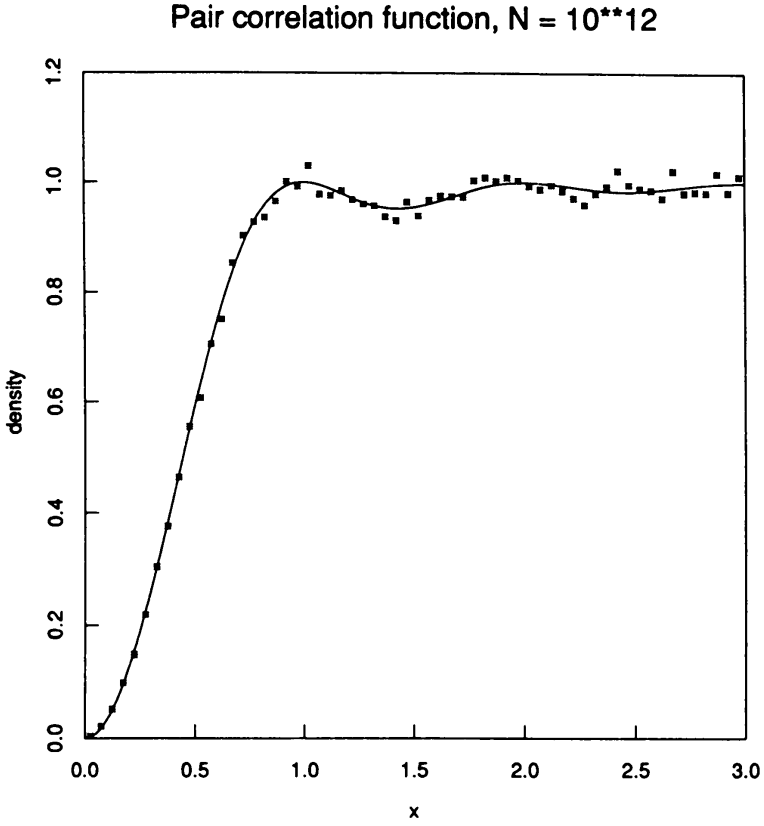

Figure 1: Odlyzko's numerical calculation of the pair correlation function of the Riemann zeta zeroes (black squares) plotted alongside the GUE pair correlation function (2.10). Figure taken from [Odlyzko, 1987].

Odlyzko's numerical corroboration of the pair correlation conjecture thus seems to suggest that, to a certain extent, the Riemann zeta zeroes obey GUE statistics. That is, if the zeroes were sampled from a distribution, then that distribution would seem to have GUE statistics. This supports the existence of an infinite-dimensional Hermitian matrix (a self-adjoint operator on an infinite-dimensional Hilbert space) having the zeroes as eigenvalues, as GUE statistics are characteristic of the spectra of random Hermitian matrices.

2.2.2 Quantum chaos

It turns out that the counting function $N(T)$ of the Riemann zeta zeroes is also a 'statistic' of the zeroes that can be given a physical interpretation. This was first realised by [Berry, 1986] and requires some knowledge of chaotic systems. Recall that a classical system is said to be integrable if it has enough independent conserved quantities to restrict the orbits to a low-dimensional submanifold of the phase space. Non-integrable systems, which do not have enough conserved quantities to tame its orbits, are said to exhibit chaotic behaviour. While there may exist tame periodic orbits in such systems, there will also be a lot of unstable orbits which are very sensitive to initial conditions. A good example of such a system is billiards on a non-symmetric table.

Given a classical system, one may quantise it to obtain the corresponding quantum system. The question may then be asked what the relation is between chaos in the classical system and chaos in the quantum system. A famous and important conjecture on this matter, which holds good for many systems, is the Bohigas-Giannoni-Schmit conjecture (see [Weidenmüller and Mitchell, 2009]), which states that the energy spectrum of a chaotic quantum system is actually distributed according to one of the fundamental ensembles of random matrix theory (see Table 1), while the eigenvalues of a quantisation of an integrable system are expected to be independently distributed. From this, one can already see that the Riemann zeta zeroes might have some relation to quantum chaos from the fact that they obey GUE statistics, as we saw earlier.

Berry gave a more direct argument for the analogy with quantum chaos (see [Berry, 1986] and [Berry and Keating, 1999b]). Given a quantum system, chaotic or not, one defines the energy level counting function $N(E)$ as the number of energy levels in the interval $[0, E]$[2]. As with the counting function of the Riemann zeta zeroes, it will generally be decomposable into a mean part and a fluctuating part,

$$N(E) = \langle N(E) \rangle + N_{\text{fl}}(E).$$

The asymptotics of $N(E)$ can obtained using semiclassical techniques, which involve the approximation of the quantum system by a corresponding classical system. The Wilson-Sommerfeld quantisation rule and the WKB approximation, two famous semiclassical methods, are not applicable to chaotic systems, as pointed out by Einstein (see [Stone, 2005]). However, a method for semiclassically analysing chaotic quantum systems has been developed by Gutzwiller in the 1970's. His method yields asymptotic information on the energy spectrum by relating it to the periodic orbits of the corresponding classical system. More precisely, the periodic orbits determine the fluctuating part, giving the asymptotic formula

$$N_{\text{fl}}(E) \sim \frac{1}{\pi} \sum_p \sum_{m=1}^{\infty} \frac{\sin\left(mS_p(E)/\hbar - \pi m \mu_p/2\right)}{m\sqrt{\left|\det\left(M_p^m - I\right)\right|}} \tag{2.12}$$

as $E \to \infty$. There is quite a lot to explain in this complicated formula. First, p labels the primitive periodic orbits of the classical system and

$$S_p(E) = \oint_p \mathbf{p} \cdot d\mathbf{q}$$

is the action of the orbit. The qualifier 'primitive' means that the orbit does not return to its starting point more than once. Repetitions of these primitive orbits contribute to the sum and are indexed

[2]Because energy may be freely shifted, we may as well define the lowest energy level to be at zero.

by m. The matrix M_p is called the monodromy matrix and essentially quantifies how orbits nearby p diverge from p (I is the identity matrix and det is the determinant operation). Finally, the numbers μ_p are the Maslov phases of the orbits, which are related to Maslov corrections appearing for example in the WKB approximation. For long orbits, the determinant involving the monodromy matrix may be approximated in terms of the Lyapunov exponent λ_p of the orbit, which measures the exponential divergence of orbits near p, giving

$$\det(M_p^m - I) \sim \exp(m\lambda_p T_p),$$

with T_p the period of the orbit p. The use of this approximation in Gutzwiller's formula (2.12) yields the asymptotic formula

$$N_{\text{fl}}(E) \sim \frac{1}{\pi} \sum_p \sum_{m=1}^{\infty} \frac{\exp(-\frac{1}{2}m\lambda_p T_p)}{m} \sin\left(mS_p(E)/\hbar - \pi m\mu_p/2\right). \tag{2.13}$$

Berry observes that this asymptotic formula has the same form as the expression (2.7) for the fluctuating part of the Riemann zeta zeroes counting function which we mentioned earlier. This may be taken as evidence that there is some underlying chaotic quantum system which has for its energy spectrum the zeroes of the Riemann zeta function. Because Gutzwiller's formula (2.12) assumes a corresponding classical system exists, this system should be a quantisation of some chaotic classical system, which Berry calls the 'Riemann dynamics'. One problem with the analogy is that (2.7) has a minus sign while (2.13) does not. Connes claims to have solved this discrepancy, by interpreting the minus sign to mean that the Riemann zeta zeroes form an 'absorption spectrum', not an 'emission spectrum' (see [Connes, 1997]).

By comparing terms in (2.13) and (2.7), we may read off properties of the hypothetical Riemann dynamics. For example, the primitive orbits and their repetitions, which label summands in (2.13), correspond to prime powers p^m, as in (2.7). The period of the orbit corresponding to p^m is $m \log p$ and each orbit has Lyapunov exponent 1, which means that the Riemann dynamics is 'homogeneously unstable'. Another important conclusion is that the Riemann dynamics should not be time reversible. This follows from (2.7), but may also be seen as a consequence of the fact that the Riemann zeta zeroes appear to be modelled by GUE statistics, which are used in the modelling of systems that lack time reversibility.

2.2.3 Berry-Keating Hamiltonian

The analogy discovered by Berry certainly supports the idea that there should be some system whose Hamiltonian has the Riemann zeta zeroes as its spectrum. However, the analogy itself does not give any possible candidates for such a system. Nevertheless, Berry and Keating were able to come up with a classical system whose quantisation comes close the reproducing the Riemann zeta zeroes as an energy spectrum (see [Berry and Keating, 1999a] and [Berry and Keating, 1999b]). Their proposal was that the sought-after Hilbert-Pólya operator is some quantisation of the classical Hamiltonian

$$H(q,p) = qp. \tag{2.14}$$

This Hamiltonian yields the equations of motion $\dot{q} = q$ and $\dot{p} = -p$, which have solutions $q(t) = q(0)\exp(t)$ and $p(t) = p(0)\exp(-t)$. It follows from these equations that the motion is unstable and one can also prove that the Lyapunov exponents are all equal to 1. Furthermore, because of the

connection $\dot{q} = q$ between position and velocity, the motion is not time-reversible. That is, the velocity cannot be reversed without also changing the position. As explained in the previous subsection, these are properties we should expect of any Hamiltonian having bearing on the Riemann dynamics. It is furthermore interesting to note that the Berry-Keating Hamiltonian (2.14) can be transformed into the Hamiltonian $\frac{1}{2}(P^2 - Q^2)$ of the inverted harmonic oscillator by the canonical transformation

$$\begin{pmatrix} Q \\ P \end{pmatrix} = \begin{pmatrix} \cos\alpha & -\sin\alpha \\ \sin\alpha & \cos\alpha \end{pmatrix} \begin{pmatrix} q \\ p \end{pmatrix}$$

with $\alpha = \pi/4$. The inverted harmonic oscillator itself has interesting physics and one speculate as to whether it could somehow be involved with Riemann zeta zeroes, just as the Berry-Keating Hamiltonian (see [Subramanyan et al., 2021]).

We now want to perform a semiclassical analysis of the proposed Hamiltonian. Specifically, we will compute the mean part $\langle N(E)\rangle$ of the energy counting function belonging to quantisations of (2.14). For this, a semiclassical technique called Weyl's law[3] will be useful. It states that for a (one-dimensional) classical Hamiltonian with bounded motion, the mean part of the counting function can be expressed as

$$\langle N(E)\rangle = \frac{A(E)}{2\pi\hbar},$$

in which $A(E)$ is the phase space area within the contour given by $H(q,p) = E$. In other words, each quantum state corresponds approximately to a Planck unit cell in the phase space, which has area $2\pi\hbar$. The Berry-Keating Hamiltonian has the problem that its orbits are unbounded, hence Weyl's law does not apply. Indeed, unbounded motion implies that corresponding quantisations will have scattering states, meaning the spectrum will have a continuous part. This is undesirable, as we are interested in reproducing the discrete Riemann zeta zeroes. An ad hoc solution is to truncate both variables by restricting their range. Introducing the lower bounds $q \geq l_q, p \geq l_p$ also yields upper bounds $q \leq E/l_p, p \leq E/l_q$ for all states within the contour $H(q,p) = E$. With this truncation, the area within the contour $H(q,p) = E$ is calculated simply by integration and is given by

$$A(E) = E\left(\log\left(\frac{E}{2\pi\hbar}\right) - 1\right) + 2\pi\hbar,$$

giving

$$\langle N(E)\rangle = \frac{E}{2\pi\hbar}\left(\log\left(\frac{E}{2\pi\hbar}\right) - 1\right) + 1.$$

Apart from a constant $-1/8$, which Berry and Keating claim one can obtain as a Maslov correction, this asymptotic formula agrees with the mean part of the Riemann zeta zeroes counting function (2.5) upon setting $\hbar = 1$. This seems to suggest that the Berry-Keating Hamiltonian is indeed somehow related to the Riemann zeta zeroes.

Taking everything we have seen thus far into account, the physical picture that now emerges of the Riemann zeta zeroes is the following. Both the mean part and fluctuating part of the Riemann zeta zeroes asymptotics (2.4) seem to have a physical origin. The mean part appears to arise through Weyl's law from a quantisation of the Berry-Keating Hamiltonian (2.14), while the fluctuating part is

[3]Weyl's law can actually be made into a rigorous result, but may not hold for all differential operators and needs to be proven for each (family of) operator separately (see [Victor, 2019]).

given by Gutzwiller's formula (2.13). Especially the latter part suggests that a classical system exists, the 'Riemann dynamics', whose corresponding quantum system is chaotic and that has energy levels which reproduce the Riemann zeta zeroes. This chaotic nature seems to be corroborated by the GUE statistics followed by the Riemann zeta zeroes.

We should note, however, that there are still problems with the Berry-Keating approach. One major problem, apart from the expedient truncation, is that for the quantum chaos analogy to work, the orbits of the Riemann dynamics should be periodic, while those of the Berry-Keating Hamiltonian are not. The Hamiltonian $H(q,p) = q(p + l_p^2/p)$ was proposed by [Sierra and Rodríguez-Laguna, 2011] to fix the truncation problem. This Hamiltonian does not need to be truncated yet still has the same asymptotics as the Riemann zeta zeroes. However, it too suffers from the problem of not having periodic orbits.

One question which remains is precisely what quantisation of (2.14) could be the Hilbert-Pólya operator. Berry and Keating considered the obvious quantisation $\frac{1}{2}(XP + PX)$, in which X and P are the standard position and momentum operators on $L^2(\mathbb{R})$, but this proved to be fruitless. More recent proposals have been made such as [Yakaboylu, 2022]. An interesting proposal is due to [Bender et al., 2017], which makes use of Benders PT-symmetric generalisation of quantum mechanics. However, both of these proposals remain formal, lacking rigorous analytical proofs.

3 The Prolate Spheroidal Operator

The mathematical context of [Connes and Moscovici, 2022] is Connes' previous work on the Hilbert-Pólya conjecture, culminating in the publication of his trace formula [Connes, 1997]. This work was partly inspired by the physical indications presented in Section 2, though mathematical motivations, such as the Selberg trace formula, were important as well. We cannot enter into the details of Connes' trace formula or that of Selberg, as these are too advanced for the level of this thesis.

What is relevant here, is that in the process of deriving his trace formula, Connes had to make use of a cutoff argument, in which functions $\xi \in L^2(\mathbb{R})$ together with their Fourier transforms $F\xi$ needed to be restricted to the interval $(-\lambda, \lambda)$. However, it is not possible for both a non-zero function and its Fourier transform to vanish outside of a bounded interval. To overcome this problem, Connes considers the cutoff projections

$$P : L^2(\mathbb{R}) \to \left\{\xi \in L^2(\mathbb{R}) \mid \xi(x) = 0, |x| \geq \lambda\right\}$$
$$\widehat{P} : L^2(\mathbb{R}) \to \left\{\xi \in L^2(\mathbb{R}) \mid F\xi(x) = 0, |x| \geq \lambda\right\}$$

The fact that these do not commute with each other expresses the fact that one cannot perform both cutoffs at the same time. However, they do commute with the prolate spheroidal operator

$$W = -\frac{d}{dx}\left((\lambda^2 - x^2)\frac{d}{dx}\right) + (2\pi\lambda x)^2$$

and Connes uses its eigenfunctions on the interval $(-\lambda, \lambda)$ to construct an approximate cutoff in both space and Fourier domain, sufficient for his purposes. These eigenfunctions, called prolate spheroidal wave functions, were already considered by [Slepian and Pollak, 1961] with regards to questions of signal analysis. These authors were confronted with the similar problem of signals which are restricted to an interval in both the time domain and the frequency domain. Even before this, the prolate spheroidal wave functions were used to solve the Helmholtz equation, which often appears in mathematical physics, by separation of variables in prolate spheroidal coordinates, from which the operator W and its eigenfunctions get their names.

Since their original use in [Connes, 1997], the prolate spheroidal operator on the interval $(-\lambda, \lambda)$ and its eigenfunctions have remained an important part of Connes spectral framework for the Riemann hypothesis. Connes also defined the operator on the larger domain $(-\infty, \infty)$ and showed that it has a unique self-adjoint realisation commuting with $P, \widehat{P}$. However, the spectrum of this operator was not analysed until [Connes and Moscovici, 2022]. We will detail in this section Connes and Moscovici's construction of this operator and show that its spectrum is related to the squares of the Riemann zeta zeroes. We also indicate how a Dirac square root of this operator may be constructed, giving an approximate Hilbert-Pólya operator.

3.1 Self-adjoint extensions

The most important operator-theoretic tool used in [Connes and Moscovici, 2022] is the theory of self-adjoint extensions of symmetric operators, which we detail in this subsection before moving onto the actual construction of Connes and Moscovici's prolate spheroidal operator.

Let A be an operator on a Hilbert space $\mathcal{H}$. We assume throughout this subsection that A has dense domain $D(A)$ and is symmetric, unless stated otherwise. Recall that symmetry means that

$$\langle Ax, y\rangle = \langle x, Ay\rangle$$

for all $x, y \in D(A)$. An important consequence is that A is extended[4] by its adjoint A^*. Consequently, A is closable, meaning we may as well assume A is closed. A self-adjoint operator is necessarily symmetric. However, an operator may be symmetric without being self-adjoint. In such a case, to still be able to exploit self-adjointness, one may try to extend the operator to a self-adjoint operator. The first question then is whether self-adjoint extensions exist in the first place. For this, we have the following definition and theorem.

Definition 3.1. Let A be a densely-defined operator (not necessarily symmetric) on a Hilbert space $\mathcal{H}$. Its deficiency indices are defined as the numbers

$$n_+ = \dim\ker(A^* - i)$$
$$n_- = \dim\ker(A^* + i).$$

Theorem 3.1. Let A be a densely-defined closed symmetric operator on a Hilbert space $\mathcal{H}$. Suppose its deficiency indices are finite.

(i) If $n_+ = n_-$, there exist self-adjoint extensions of A;

(ii) if $n_+ = n_- = 0$, then A is already self-adjoint;

(iii) if $n_+ \neq n_-$, then no extension of A is self-adjoint.

One may consult [Akhiezer and Glazman, 1981b] for a more detailed exposition of extension theory, including a proof of Theorem 3.1. The same reference also gives a method of constructing all self-adjoint extensions in the case that $n_+ = n_-$. However, Connes and Moscovici's article uses a different method, which we now describe, following [Katsnelson, 2018]. We introduce the sesquilinear form $\Omega : D(A^*) \times D(A^*) \to \mathbb{C}$, defined by

$$\Omega(x, y) = \frac{\langle A^*x, y\rangle - \langle x, A^*y\rangle}{i}.$$

One may easily verify that Ω is conjugate symmetric, meaning $\overline{\Omega(x, y)} = \Omega(y, x)$ for all $x, y \in D(A^*)$. Furthermore, because $A^*x = Ax$ for $x \in D(A)$, we have $\Omega(x, y) = 0$ whenever $x \in D(A)$ and $y \in D(A^*)$. Consequently, Ω descends to a well-defined form on the quotient space $\mathcal{E} = D(A^*)/D(A)$ (which we denote by the same symbol). That is, given $[x], [y] \in \mathcal{E}$, we define

$$\Omega([x], [y]) = \Omega(x, y).$$

We call the sesquilinear form Ω the boundary space and the quotient space $\mathcal{E}$ upon which it is defined the boundary space[5]. According to [Akhiezer and Glazman, 1981b], the dimension of the latter is given by

$$\dim\mathcal{E} = n_+ + n_-. \tag{3.1}$$

[4] Recall that an operator B extends an operator A if $D(A) \subseteq D(B)$ and $Bx = Ax$ for all $x \in D(A)$. We denote this by $A \subseteq B$.

[5] The reason for these names will become apparent in Subsection 3.5, when it will be seen that linear functionals like $\Omega(x, \cdot)$ correspond to boundary conditions, when applying the presently developed extension theory to a differential operator on an interval in $\mathbb{R}$.

Lemma 3.2. The boundary form Ω is non-degenerate on $\mathcal{E}$. That is, if $\Omega([x],[y]) = 0$ for all $[y] \in \mathcal{E}$, then $[x] = 0$.

Proof. Suppose $\Omega(x,y) = 0$ for all $y \in D(A^*)$. This equivalent to

$$\langle A^*x, y\rangle = \langle x, A^*y\rangle$$

for all $y \in D(A^*)$. This equality means that $x \in D(A^{**})$. Because we assume A to be closed, we have $A^{**} = A$. Hence, $x \in D(A)$, from which $[x] = 0$ follows. □

The operator A is not self-adjoint insofar as $D(A^*)$ is larger than $D(A)$. Because the boundary space $\mathcal{E} = D(A^*)/D(A)$ essentially measures how much larger $D(A^*)$ is, it is plausible that we can use it to parameterise all self-adjoint extensions of A. Let $\pi : D(A^*) \to \mathcal{E}$ be the quotient map. To each linear subspace $S \subseteq \mathcal{E}$, we associate an operator A_S on $\mathcal{H}$ defined by

$$D(A_S) = \pi^{-1}(S)$$
$$A_S x = A^* x.$$

It is obvious that $D(A) \subseteq D(A_S) \subset D(A^*)$. These three maps all have the action $x \mapsto A^*x$. This means that we have $A \subseteq A_S \subseteq A^*$. Conversely, we have the following proposition.

Proposition 3.3. Suppose B is an operator on $\mathcal{H}$ such that $A \subseteq B \subseteq A^*$. Then there exist some $S \subseteq \mathcal{E}$ such that $B = A_S$.

Proof. Setting $S = \pi(D(B))$, it follows from $A \subseteq B$ that $D(A_S) = D(B)$. If $x \in D(B)$, it follows from $B \subseteq A^*$ that $Bx = A^*x$. But $A^*x = A_S x$, because $x \in D(A_S)$ as well. We conclude $A_S = B$. □

Hence, the operators A_S are precisely those operators B which sit between A and A^*. We do not expect that every extension of A is a restriction of A^*. However, this is true for symmetric extensions. For suppose $A \subseteq B$ and that B is a symmetric operator. Taking adjoints, we get $B^* \subseteq A^*$. Because B is symmetric, we also have $B \subseteq B^*$, hence $B \subseteq A^*$ by transitivity. In particular, it follows that all self-adjoint extensions of A are obtained in this way. We now indicate how to obtain these self-adjoint extensions.

Proposition 3.4. The adjoint of A_S is given by $A_{S^\perp}$, in which $S^\perp$ is the orthogonal complement of S with respect to Ω, defined by

$$S^\perp = \{[x] \in \mathcal{E} : \Omega([x],[y]) = 0 \text{ for all } [y] \in S\}.$$

Proof. We prove that $D(A_{S^\perp}) = D(A_S^*)$. Suppose that $y \in D(A_{S^\perp})$. This means that $[y] \in S^\perp$, which is to say that $\Omega(x,y) = 0$ for all $x \in \pi^{-1}(S)$. Because $D(A_S) = \pi^{-1}(S)$ and $A_S x = A^*x$ for all $x \in D(A_S)$, this equality $\Omega(x,y) = 0$ may be written as

$$\langle Ax, y\rangle = \langle x, A^*y\rangle$$

implying that $y \in D(A_S^*)$. Hence $D(A_{S^\perp}) \subseteq D(A_S^*)$. The reverse inclusion $D(A_S^*) \subseteq D(A_{S^\perp})$ is proven by reversing all the steps in the previous chain of implications. Thus, $D(A_{S^\perp}) = D(A_S^*)$. Because both operators are extended by A^*, they have the same action. We conclude that $A_S^* = A_{S^\perp}$. □

It follows from Propositions 3.4 that the problem of constructing all self-adjoint extensions of A is equivalent to the problem of determining all self-orthogonal subspaces $S \subseteq \mathcal{E}$, meaning $S^\perp = S$

3.2 Minimal and maximal operators

The prolate spheroidal differential expression, in the context of Connes and Moscovici's article, is defined as a differential expression of Sturm-Liouville type

$$(W\xi)(x) = -\frac{d}{dx}\left(p(x)\frac{d\xi}{dx}(x)\right) + q(x)\xi(x) \tag{3.2}$$

with variable coefficients given by $p(x) = \lambda^2 - x^2$ and $q(x) = (2\pi\lambda x)^2$. Here λ is a parameter, which in applications to Connes' trace formula is interpreted as a cutoff parameter. The points $\pm\lambda$ are zeroes of $p(x)$, hence are said to be singular points of W. We stress that (3.2) is a differential expression, not an operator. The expression is defined pointwise for all functions such that ξ and $p\xi'$ are differentiable on $\mathbb{R}$. It will be our goal to construct operator realisations of the expression (3.2). That is, we seek to construct operators A on a suitable function space such that the action $A\xi$ is given by (3.2). A natural choice for the function space is the Hilbert space $L^2(\mathbb{R})$, which has inner product given by

$$\langle \xi, \eta \rangle = \int_{\mathbb{R}} \overline{\xi(x)}\eta(x)\, dx.$$

Because the action is the same for all realisations, the real content of constructing operator realisations is the specification of the domain $D(A)$. This makes it easy to find operator realisations. One can for example take as domain simply all functions $\xi \in L^2(\mathbb{R})$ for which (3.2) makes pointwise sense and is square-integrable. However, what is harder and more useful, is the construction of self-adjoint realisations, in which the operator A is self-adjoint. These are useful when one wants to study the eigenvalues and eigenfunctions of (3.2). That is, one wants to find $\mu \in \mathbb{C}$ such that the differential equation $W\xi = \mu\xi$ has solutions when imposing certain boundary conditions. This is equivalent to determining the eigenvalues of the self-adjoint realisation A for which the boundary conditions have been incorporated into its domain $D(A)$. This manner of studying (second-order) differential expressions like (3.2) is often called Sturm-Liouville theory and one may consult [Naimark, 1967] and [Zettl, 2005] for a fuller introduction and major results.

To construct self-adjoint realisations of (3.2), we first consider a class of very well-behaved functions which should be contained in the domain of each operator realisation. Specifically, we define the preminimal operator W_0, having the Schwartz space $\mathcal{S}(\mathbb{R})$ (see Appendix C) as domain and action given by

$$\varphi \mapsto W\varphi.$$

The differential expression $W\varphi$ is obviously pointwise defined for Schwartz functions. We will shortly prove that this operator is symmetric, which sets us in a position to construct self-adjoint realisations by finding self-adjoint extensions of W_0 using the theory described in Subsection 3.1. Because extension theory requires the operator to be closed, we define the so-called minimal operator $W_{\min} = \overline{W_0}$ as its closure. In addition, we define the so-called maximal operator $W_{\max} = W_0^*$ as its adjoint operator. Because $\mathcal{S}(\mathbb{R})$ is dense in $L^2(\mathbb{R})$, we may indeed speak of the adjoint of W_0. By a standard operator theoretic result, these operators are mutually adjoint, meaning

$$W_{\min}^* = W_{\max}, \quad W_{\max}^* = W_{\min}. \tag{3.3}$$

Following the extension theory described in Subsection 3.1, we look for self-adjoint operators W_{sa} such that $W_{\min} \subseteq W_{\text{sa}} \subseteq W_{\max}$. We interpret the domain $D(W_{\max})$ as the largest domain for which (3.2)

makes pointwise sense (almost everywhere) as an element of $L^2(\mathbb{R})$, subject to the condition that $W_{\max}$ be adjoint to $W_{\min}$. Hence, to be an element of $D(W_{\max})$ requires a function to satisfy some regularity properties. Restricting this maximal domain to the domain of some (self-adjoint) operator realisation amounts to adding (self-adjoint) boundary conditions to the regularity. The rest of this subsection will be devoted to proving basic properties of the three operators which have just been defined. We come back to the construction of self-adjoints realisations in Subsections 3.4 and 3.5.

Proposition 3.5. The operator W_0 is symmetric. The same holds for $W_{\min}$.

Proof. For W_0, we simply perform a calculation in which we use integration by parts twice to show that $\langle W_0\varphi, \psi\rangle = \langle \varphi, W_0\psi\rangle$ for all $\varphi, \psi \in \mathcal{S}(\mathbb{R})$. Specifically, one has

$$\begin{aligned}
\langle W_0\varphi, \psi\rangle &= \int_{\mathbb{R}} \overline{(-(p\varphi')'(x) + q(x)\varphi(x))}\psi(x)\,dx \\
&= \int_{\mathbb{R}} \Big(p(x)\overline{\varphi'(x)}\psi'(x) + q(x)\overline{\varphi(x)}psi(x)\Big)\,dx \\
&= \int_{\mathbb{R}} \Big(-\overline{\varphi(x)}(p\psi')'(x) + \overline{\varphi(x)}q(x)\psi(x)\Big)\,dx \\
&= \int_{\mathbb{R}} \overline{\varphi(x)}\,(-(p\psi')'(x) + q(x)\psi(x))\,dx \\
&= \langle \varphi, W_0\psi\rangle.
\end{aligned}$$

The integration by parts are justified by Propositions C.4 and C.6. We also made us of the fact that p and q are real, to take them from under the conjugation bars.

For $W_{\min}$, we use the fundamental property of closures. Let $\xi, \eta \in D(W_{\min})$. Then there exist sequences (ξ_n) and (η_n) in $\mathcal{S}(\mathbb{R})$ such that $\xi_n \to \xi$ and $W_0\xi_n \to W_{\min}\xi$ in $L^2(\mathbb{R})$ and similarly for η. Continuity of the inner product entails $\langle W_0\xi_n, \eta_n\rangle \to \langle W_{\min}\xi, \eta\rangle$ and $\langle \xi_n, W_0\eta_n\rangle \to \langle \xi, W_{\min}\eta\rangle$. The already proven equality $\langle W_0\xi_n, \eta_n\rangle = \langle \xi_n, W_0\eta_n\rangle$ then yields that $\langle W_{\min}\xi, \eta\rangle = \langle \xi, W_{\min}\eta\rangle$. □

Two auxiliary operators which will play an important role are the parity operator T, which is defined by $(T\xi)(x) = \xi(-x)$, and the Fourier transform F, defined for $\xi \in L^1(\mathbb{R})$ by

$$(F\xi)(y) = \int_{\mathbb{R}} \xi(x)\exp(-2\pi i x y)\,dx \tag{3.4}$$

and extended to an operator on $L^2(\mathbb{R})$ (see Section 5.5 in [van Neerven, 2022]). Both T and F are everywhere-defined bounded operators on $L^2(\mathbb{R})$. The operator T is self-adjoint, while F is unitary. The inverse of F, which is the inverse Fourier transform, is related to F as

$$F^{-1} = TF. \tag{3.5}$$

The time-reversal properties of the Fourier transform express the fact that F and T commute. The following two propositions will show that W_0 and the derived minimal and maximal operators commute with F and T. An operator A with domain $D(A)$ is said to commute with an everywhere-defined operator B if its domain is invariant under B, meaning $x \in D(A)$ implies $Bx \in D(A)$, and if $ABx = BAx$ for all $x \in D(A)$.

Proposition 3.6. The operator W_0 commutes with the parity exchange operator T. The same holds for $W_{\min}$ and $W_{\max}$.

Proof. For W_0, this is an easy application of the chain rule, specifically $(T\varphi)'(x) = -(T\varphi')(x)$, and the fact that $\mathcal{S}(\mathbb{R})$ is obviously invariant under T.

Now let $\xi \in D(W_{\min})$. There is a sequence (ξ_n) in $\mathcal{S}(\mathbb{R})$ such that $\xi_n \to \xi$ and $W_0\xi_n \to W_{\min}\xi$. The boundedness of T together with the fact that W_0 and T commute yields the convergences $T\xi_n \to T\xi$ and $W_0T\xi_n \to TW_{\min}\xi$. This means that $T\xi \in D(W_{\min})$ and $W_{\min}T\xi = TW_{\min}\xi$.

Finally, let $\xi \in D(W_{\max})$. By the definition of the adjoint, we have $\langle W_0\varphi, \xi\rangle = \langle \varphi, W_{\max}\xi\rangle$ for all $\varphi \in \mathcal{S}(\mathbb{R})$. Using the self-adjointness of T and the fact that W_0 and T commute, we calculate that $\langle W_0\varphi, T\xi\rangle = \langle \varphi, TW_{\max}\xi\rangle$. This means that $T\xi \in D(W_{\max})$ and $W_{\max}T\xi = TW_{\max}\xi$. □

Proposition 3.7. The operator W_0 commutes with the Fourier transform F and with the inverse Fourier transform F^{-1}. The same holds for $W_{\min}$ and $W_{\max}$.

Proof. Notice that we only need to prove the commutation with F, due to formula (3.5) and Proposition 3.6. We already know that $\mathcal{S}(\mathbb{R})$ is invariant under the Fourier transform. To prove that W_0 and F commute, we will need the differentiation rules for the Fourier transform. Making use of these rules yields for $\varphi \in \mathcal{S}(\mathbb{R})$

$$(FW_0\varphi)(x) = \int_{\mathbb{R}} \varphi(t)\left(4\pi^2x^2p(t)^2 + 2\pi ixp'(t) + q(t)\right)\exp(-2\pi ixt)\,dt$$
$$(W_0F\varphi)(x) = \int_{\mathbb{R}} \varphi(t)\left(4\pi^2t^2p(x)^2 + 2\pi itp'(x) + q(x)\right)\exp(-2\pi ixt)\,dt.$$

From this, we see that W_0 and F will commute when the function $4\pi^2x^2p(t)^2 + 2\pi ixp'(t) + q(t)$ is symmetric in the variables x and t. As the reader may easily verify, this is the case for the p and q in the prolate spheroidal expression (3.2). Hence, W_0 and F commute. The proof that $W_{\min}$ commutes with F is exactly the same as in the proof of Proposition 3.6 with T replaced by F.

Finally, let $\xi \in D(W_{\max})$. Notice that the fact that W_0 commutes with T and F, combined with equation (3.5), implies that W_0 also commutes with F^{-1}. Together with the unitarity of F, this gives $\langle W_0\varphi, F\xi\rangle = \langle \varphi, FW_{\max}\xi\rangle$, meaning that $F\xi \in D(W_{\max})$ and $W_{\max}F\xi = FW_{\max}\xi$. □

Two additional operators that play an important role are the projections $P, \widehat{P}$ on $L^2(\mathbb{R})$, which we mentioned in the introduction to this section. The first is defined by $(P\xi)(x) = \xi(x)\mathbf{1}_{(-\lambda,\lambda)}(x)$, while the second is the conjugate of the first by the Fourier transform, meaning $\widehat{P} = FPF^{-1}$. The following proposition will be useful later on.

Proposition 3.8. If $\xi \in D(W_{\min})$, then $P\xi \in D(W_{\max})$ and $W_{\max}P\xi = PW_{\min}\xi$. The same holds for $\widehat{P}$.

Proof. In view of Proposition 3.7, we only need to prove it for P. Let $\psi \in \mathcal{S}(\mathbb{R})$. For all $\varphi \in \mathcal{S}(\mathbb{R})$, using integration by parts twice yields $\langle W_0\varphi, P\psi\rangle = \langle \varphi, PW_0\psi\rangle$, which by the definition of the adjoint shows that $P\psi \in D(W_{\max})$ and $W_{\max}P\psi = PW_0\psi$. Now let $\xi \in D(W_{\min})$ and take a sequence (ξ_n) in $\mathcal{S}(\mathbb{R})$ such that $\xi_n \to \xi$ and $W_0\xi \to W_{\min}\xi$. Using continuity, for all $\varphi \in \mathcal{S}(\mathbb{R})$ we have the

convergences $\langle W_0\varphi, P\xi_n\rangle \to \langle W_0\varphi, P\xi\rangle$ and $\langle \varphi, PW_0\xi_n\rangle \to \langle \varphi, PW_{\min}\xi\rangle$. Because we have already proven $\langle W_0\varphi, P\xi_n\rangle = \langle \varphi, PW_0\xi_n\rangle$, this gives $\langle W_0\varphi, P\xi\rangle = \langle \varphi, PW_{\min}\xi\rangle$. Hence, $P\xi \in D(W_{\max})$ and $W_{\max}P\xi = PW_{\min}\xi$. □

Proposition 3.9. The domain of $W_{\max}$ is given by

$$D(W_{\max}) = \{\xi \in L^2(\mathbb{R}) \mid W\xi \in L^2(\mathbb{R})\}.$$

The inclusion $W\xi \in L^2(\mathbb{R})$ is to be understood here in distributional sense. One may define the tempered distribution $W\xi$, even when the differential expression (3.2) does not make pointwise sense, by the action

$$\varphi \mapsto \int_{\mathbb{R}} (W\varphi)(x)\xi(x)\,dx$$

on Schwartz functions. A proof that this is indeed a tempered distribution may be found in Appendix C, as well as a brief introduction to distributions in general. Take care to not confuse the tempered distribution $W\xi$ with the pointwise expression (3.2), for which we use the same symbol. Context should suffice to differentiate between these two meanings. We will use the pointwise sense more than the distributional sense in this thesis, the latter being restricted to Propositions 3.9, 3.10, 3.14 and Lemma 3.40. We take $W\xi \in L^2(\mathbb{R})$ to mean that there is some function $\theta \in L^2(\mathbb{R})$ which defines a tempered distribution

$$\varphi \mapsto \int_{\mathbb{R}} \varphi(x)\theta(x)\,dx$$

that is equal to $W\xi$. Notice that we only need to prove the equality, as from the fact that $W\xi$ is a tempered distribution it will follow that θ is a tempered distribution.

Proof. By definition, $\xi \in D(W_{\max})$ is equivalent to the existence of some function $\theta \in L^2(\mathbb{R})$ such that $\langle W_0\varphi, \xi\rangle = \langle \varphi, \theta\rangle$ for all $\varphi \in \mathcal{S}(\mathbb{R})$. Because $\mathcal{S}(\mathbb{R})$ is obviously invariant under conjugation, we may apply this to $\overline{\varphi}$, so as to remove the conjugation in the inner product. This gives for all $\varphi \in \mathcal{S}(\mathbb{R})$ the equality

$$\int_{\mathbb{R}} (W_0\varphi)(x)\xi(x)\,dx = \int_{\mathbb{R}} \varphi(x)\theta(x)\,dx,$$

which is precisely what the tempered distributional equality $W\xi = \theta$ means. □

We now work to give a concrete characterisation of the maximal domain $D(W_{\max})$ in terms of regularity. Because we are working with functions that are defined only up to sets of measure zero, we need to be more careful about the way we define regularity. We discuss this in Appendix B.

Proposition 3.10. For any $\xi \in D(W_{\max})$, the functions $p\xi$ and $p\xi'$ are locally absolutely continuous on $\mathbb{R}$. Furthermore, the pointwise differential expression $W\xi$ is almost everywhere defined, is an element of $L^2(\mathbb{R})$ and $W_{\max}\xi$ is almost everywhere equal to $W\xi$.

Proof. Because $\xi \in D(W_{\max})$, there is a function $\theta \in L^2(\mathbb{R})$ such that the tempered distributional equality $W\xi = \theta$ holds. We may restrict the test functions φ to the class $\mathcal{D}(\mathbb{R})$ of compactly supported smooth functions, yielding a distributional equality. For all $\varphi \in \mathcal{D}(\mathbb{R})$ we have

$$\int_{\mathbb{R}} (W_0\varphi)(x)\xi(x)\,dx = \int_{\mathbb{R}} \varphi(x)\theta(x)\,dx,$$

which we will write, replacing the variable x by t, as

$$\int_{\mathbb{R}} \left(-p(t)\varphi''(t) - p'(t)\varphi'(t) + q(t)\varphi(t)\right)\xi(t)\,dt = \int_{\mathbb{R}} \varphi(t)\theta(t)\,dt.$$

Using Proposition C.8, we raise the derivatives of φ and collect terms to obtain

$$\int_{\mathbb{R}} \varphi''(t)\left(p(t)\xi(t) + H(t) - F(t) - G(t)\right)\,dt = 0, \tag{3.6}$$

in which we have defined, for some arbitrary x_0, the functions

$$F(x) = \int_{x_0}^{x} p'(t)\xi(t)\,dt \qquad g(x) = \int_{x_0}^{x} q(t)\xi(t)\,dt$$
$$G(x) = \int_{x_0}^{x} g(t)\,dt \qquad h(x) = \int_{x_0}^{x} \theta(t)\,dt.$$
$$H(x) = \int_{x_0}^{x} h(t)\,dt$$

The functions ξ, θ are elements of $L^2(\mathbb{R})$, hence are locally integrable on $\mathbb{R}$ (this follows from Hölder's inequality applied on a compact interval). Because p, q' are continuous, $q\xi$ and $p'\xi$ are locally integrable as well. Finally, g, h are locally integrable due to their continuity. Because the equality (3.6) holds for all $\varphi \in \mathcal{D}(\mathbb{R})$, Proposition C.7 implies that there are complex numbers a, b such that for almost every t we have

$$p(t)\xi(t) = at + b + F(t) + G(t) - H(t),$$

which may be written as

$$p(t)\xi(t) = ax_0 + b + \int_{x_0}^{t} \left(a + p'(s)\xi(s) + g(s) - h(s)\right)\,ds. \tag{3.7}$$

Because the integrand is locally integrable on $\mathbb{R}$, the function on the right-hand side of equation (3.7) is locally absolutely continuous $\mathbb{R}$, meaning so is $p\xi$. This implies that ξ is almost every differentiable. Differentiating (3.7) and using the product rule, we obtain

$$p(t)\xi'(t) = a + \int_{x_0}^{t} \left(q(s)\xi(s) - \theta(s)\right)\,ds \tag{3.8}$$

for almost all t. As before, the function on the right-hand side of equation (3.8) is locally absolutely continuous on $\mathbb{R}$, hence so is $p\xi'$. This means that $p\xi'$ is almost everywhere differentiable. As a consequence, the pointwise differential expression $W\xi$ is almost everywhere defined. Finally, differentiating (3.8) gives $-(p\xi')'(t) + q(t)\xi(t) = \theta(t)$ for almost all t, meaning $W_{\max}\xi = \theta$ is almost everywhere equal to $W\xi$. □

Corollary 3.11. If $\xi \in D(W_{\max})$, then ξ is continuously differentiable on each of the three intervals which partition $\mathbb{R} \setminus \{\pm\lambda\}$.

Proof. Let I be one of the intervals making up $\mathbb{R} \setminus \{\pm\lambda\}$. Because p is locally absolutely continuous on $\mathbb{R}$ and does not have zeroes in I, $1/p$ is locally absolutely continuous on $\mathbb{R} \setminus \{\pm\lambda\}$, hence so are ξ and ξ'. Thus, ξ' is continuous and ξ is a locally absolutely continuous function with a continuous derivative. By Proposition B.8, it follows that ξ is continuously differentiable. □

The next goal is to prove that the necessary conditions proven in Proposition 3.10 are actually sufficient for $\xi \in D(W_{\max})$. For this and future use, we will require a version of Green's formula. First, we take functions ξ and η such that $p\xi$ and $p\xi'$ are locally absolutely continuous on $\mathbb{R}$ and similarly for η. The function $1/p$ is locally absolutely continuous on $\mathbb{R} \setminus \{\pm\lambda\}$ and hence ξ and η as well. As a consequence, the generalised Wronskian

$$[\xi, \eta] = p(\xi'\eta - \xi\eta')$$

is also locally absolutely continuous on $\mathbb{R} \setminus \{\pm\lambda\}$. By a standard calculation, its almost everywhere defined derivative satisfies the Lagrange identity

$$[\xi, \eta]' = \xi W \eta - \eta W \xi.$$

For any compact interval $[a, b] \subseteq \mathbb{R} \setminus \{\pm\lambda\}$ we obtain the standard Green's formula by absolute continuity,

$$\int_a^b (\xi W\eta - \eta W\xi)(x)\, dx = [\xi, \eta](b) - [\xi, \eta](a).$$

We define for any open interval $(a, b) \subseteq \mathbb{R}$, including infinite intervals, the expression

$$[\xi, \eta]|_a^b = \lim_{x \to b^-} [\xi, \eta](x) - \lim_{x \to a^+} [\xi, \eta](x),$$

assuming these limits exist.

Lemma 3.12. Suppose that $\xi, \eta \in L^2(\mathbb{R})$ are such that $p\xi$ and $p\xi'$ are locally absolutely continuous on $\mathbb{R}$ and such that $W\xi \in L^2(\mathbb{R})$, similarly for η. Then the following version of Green's formula holds,

$$\int_{\mathbb{R}} (\xi W\eta - \eta W\xi)(x)\, dx = [\xi, \eta]|_{-\infty}^{-\lambda} + [\xi, \eta]|_{-\lambda}^{\lambda} + [\xi, \eta]|_{\lambda}^{\infty}. \tag{3.9}$$

Proof. First, notice that the integrand in (3.9) is integrable by Hölder's inequality. We may split the integral over the three intervals which partition $\mathbb{R} \setminus \{\pm\lambda\}$. For example, we will treat (λ, ∞) and the other two intervals are treated similarly. By Proposition B.2, for any $a, b \in (\lambda, \infty)$ with $a < b$ we have

$$\begin{aligned}\int_a^{\infty} (\xi W\eta - \eta W\xi)(x)\, dx &= \lim_{b \to \infty} \int_a^b (\xi W\eta - \eta W\xi)(x)\, dx. \\ &= \lim_{b \to \infty} [\xi, \eta](b) - [\xi, \eta](a).\end{aligned}$$

Similarly, we also have

$$\begin{aligned}\int_{\lambda}^{\infty} (\xi W\eta - \eta W\xi)(x)\, dx &= \lim_{a \to \lambda^+} \int_a^{\infty} (\xi W\eta - \eta W\xi)(x)\, dx \\ &= \lim_{b \to \infty} [\xi, \eta](b) - \lim_{a \to \lambda^+} [\xi, \eta](a).\end{aligned}$$

These two calculations show that the limits of $[\xi, \eta](x)$ as $x \to \infty$ and $x \to \lambda^+$ exist and that

$$\int_{\lambda}^{\infty} (\xi W\eta - \eta W\xi)(x)\, dx = [\xi, \eta]|_{\lambda}^{\infty}.$$

□

Lemma 3.13. If $\xi \in L^2(\mathbb{R})$ is such that $p\xi$ and $p\xi'$ are locally absolutely continuous on $\mathbb{R}$ and such that $W\xi \in L^2(\mathbb{R})$, then the functions $p\xi$ and $p\xi'$ are of polynomially bounded growth at $\pm\infty$.

Proof. We will prove the growth bound only for $x \to \infty$. The case $x \to -\infty$ is similar. Take an arbitrary x_0. Then, because $p\xi'$ is locally absolutely continuous, we have for all $x > x_0$

$$\begin{aligned}(p\xi')(x) &= (p\xi')(x_0) + \int_{x_0}^{x} (p\xi')'(t)\,dt \\ &= (p\xi')(x_0) + \int_{x_0}^{x} q(t)\xi(t)\,dt - \int_{x_0}^{x} (W\xi)(t)\,dt.\end{aligned}$$

Using Hölder's inequality on the functions $1_{(x_0,x)}q\xi$ and $1_{(x_0,x)}W\xi$ yields the estimate

$$|(p\xi')(x)| \leq |(p\xi')(x_0)| + \frac{(2\pi\lambda)^2}{\sqrt{5}}\|\xi\|_{L^2}\sqrt{x^5 - x_0^5} + \|W\xi\|_{L^2}\sqrt{x - x_0},$$

which is bounded by polynomial growth as $x \to \infty$. For $p\xi$, we again have

$$(p\xi)(x) = (p\xi)(x_0) + \int_{x_0}^{x} (p\xi)'(t)\,dt.$$

Using $(p\xi)' = p'\xi + p\xi'$ and the fact that we already know that $p\xi'$ is of polynomially bounded growth, hence its integral as well, it suffices to bound the integral of $p'\xi$. This is again accomplished using Hölder's inequality,

$$\int_{x_0}^{x} |p'(t)\xi(t)|\,dt \leq \frac{2}{\sqrt{5}}\|\xi\|_{L^2}\sqrt{x^5 - x_0^5}.$$

□

Proposition 3.14. Suppose that $\xi \in L^2(\mathbb{R})$ satisfies the same hypotheses as in the previous lemma. Then $\xi \in D(W_{\max})$.

Proof. Let $\varphi \in \mathcal{S}(\mathbb{R})$ be arbitrary. Because $\mathcal{S}(\mathbb{R})$ is invariant under differentiation and multiplication by polynomials, ξ and φ together satisfy the hypotheses of Lemma 3.12. Hence, we may apply Green's formula (3.9). We will show that all terms on the right-hand side of (3.9) vanish, which implies

$$\int_{\mathbb{R}} (W\varphi)(x)\xi(x)\,dx = \int_{\mathbb{R}} \varphi(x)(W\xi)(x)\,dx,$$

allowing us to conclude that $\xi \in D(W_{\max})$ by Proposition 3.9. The one-sided limits of $[\xi, \varphi]$ at $\pm\lambda$ cancel due to the continuity of $[\xi, \varphi]$. By Lemma 3.13 and the fact that Schwartz functions decay faster than any polynomial, $p\xi'\varphi$ and $p\xi\varphi'$ go to zero at $\pm\infty$, hence $[\xi, \varphi]$ as well. Thus, the right-hand side of (3.9) vanishes. □

Corollary 3.15. The domain $D(W_{\max})$ is precisely the set of $\xi \in L^2(\mathbb{R})$ such that $p\xi$ and $p\xi'$ are locally absolutely continuous on $\mathbb{R}$ and such that $W\xi \in L^2(\mathbb{R})$. The pointwise differential expression $W\xi$ is almost everywhere defined and $W_{\max}\xi$ is almost everywhere equal to it.

3.3 Deficiency indices

To find out whether self-adjoint extensions of $W_{\min}$ exist, we calculate its deficiency indices and use Theorem 3.1. Recall that these are defined as the dimensions of the subspaces $\ker(W_{\max} \pm i)$. The next lemma will relate the more general subspaces $\ker(W_{\max} - \mu)$ to the solution set of the differential equation $W\xi = \mu\xi$, which will help in calculating the deficiency indices. By 'solution' we mean a twice continuously differentiable function ξ such that $W\xi = \mu\xi$. That is to say, a classical solution (rather than a weak solution).

Lemma 3.16. The subspace $\ker(W_{\max} - \mu)$ is precisely the set of $\xi \in D(W_{\max})$ that are solutions of the differential equation $W\xi = \mu\xi$ on $\mathbb{R} \setminus \{\pm\lambda\}$.

Proof. Suppose $\xi \in \ker(W_{\max} - \mu)$. Let J be one of the intervals which partition $\mathbb{R} \setminus \{\pm\lambda\}$. According to Proposition 3.10, $W_{\max}\xi$ is almost everywhere equal to the pointwise differential expression $W\xi$, hence

$$-(p\xi')'(x) + q(x)\xi(x) = \mu\xi(x) \tag{3.10}$$

for almost all $x \in J$, meaning that $p\xi'$ is a locally absolutely continuous function on J whose almost everywhere defined derivative is almost everywhere equal to a continuous function. It follows from Proposition B.8 that $p\xi'$ is continuously differentiable on J, hence ξ' as well and ξ is twice continuously differentiable. This means that both sides of equation (3.10) are continuous, which means that the equality will hold for all $x \in J$ (see Proposition B.4). Thus, we conclude that ξ is a twice continuously differentiable function satisfying $W\xi = \mu\xi$ on $\mathbb{R} \setminus \{\pm\lambda\}$, meaning it is a solution.

On the other hand, suppose that $\xi \in D(W_{\max})$ is a solution of $W\xi = \mu\xi$ on $\mathbb{R} \setminus \{\pm\lambda\}$. By Proposition 3.10, $W_{\max}\xi$ is almost everywhere equal to $W\xi$, yielding the equality $W_{\max}\xi = \mu\xi$ in $L^2(\mathbb{R})$. Hence $\xi \in \ker(W_{\max} - \mu)$. □

The previous lemma thus identifies $\ker(W_{\max} - \mu)$ with a subspace of the solution set of $W\xi = \mu\xi$ over $\mathbb{R} \setminus \{\pm\lambda\}$. Notice that this solution set is the direct sum of the three solutions sets over the intervals partitioning $\mathbb{R} \setminus \{\pm\lambda\}$. On each of these intervals, the standard theory of linear differential equations is applicable. In particular, this means that these solution sets have dimension 2. Hence, the entire solution set has a dimension of 6.

To get more insight into the behaviour of the solutions near the singular points $\pm\lambda$, we apply the Frobenius method (see for example [Braun, 1992]). The differential equation, when written out in full and normalised so as to have leading coefficient 1, is given by

$$\xi''(x) + \frac{p'(x)}{p(x)}\xi'(x) + \frac{\mu - q(x)}{p(x)}\xi(x) = 0. \tag{3.11}$$

Looking for example at λ, the case of $-\lambda$ being completely similar, and recalling that $p(x) = \lambda^2 - x^2$ and $q(x) = (2\pi\lambda x)^2$, one easily sees that the functions $(x-\lambda)p'(x)/p(x)$ and $(x-\lambda)^2(\mu - q(x)/p(x)$ are analytic at λ. Hence λ is a regular singular point. Using the values of these functions at λ, one constructs the indicial equation, which is given by $r^2 = 0$. It has solution $r = 0$ of multiplicity 2, which implies that there exists some $R > 0$ and functions f, g which are analytic at λ such that the functions

$$f(x)$$
$$f(x)\log(x-\lambda) + g(x)$$

form a basis for all solutions of $W\xi = \mu\xi$ on the half-open interval $(\lambda, \lambda + R)$, and similarly the functions

$$\begin{gathered} f(x) \\ f(x)\log(\lambda - x) + g(x) \end{gathered}$$

form a basis for all solutions on the half-open interval $(\lambda - R, \lambda)$. Furthermore, f, g may be chosen such that $f(\lambda) = 1$, $g(\lambda) = 0$ and $g'(\lambda) = 1$. The situation at $-\lambda$ is completely similar. Thus, the Frobenius method shows that to the left and right of $\pm\lambda$, any solution has analytic behaviour or else has a logarithmic singularity.

We will now use the bases obtained by the Frobenius method to investigate how solutions behave at the singular points $\pm\lambda$. Let $f^{\pm}, g^{\pm}$ be the analytic functions obtained from the Frobenius method at $\pm\lambda$, as earlier. Any solution ξ of (3.11) can be expressed as

$$\begin{aligned} \xi(x) &= a_1^{\pm} f^{\pm}(x) + b_1^{\pm}\left(f^{\pm}(x)\log(\pm\lambda - x) + g^{\pm}(x)\right) \\ \xi(x) &= a_2^{\pm} f^{\pm}(x) + b_2^{\pm}\left(f^{\pm}(x)\log(\mp\lambda + x) + g^{\pm}(x)\right) \end{aligned} \tag{3.12}$$

on the left and right half-open intervals at $\pm\lambda$, respectively. The coefficients in these expansions may be regarded as linear functions of ξ and they control the behaviour of the solution around the singular points $\pm\lambda$. In particular, they control the continuity of $p\xi$ and $p\xi'$ at these points. It is obvious that the only term which could introduce a discontinuity is the logarithmic term. A standard limit calculation shows that the one-sided limits of the logarithmic term in $p\xi$ at $\pm\lambda$ are both equal to zero, meaning $p\xi$ is always continuous. A similar limit calculation for $p\xi'$ yields

$$\lim_{x\to\pm\lambda^+} p(x)\xi'(x) - \lim_{x\to\pm\lambda^-} p(x)\xi'(x) = \mp 2\lambda(b_2^{\pm} - b_1^{\pm}). \tag{3.13}$$

We have thus proven the following lemma.

Lemma 3.17. For any solution of $W\xi = \mu\xi$, $p\xi$ is continuous at $\pm\lambda$ and $p\xi'$ is continuous at $\pm\lambda$ if and only if ξ belongs to the subspace determined by $b_1^{\pm} = b_2^{\pm}$.

Lemma 3.18. Any solution of $W\xi = \mu\xi$ over $\mathbb{R} \setminus \{\pm\lambda\}$ belongs to $L^2(\mathbb{R})$.

Proof. We only need to prove that ξ is square integrable in a neighbourhood of each the points $\pm\lambda$ and $\pm\infty$, as ξ is continuous on compact intervals in between these points. For $\pm\lambda$, the square-integrability follows from the representation (3.12) obtained from the Frobenius method and the fact that logarithmic singularities are square integrable. For $\pm\infty$, one applies Corollary 3.5 from [Zettl et al., 1977]. □

Now that we know what properties solutions of $W\xi = \mu\xi$ have, we will work on finding a different description of the subspace of solutions satisfying $\xi \in D(W_{\max})$, which we have identified with $\ker(W_{\max} - \mu)$ according to Lemma 3.16.

Lemma 3.19. For a solution of $W\xi = \mu\xi$ over $\mathbb{R} \setminus \{\pm\lambda\}$, the condition $\xi \in D(W_{\max})$ is equivalent to the continuity of $p\xi'$ at $\pm\lambda$ if $\mu \neq 0$.

Proof. If $\xi \in D(W_{\max})$, then the continuity at $\pm\lambda$ follows readily from Proposition 3.10. Thus, let ξ be a solution of $W\xi = \mu\xi$ such that $p\xi'$ is continuous at $\pm\lambda$. We show that $p\xi$ and $p\xi'$ are absolutely

continuous on each compact interval $[a, b]$ containing λ, the case of $-\lambda$ being similar. From this it will follow that $p\xi$ and $p\xi'$ are locally absolutely continuous on $\mathbb{R}$.

According to Lemma 3.16, ξ is twice continuously differentiable on $\mathbb{R} \setminus \{\pm\lambda\}$, hence locally absolutely continuous on the same domain. The same conclusion holds for $p\xi$ and $p\xi'$. As a result of Lemma 3.17, $p\xi$ is continuous on $[a, b]$. The continuity of $p\xi'$ is part of the assumptions. Hence, by Proposition B.9, we only need to show that $p\xi$ and $p\xi'$ have derivatives which are integrable on $[a, b]$. First, $(p\xi)' = p'\xi + p\xi'$. By Lemma 3.18, $\xi \in L^2(\mathbb{R})$, hence the first term is integrable by Hölder's inequality and the second due to continuity. Secondly, $(p\xi')' = (q - \mu)\xi$, which is integrable, again by Hölder's inequality. Finally, because $W\xi = \mu\xi$ and $\xi \in L^2(\mathbb{R})$, we get $W\xi \in L^2(\mathbb{R})$ as well. Proposition 3.14 now shows that $\xi \in D(W_{\max})$. □

Proposition 3.20. The deficiency indices of $W_{\min}$ are $(4, 4)$.

Proof. Using Lemmas 3.16 and 3.19, the deficiency subspace $\ker(W_{\max} - \mu)$ for $\mu \notin \mathbb{R}$ is equal to the set of solutions of the differential equation $W\xi = \mu\xi$ on $\mathbb{R} \setminus \{\pm\lambda\}$ for which $p\xi'$ is continuous at $\pm\lambda$. By Lemma 3.17, this is equivalent to the two conditions $b_1^{\pm} = b_2^{\pm}$, which are obviously linearly independent and hence determine a subspace of dimension 4. □

3.4 Boundary form

It follows from Proposition 3.20 and Theorem 3.1 that self-adjoint extensions of $W_{\min}$ exist. In this subsection, we will construct and study the boundary form used to determine all of these self-adjoint extensions. Recall from Subsection 3.1 that this form is defined on $D(W_{\max})$ by the action

$$\Omega(\xi, \eta) = \frac{\langle W_{\max}\xi, \eta\rangle - \langle \xi, W_{\max}\eta\rangle}{i}, \tag{3.14}$$

and descends to a non-degenerate form on the quotient space $\mathcal{E} = D(W_{\max})/D(W_{\min})$, which has dimension 8 by Proposition 3.20 and equation (3.1). We will generally denote this form and its descended version by the same symbol, as well as use the same notation for functions in $D(W_{\max})$ and their equivalence classes in $\mathcal{E}$. Using Green's formula (3.9), which we may apply by Proposition 3.10 and Lemma 3.12, the boundary form may be expressed as

$$i\Omega(\xi, \eta) = [\overline{\xi}, \eta]|_{-\infty}^{-\lambda} + [\overline{\xi}, \eta]|_{-\lambda}^{\lambda} + [\overline{\xi}, \eta]|_{\lambda}^{\infty}. \tag{3.15}$$

We will now proceed to construct a basis for the boundary space $\mathcal{E}$. To do this, it will be useful to take advantage of the fact that the operators $W_{\min}$ and $W_{\max}$ commute with the parity operator T and the Fourier transform F. The operator T induces an orthogonal decomposition $L^2(\mathbb{R}) = L^2_+(\mathbb{R}) \oplus L^2_-(\mathbb{R})$ into even and odd functions, respectively. Because $W_{\max}$ commutes with T, we may orthogonally decompose

$$W_{\max} = W_{\max}^+ \oplus W_{\max}^-$$

along the decomposition into even and odd functions. The reader is referred to Appendix A for how such a decomposition works. There is a similar decomposition for $W_{\min}$. The boundary form Ω also has a decomposition $\Omega = \Omega_+ \oplus \Omega_-$, in the following sense. Because even and uneven functions are orthogonal and $W_{\max}$ commutes with T, we have $\langle W_{\max}\xi, \eta\rangle = 0$ and $\langle \xi, W_{\max}\eta\rangle = 0$ for $\xi \in D(W_{\max}^{\pm})$

and $\eta \in D(W_{\max}^{\mp})$. Thus $\Omega(\xi, \eta) = 0$. In other words, the subspaces $D(W_{\max}^{\pm})$ are Ω-orthogonal. Hence, for arbitrary $\xi, \eta \in D(W_{\max})$, the decomposition into even and odd functions yields

$$\Omega(\xi, \eta) = \Omega(\xi^+, \eta^+) + \Omega(\xi^-, \eta^-).$$

We now see that we have a decomposition $\Omega = \Omega_+ \oplus \Omega_-$ if we define $\Omega_\pm$ on $D(W_{\max}^{\pm})$ by the same action (3.14). These forms similarly descend to non-degenerate forms on the quotient spaces $\mathcal{E}_\pm = D(W_{\max}^{\pm})/D(W_{\min}^{\pm})$, which also give a decomposition of $\mathcal{E}$, in the sense of the following lemma.

Lemma 3.21. The boundary space $\mathcal{E}$ is isomorphic to the direct sum $\mathcal{E}_+ \oplus \mathcal{E}_-$.

Proof. Consider the map $D(W_{\max}) \to \mathcal{E}_+ \oplus \mathcal{E}_-$ given by $\xi \mapsto (\pi_+(\xi^+), \pi_-(\xi^-))$, in which $\pi_\pm : D(W_{\max}^{\pm}) \to \mathcal{E}_\pm$ is the canonical projection map and $\xi = \xi^+ + \xi^-$ is the decomposition into even and odd functions. This map is obviously linear and surjective with kernel $D(W_{\min})$. Hence, the first isomorphism theorem gives the desired isomorphism. □

Now we consider the Fourier transform F in relation to the boundary form. First, because the Fourier transform is unitary with respect to the inner product on $L^2(\mathbb{R})$ and $W_{\max}$ commutes with F and F^{-1} by Proposition 3.7, it follows that F is also unitary with respect to Ω, in the sense that

$$\Omega(\xi, F\eta) = \Omega(F^{-1}\xi, \eta) \tag{3.16}$$

for all $\xi, \eta \in D(W_{\max})$. Furthermore, $D(W_{\max})$ is invariant under F, hence the Fourier transform restricts to a map $D(W_{\max}) \to D(W_{\max})$. Because $D(W_{\min})$ is also invariant under F, this map descends to a map $\mathcal{E} \to \mathcal{E}$, given by $[\xi] \mapsto [F\xi]$ on equivalence classes. Hence, we may speak of Fourier transforms of elements of $\mathcal{E}$. Because F commutes with T, which also leaves $D(W_{\max})$ and $D(W_{\min})$ invariant, the descended Fourier transform respects the decomposition into even and odd functions, meaning it maps $\mathcal{E}_\pm$ into $\mathcal{E}_\pm$.

Now we construct a basis for $\mathcal{E}$. We will do so by constructing bases for $\mathcal{E}_\pm$ separately. First, we take an even function $\alpha_+ \in \mathcal{D}(\mathbb{R})$ which on $[0, \infty)$ has support in $(\frac{1}{2}\lambda, \frac{3}{2}\lambda)$ and on $(\frac{3}{4}\lambda, \frac{5}{4}\lambda)$ coincides with $\log|\lambda^2 - x^2|$. Secondly, we define $\beta_+ = \mathbf{1}_{(-\lambda,\lambda)}$. Corresponding odd versions are given by $\alpha_-(x) = x\alpha_+$ and $\beta_-(x) = x\beta_+(x)$. We now state and prove some important properties of these functions.

Lemma 3.22. The functions $\alpha_\pm, \beta_\pm, \widehat{\alpha}_\pm, \widehat{\beta}_\pm$ are elements of $D(W_{\max})$. The functions $\beta_\pm$ belong to $P(\mathcal{S}(\mathbb{R}))$ and $\widehat{\beta}_\pm$ to $\widehat{P}(\mathcal{S}(\mathbb{R}))$. The Fourier transforms $\widehat{\alpha}_\pm, \widehat{\beta}_\pm$ are continuously differentiable on $\mathbb{R}$.

Proof. By explicit calculation, one verifies that α_+, β_+ satisfy the hypotheses of Proposition 3.14, hence belong to $D(W_{\max})$. Because $D(W_{\max})$ is invariant under Fourier transform, it follows that $\widehat{\alpha}_+, \widehat{\beta}_+$ are also elements of $D(W_{\max})$. Similar reasoning holds for the odd functions.

We may obviously find functions $f_\pm \in \mathcal{D}(\mathbb{R}) \subseteq \mathcal{S}(\mathbb{R})$ such that $f_\pm$ coincides with $\beta_\pm$ on $(-\lambda, \lambda)$, hence $Pf_\pm = \beta_\pm$. Because $\mathcal{S}(\mathbb{R})$ is invariant under the Fourier transform, we have $Ff_\pm \in \mathcal{S}(\mathbb{R})$, hence $\widehat{P}(Ff_\pm) = FPf_\pm = F\beta_\pm = \widehat{\beta}_\pm$.

Because $\alpha_\pm, \beta_\pm$ are compactly supported, their Fourier transforms will be very regular, in particular continuously differentiable. This is the content of a Paley-Wiener theorem (see [Rudin, 1986]). □

Before proving that $\alpha_\pm, \beta_\pm, \widehat{\alpha}_\pm, \widehat{\beta}_\pm$ constitute a basis of $\mathcal{E}_\pm$, it will be useful to consider the linear functionals corresponding to these functions through Ω. That is, we define for $\xi \in D(W_{\max})$

$$\begin{aligned} L_{\alpha_\pm}(\xi) &= i\Omega(\alpha_\pm, \xi) \\ L_{\beta_\pm}(\xi) &= i\Omega(\beta_\pm, \xi) \\ L_{\widehat{\alpha}_\pm}(\xi) &= i\Omega(\widehat{\alpha}_\pm, \xi) \\ L_{\widehat{\beta}_\pm}(\xi) &= i\Omega(\widehat{\beta}_\pm, \xi). \end{aligned}$$

Just like Ω, these linear functionals descend to linear functionals on $\mathcal{E}$. Using (3.15), we can obtain explicit representations in terms of limits at $\pm\lambda$ and $\pm\infty$. Because all functions involved are either even or odd, it is possible to restrict calculations to $(0, \infty)$. For example, for α_+, β_+ these calculations yield

$$\begin{aligned} L_{\alpha_+}(\xi) = \; & 4\lambda \lim_{x \to \lambda^-} ((x-\lambda)\log(\lambda - x)\xi'(x) - \xi(x)) \\ & - 4\lambda \lim_{x \to \lambda^+} ((x-\lambda)\log(x-\lambda)\xi'(x) - \xi(x)) \\ L_{\beta_+}(\xi) = \; & -2 \lim_{x \to \lambda} p(x)\xi'(x). \end{aligned} \tag{3.17}$$

Notice that for $L_{\beta_+}(\xi)$, the one-sided limits have been replaced by usual limits, because the function $p\xi'$ is continuous as a consequence of Proposition 3.10.

Proposition 3.23. The functions $\alpha_\pm, \beta_\pm, \widehat{\alpha}_\pm, \widehat{\beta}_\pm$ constitute a basis for $\mathcal{E}_\pm$. Together, they constitute a basis for $\mathcal{E}$.

Proof. We first deal with the even case. We first calculate the Gram matrix of the functions $\alpha_+, \beta_+, \widehat{\alpha}_+, \widehat{\beta}_+$ with respect to Ω_+, that is, the matrix consisting of all Ω_+-products of these functions, in the given order. Because Ω is conjugate symmetric, this matrix will be Hermitian.

For $\Omega_+(\alpha_+, \beta_+)$, we use the representations (3.17) to calculate that $\Omega_+(\alpha_+, \beta_+) = 4\lambda i$. Any product involving a Fourier transform and non-Fourier transform will be zero, because the Fourier transforms of the functions α_+ and β_+ are continuously differentiable on $\mathbb{R}$ by Lemma 3.22, hence make (3.17) vanish. Finally, using unitarity (3.16), we get $\Omega_+(\widehat{\alpha}_+, \widehat{\beta}_+) = \Omega_+(\alpha_+, \beta_+)$. Thus, the matrix representation is

$$4\lambda i \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix}. \tag{3.18}$$

From this it follows that $\alpha_+, \beta_+, \widehat{\alpha}_+, \widehat{\beta}_+$ are linearly independent, because in any linear relation among these functions one can use (3.18) to isolate and equate to zero all the coefficients. In the same way we prove that in the odd case $\alpha_-, \beta_-, \widehat{\alpha}_-, \widehat{\beta}_-$ is a basis of $\mathcal{E}_-$. By a similar argument, any product of a Fourier transform and a non-Fourier transform is zero. The non-zero entries $\Omega_-(\alpha_-,\beta_-) = \Omega_-(\widehat{\alpha}_-, \widehat{\beta}_-)$ can be obtained from the even case from the relation $[\alpha_-, \beta_-](x) = x^2[\alpha_+, \beta_+](x)$, giving the matrix representation

$$4\lambda^3 i \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix}. \tag{3.19}$$

Because $\alpha_\pm, \beta_\pm, \widehat{\alpha}_\pm, \widehat{\beta}_\pm$ are linearly independent, it follows that the dimension of $\mathcal{E}_\pm$ is at least 4. But by Lemma 3.2 and Proposition 3.20, $\mathcal{E}$ has dimension 8. As a consequence of the decomposition $\mathcal{E} = \mathcal{E}_+ \oplus \mathcal{E}_-$, the dimension of $\mathcal{E}_\pm$ must be 4, meaning $\alpha_\pm, \beta_\pm, \widehat{\alpha}_\pm, \widehat{\beta}_\pm$ is a basis. □

Corollary 3.24. The domain of $W^\pm_{\min}$ may be expressed in the terms of the linear functionals by

$$D(W^\pm_{\min}) = \ker L_{\alpha_\pm} \cap \ker L_{\beta_\pm} \cap \ker L_{\widehat{\alpha}_\pm} \cap \ker L_{\widehat{\beta}_\pm}.$$

Proof. Because $\Omega_\pm$ is non-degenerate on $\mathcal{E}_\pm$, we have $\Omega_\pm(\xi, \eta) = 0$ for all $\eta \in D(W^\pm_{\max})$ if and only if $\xi \in D(W^\pm_{\min})$. Because $\alpha_\pm, \beta_\pm, \widehat{\alpha}_\pm, \widehat{\beta}_\pm$ is a basis of $\mathcal{E}_\pm$, the former condition is clearly equivalent to $\xi \in \ker L_{\alpha_\pm} \cap \ker L_{\beta_\pm} \cap \ker L_{\widehat{\alpha}_\pm} \cap \ker L_{\widehat{\beta}_\pm}$. From this, the result follows. □

3.5 Self-adjoint realisation

We are now in a position to construct self-adjoint realisations of the prolate spheroidal expression (3.2). Using the basis of the boundary space $\mathcal{E}$ constructed in the previous subsection, the following two self-orthogonal subspaces clearly present themselves:

$$\begin{aligned} \mathcal{L}_\alpha &= \ker L_{\alpha_+} \cap \ker L_{\alpha_-} \cap \ker L_{\widehat{\alpha}_+} \cap \ker L_{\widehat{\alpha}_-} \\ \mathcal{L}_\beta &= \ker L_{\beta_+} \cap \ker L_{\beta_-} \cap \ker L_{\widehat{\beta}_+} \cap \ker L_{\widehat{\beta}_-}. \end{aligned} \tag{3.20}$$

Lemma 3.25. $\mathcal{L}_\beta$ is the linear span of $\beta_\pm, \widehat{\beta}_\pm$, from which it follows that $\mathcal{L}_\beta$ is self-orthogonal. Similar statements hold for $\mathcal{L}_\alpha$.

Proof. We only proof that $\mathcal{L}_\beta$ is self-orthogonal, as the proof for $\mathcal{L}_\alpha$ is completely similar. It follows from the matrix representations (3.18) and (3.19) that $\beta_\pm, \widehat{\beta}_\pm \in \mathcal{L}_\beta$. Also using Proposition 3.23 to write $\xi \in \mathcal{L}_\beta$ as a linear combination of $\alpha_\pm, \beta_\pm, \widehat{\alpha}_\pm, \widehat{\beta}_\pm$, we can isolate and equate to zero the coefficients of $\alpha_\pm, \widehat{\alpha}_\pm$. Thus, $\mathcal{L}_\beta$ is equal to the linear span of $\beta_\pm, \widehat{\beta}_\pm$. It is obvious that ξ is orthogonal to this linear span if and only if it satisfies $\Omega(\beta_\pm, \xi) = 0$ and $\Omega(\widehat{\beta}_\pm, \xi) = 0$, which is precisely the condition that defines $\mathcal{L}_\beta$. We conclude $\mathcal{L}_\beta^\perp = \mathcal{L}_\beta$. □

Definition 3.26. Connes and Moscovici's self-adjoint realisation W_{sa} is defined as the extension of $W_{\min}$ with domain $D(W_{\text{sa}})$ corresponding to the self-orthogonal subspace $\mathcal{L}_\beta$. Recall from Subsection 3.1 that this amounts to restricting $W_{\max}$ to $\mathcal{L}_\beta$, regarding it as a subspace of $D(W_{\max})$ instead of $\mathcal{E}$. This choice of self-orthogonal subspace corresponds to the self-adjoint boundary conditions

$$\begin{aligned} L_{\beta_\pm}(\xi) &= 0 \\ L_{\widehat{\beta}_\pm}(\xi) &= 0. \end{aligned} \tag{3.21}$$

That is to say, the domain $D(W_{\mathrm{sa}})$ consists of those functions $\xi \in D(W_{\mathrm{max}})$ which satisfy the boundary conditions (3.21). These can be explicitly written out using limits, using the fact that $\widehat{\beta}_+(y) = \sin(2\pi\lambda y)/\pi y$, which is a standard Fourier transform. Using the decomposition $\xi = \xi^+ + \xi^-$ into even and odd functions, we have

$$\begin{aligned} &\lim_{x\to\pm\lambda} p(x)\xi'(x) = 0 \\ &\lim_{x\to\infty} \big(x\sin(2\pi\lambda x)(\xi^+)'(x) - (2\pi\lambda x\cos(2\pi\lambda x) - \sin(2\pi\lambda x))\xi^+(x)\big) = 0 \\ &\lim_{x\to\infty} \big(x\cos(2\pi\lambda x)(\xi^-)'(x) + (2\pi\lambda x\sin(2\pi\lambda x) + \cos(2\pi\lambda x))\xi^-(x)\big) = 0. \end{aligned} \tag{3.22}$$

Proposition 3.27. The operator W_{sa} commutes with the parity operator T, the Fourier transform F and with the projections $P, \widehat{P}$. In addition, it is the only self-adjoint extension of W_{min} which commutes with $P, \widehat{P}$.

Proof. Because W_{sa} is a restriction of W_{max}, which commutes with T by Proposition 3.6, it suffices to prove that $D(W_{\mathrm{sa}})$ is invariant under T. By Lemma 3.25, each element of $D(W_{\mathrm{sa}})$ is the sum of an element of $D(W_{\mathrm{min}})$ and a linear combination of $\beta_\pm, \widehat{\beta}_\pm$. We already know that $D(W_{\mathrm{min}})$ is invariant under T by Proposition 3.6. That $\beta_\pm, \widehat{\beta}_\pm$ are mapped into $D(W_{\mathrm{sa}})$ by T is easily verified. Hence, W_{sa} commutes with T. The proof that it commutes with F is similar.

To prove W_{sa} commutes with the projections, it suffices to prove it for P, as $\widehat{P} = FPF^{-1}$. We first prove $D(W_{\mathrm{sa}})$ is invariant under P. If $\xi \in D(W_{\mathrm{min}})$, then $P\xi \in D(W_{\mathrm{max}})$ by Proposition 3.8. Because $D(W_{\mathrm{min}}) \subseteq D(W_{\mathrm{sa}})$, ξ satisfies the boundary conditions (3.21), and it is plain to see then that $P\xi$ does as well. Thus, $P\xi \in D(W_{\mathrm{sa}})$. For the functions $\beta_\pm, \widehat{\beta}_\pm$, we obviously have $P\beta_\pm = \beta_\pm$. Explicit calculation shows that $P\widehat{\beta}_\pm$ satisfies the hypotheses of Proposition 3.14 and the conditions (3.21), hence $P\widehat{\beta}_\pm \in D(W_{\mathrm{sa}})$. Finally, it is trivial to prove that $PW_{\mathrm{max}}\xi = W_{\mathrm{max}}P\xi$ whenever $\xi \in D(W_{\mathrm{max}})$ such that $P\xi \in D(W_{\mathrm{max}})$, from which it follows that W_{sa} commutes with P.

Suppose A is a self-adjoint extension of W_{min} which commutes with $P, \widehat{P}$. Its domain $D(A)$ contains $D(W_{\mathrm{min}})$, hence $\mathcal{S}(\mathbb{R})$ as well. Because it is invariant under $P, \widehat{P}$, it will contain $\beta_\pm, \widehat{\beta}_\pm$ by Lemma 3.22. Thus, $D(A)$ contains $D(W_{\mathrm{sa}})$ and it follows that A is an extension of W_{sa}. Using self-adjointness, we conclude that $A = W_{\mathrm{sa}}$. □

We now study the spectrum of W_{sa}. Our main goal here is to show that its spectrum is discrete and unbounded. Because W_{sa} commutes with the projection P, we may orthogonally decompose W_{sa} over the range of P and its orthogonal complement and the spectrum will be the union of the spectra of the restrictions (see Appendix A). Denoting the interval $(-\lambda, \lambda)$ by J, the range of P is the subspace of $L^2(\mathbb{R})$ consisting of functions which vanish outside of J, which we identify with the Hilbert space $L^2(J)$. That is, if $\xi \in L^2(J)$, we identify ξ with the function in $L^2(\mathbb{R})$ which coincides with ξ on J and is identically zero elsewhere. Similarly, the orthogonal complement may be identified with $L^2(\mathbb{R} \setminus J)$. We denote the restriction of W_{sa} to $L^2(J)$ by W_1 and the restriction to W_{sa} to $L^2(\mathbb{R} \setminus J)$ by W_2. To be explicit, these have the domains $D(W_1) = D(W_{\mathrm{sa}}) \cap L^2(J)$ and $D(W_2) = D(W_{\mathrm{sa}}) \cap L^2(\mathbb{R} \setminus J)$. Looking first at W_1, we characterise its domain in the following lemma.

Lemma 3.28. The domain $D(W_1)$ consists of those functions $\xi \in L^2(J)$ that are continuously differentiable, have locally absolutely continuous derivative ξ' on J, $W\xi \in L^2(J)$ and satisfy the boundary

conditions

$$\lim_{x\to\pm\lambda^{\mp}} p(x)\xi'(x) = 0.$$

Proof. A function $\xi \in L^2(J)$ is an element of $D(W_1)$ if and only if it is an element of $D(W_{\max})$, which by Corollary 3.15 is equivalent to a set of regularity properties, and satisfies the boundary conditions (3.21). Because the function vanishes outside J, these conditions have some redundancy. First, because p is locally absolutely continuous on J and has no zeroes, the condition that $p\xi$ and $p\xi'$ are locally absolutely continuous on $\mathbb{R}$ becomes equivalent to ξ being continuously differentiable on J and ξ' locally absolutely continuous on J. Obviously $W\xi \in L^2(\mathbb{R})$ if and only if $W\xi \in L^2(J)$. Finally, the two boundary conditions at infinity in (3.21) are automatically satisfied, leaving only the boundary conditions at $\pm\lambda$. □

By Lemma A.2, W_1 is a self-adjoint realisation of the prolate spheroidal differential expression (3.2) on the domain $(-\lambda, \lambda)$. It is this operator realisation whose eigenfunctions are the prolate spheroidal wave functions and which was studied in [Slepian and Pollak, 1961] with regards to questions of signal analysis. Because its domain is simply an interval, standard results of Sturm-Liouville theory may be applied. We summarise some properties of the spectrum of W_1 in the following proposition.

Proposition 3.29. The operator W_1 has discrete spectrum consisting of positive eigenvalues, each of multiplicity one.

Proof. See [Katsnelson, 2018] for a proof. The discreteness and simplicity[6] of the spectrum may also be proven as in the proof of Proposition 3.31. □

We now move on to W_2. Using the orthogonal decomposition $L^2(\mathbb{R}\setminus J) = L^2_+(\mathbb{R}\setminus J) \oplus L^2_-(\mathbb{R}\setminus J)$ into even and odd functions, we orthogonally decompose W_2 into its restrictions $W_2^{\pm}$. Both subspaces $L^2_\pm(\mathbb{R}\setminus J)$ may be identified with $L^2((\lambda,\infty))$, by mapping functions in the former space to their restrictions on (λ,∞) and functions in the latter space to their even or odd extensions on $\mathbb{R}\setminus J$. Thus, the restriction operators have the domains $D(W_2^{\pm}) = D(W_2)\cap L^2((\lambda,\infty))$. The proof of the following lemma is similar to that of Lemma 3.28.

Lemma 3.30. The domain $D(W_2^{\pm})$ consists of those functions $\xi \in L^2((\lambda,\infty))$ that are continuously differentiable, have locally absolutely continuous derivative ξ' on (λ,∞), $W\xi \in L^2((\lambda,\infty))$ and satisfy the boundary conditions

$$\lim_{x\to\lambda^+} p(x)\xi'(x) = 0$$
$$\lim_{x\to\infty} (x\sin(2\pi\lambda x)\xi'(x) - (2\pi\lambda x\cos(2\pi\lambda x) - \sin(2\pi\lambda x))\xi(x)) = 0$$

in the even case, and in the odd case

$$\lim_{x\to\lambda^+} p(x)\xi'(x) = 0$$
$$\lim_{x\to\infty} (x\cos(2\pi\lambda x)\xi'(x) + (2\pi\lambda x\sin(2\pi\lambda x) + \cos(2\pi\lambda x))\xi(x)) = 0.$$

[6] An eigenvalue is said to be 'simple' if it has multiplicity one. A spectrum is said to be simple if all its eigenvalues are simple.

Using Lemma A.2 again, the operators $W_2^{\pm}$ are self-adjoint realisations of the prolate spheroidal expression differential expression (3.2) on the interval (λ, ∞). Hence, we may again apply Sturm-Liouville theory.

Proposition 3.31. The operators $W_2^{\pm}$ have discrete spectrum consisting of eigenvalues, each of multiplicity one, unbounded from both sides. Furthermore, the spectra of $W_2^{\pm}$ are disjoint.

Proof. The discreteness of the spectrum follows from the results of section 19 in [Naimark, 1967]. It is a consequence of the remarks following Theorem 10.7 in [Weidmann, 1987] that all eigenvalues have multiplicity one. Alternatively, we know that the solution space of $W\xi = \mu\xi$ on (λ, ∞) has a basis consisting of two solutions. By the Frobenius method (see Subsection 3.3), one of these basis solutions has a logarithmic singularity at λ, while the other is regular at λ (see Subsection 3.3). Adding the boundary condition

$$\lim_{x \to \lambda^+} p(x)\xi'(x) = 0 \tag{3.23}$$

removes the solution with the logarithmic singularity, leaving a one dimensional space of solutions. Hence, eigenvalues of $W_2^{\pm}$ have multiplicity one, as their corresponding eigenfunctions belong to this one-dimensional solution space according to Lemma 3.30. It is a consequence of Theorem 10.7.1 in [Zettl, 2005] that the spectrum is unbounded from the negative side.

For the disjointness of the spectra, we only give a non-rigorous argument[7]. Suppose $\mu \in \sigma(W_2^+) \cap \sigma(W_2^-)$. The corresponding eigenfunctions are solutions of $W\xi = \mu\xi$ on (λ, ∞). As before, the boundary condition (3.23) entails these belong to a one-dimensional subspace. Hence, we may assume both $W_2^{\pm}$ have the same eigenfunction ξ corresponding to μ. Using the differential equation $W\xi = \mu\xi$, one can calculate a formal asymptotic expansion of the solution at infinity (see [Richard-Jung et al., 2017] and [Erdelyi, 1956]). Formally, this yields that the asymptotic behaviour of ξ as $x \to \infty$ is given by a linear combination

$$\xi \sim \frac{A\cos(2\pi\lambda x)}{x} + \frac{B\sin(2\pi\lambda x)}{x}. \tag{3.24}$$

If ξ is an eigenfunction to both $W_2^{\pm}$, it satisfies both boundary conditions at ∞ in Lemma 3.30. However, as one may easily check by calculation, the asymptotic form (3.24) can only satisfy both boundary conditions if $A, B = 0$, meaning ξ must be identically zero. This is a contradiction, hence no eigenvalues $\mu \in \sigma(W_2^+) \cap \sigma(W_2^-)$ exist. □

Lemma 3.32. All eigenvalues of W_1 are eigenvalues of W_2. Conversely, all positive eigenvalues of W_2 are eigenvalues of W_1, apart from possibly a finite amount of exceptions.

Proof. Suppose that $W_1\xi = \mu\xi$, in which necessarily $\mu > 0$. Because $D(W_{\mathrm{sa}})$ is invariant under F and P, we have $(I - P)F\xi \in D(W_2)$. We then get $W_2(I - P)F\xi = \mu(I - P)F\xi$ because W_{sa} commutes with F and P, W_2 being a restriction of W_{sa}. Finally, $(I - P)F\xi$ is non-zero, because ξ has compact support, meaning its Fourier transform cannot also have compact support.

For the converse, the reasoning in [Connes and Moscovici, 2022] is that the counting function of the positive W_2 eigenvalues differs from that of the W_1 eigenvalues by a $O(1)$ difference, from which it follows that there can only be a finite amount of positive eigenvalues of W_2 apart from those belonging

[7] One could try to make this argument rigorous by proving rigorous results on the asymptotics of solutions to second-order linear differential equations.

to W_1. See the references in [Connes and Moscovici, 2022] for the appropriate facts needed to prove this. □

Proposition 3.33. The spectrum of W_{sa} is discrete and unbounded on both sides and consists only of eigenvalues. The negative eigenvalues have multiplicity 1, while the positive eigenvalues have multiplicity 2, with possibly a finite amount of exceptions.

Proof. By Lemma A.1, $\sigma(W_{\text{sa}})$ is the union of $\sigma(W_1)$ and $\sigma(W_2)$. The latter is itself the disjoint union of $\sigma(W_2^{\pm})$. Because these three spectra are discrete and consist only of eigenvalues, as we have seen, the same holds for $\sigma(W_{\text{sa}})$. We have also seen that $\sigma(W_1)$ is unbounded from the right and $\sigma(W_2^{\pm})$ from the left, meaning $\sigma(W_{\text{sa}})$ is unbounded on both sides.

The spectrum $\sigma(W_2)$ is simple, being the disjoint union of the simple spectra $\sigma(W_2^{\pm})$. The negative eigenvalues of W_{sa} belong purely to W_2, hence are simple. It follows from Lemma 3.32 that there are two copies of the simple spectrum of $\sigma(W_1)$ in $\sigma(W_{\text{sa}})$, meaning these eigenvalues have multiplicity 2. Indeed, if ξ is an eigenfunction of W_1, then $(I-P)F\xi$ is an eigenfunction of W_2 with the same eigenvalue and these are obviously linearly independent. Finally, because there are only finitely many positive eigenvalues of W_2 which do not belong to $\sigma(W_1)$, only a finite number of positive eigenvalues of W_{sa} will have multiplicity 1. □

3.6 Semiclassical approximation

We now use a semiclassical approximation to study the behaviour of the negative eigenvalues of W_{sa}, which all come from the restriction W_2. We will show that their behaviour is similar to that of the squares of the Riemann zeta zeroes. As in Subsection 2.2.3, we will make use of Weyl's law to give a semiclassical estimate to the counting function of the negative eigenvalues. That is, we calculate the area in a classical phase space corresponding to the eigenfunctions. For this, we first need a classical system corresponding to the prolate spheroidal differential expression W. In [Connes and Moscovici, 2022], the classical Hamiltonian[8]

$$H(q,p) = (p^2-\lambda^2)(q^2-\lambda^2) \tag{3.25}$$

is introduced, giving the formal relation

$$W \sim -4\pi^2 H + 4\pi^2\lambda^4 \tag{3.26}$$

when identifying q and p with the position and momentum operators respectively, which are given by $\xi(x) \mapsto x\xi(x)$ and $\xi(x) \mapsto \frac{1}{2\pi i}\xi'(x)$. Now we need to identify which part of the phase space corresponds to the negative eigenvalues of W_2. For this we make use the following lemma.

Lemma 3.34. If ξ is an eigenvector of W_2 corresponding to a negative eigenvalue μ, then the Fourier transform $F\xi$ vanishes on $(-\lambda,\lambda)$.

Proof. Let $W_2\xi = \mu\xi$ with $\mu < 0$. Because $D(W_{\text{sa}})$ is invariant under F and P, we have $PF\xi \in D(W_{\text{sa}})$. Applying W_1 to this function and using the fact that W_{sa} commutes with P and F yields $W_1PF\xi = \mu PF\xi$. But W_1 only has positive eigenvalues, meaning necessarily $PF\xi = 0$. □

[8] Note that the q, p in (3.25) are canonical coordinates, not to be confused with the coefficients in the prolate spheroidal expression (3.2).

This result may be restated in terms of what Connes' calls the Sonin space, which is defined as the subspace of $L^2(\mathbb{R})$ consisting of functions which together with their Fourier transform vanish on $(-\lambda, \lambda)$ (Connes actually defines it more specifically as a subspace of $L^2_+(\mathbb{R})$). Lemma 3.34 then states that all the eigenfunctions of W_2, equivalently of W_{sa}, with negative eigenvalue belong to the Sonin space. To find out to what part of the phase space Sonin's space corresponds, recall that functions $\xi \in L^2(\mathbb{R})$ are interpreted as wave functions of particles in quantum mechanics, with $|\xi|^2$ representing the probability density of position measurements. If a wave function ξ vanishes on $(-\lambda, \lambda)$, then the particle will not be found on that interval. Hence, for such functions we should restrict the phase space to $|q| \geq \lambda$. Similarly, the Fourier transforms $F\xi$ represents the momentum wave function of the particle, because the position and momentum operators are conjugate by the Fourier transform (see for example [Talagrand, 2022]). Thus, $|F\xi|^2$ represents the probability density of momentum measurements, meaning we should restrict to $|p| \geq \lambda$ for functions whose Fourier transforms vanish on $(-\lambda, \lambda)$. Hence, Sonin's space corresponds to the region of the phase space determined by the conditions $|q| \geq \lambda$ and $|p| \geq \lambda$. Using the formal relation (3.26), the eigenfunctions with eigenvalues in the range $[-E^2, 0]$ correspond to the region

$$\left\{ (q,p) \;\middle|\; |q| \geq \lambda, |p| \geq \lambda, H(q,p) \leq \left(\frac{E}{2\pi}\right)^2 + \lambda^4 \right\}. \tag{3.27}$$

By the symmetry of $H(q,p)$, this region consists of four rotated copy's of its restriction to the first quadrant, which we denote by $\Omega_\lambda(E)$. Denoting the area of $\Omega_\lambda(E)$ by $\sigma(E,\lambda)$, the area of (3.27) is $4\sigma(E,\lambda)$.

Proposition 3.35. The area $\sigma(E,\lambda)$ satisfies the following asymptotic relation as $E \to \infty$,

$$\sigma(E,\lambda) = \frac{E}{2\pi}\left(\log\left(\frac{E}{2\pi}\right) + 2\log 2 - 2\log\lambda - 1\right) + \lambda^2 + o(1). \tag{3.28}$$

Proof. The region $\Omega_\lambda(E)$ is bounded by the coordinate curves $q = \lambda$ and $p = \lambda$ and the curve given by the equation

$$p = \sqrt{\frac{a}{q^2 - \lambda^2} + \lambda^2} = \frac{\sqrt{a + \lambda^2 q^2 - \lambda^4}}{\sqrt{q^2 - \lambda^2}},$$

in which we have defined $a = (E/2\pi)^2 + \lambda^4$. This means that the area of $\Omega_\lambda(E)$ as a function of a is given by

$$I_\lambda(a) = \int_\lambda^\infty \left(\frac{\sqrt{a + \lambda^2 q^2 - \lambda^4}}{\sqrt{q^2 - \lambda^2}} - \lambda \right) dq. \tag{3.29}$$

Let $I(a) = I_1(a)$. Substituting λq for q in (3.29) gives $I_\lambda(a) = \lambda^2 I(\lambda^{-4} a)$. Hence, we restrict our attention to the function $I(a)$. As [Connes and Moscovici, 2022] shows, this function may be expressed using the complete elliptic integrals $K(m)$ and $E(m)$ of the first and second kind, giving

$$I(a) = aK(1-a) - E(1-a) + 1. \tag{3.30}$$

The complete elliptic integrals are defined for $m < 1$ by

$$K(m) = \int_0^{\frac{\pi}{2}} \frac{d\theta}{\sqrt{1 - m\sin^2\theta}}$$

$$E(m) = \int_0^{\frac{\pi}{2}} \sqrt{1 - m\sin^2\theta}\, d\theta$$

and one may consult [Byrd and Friedman, 1971] for further properties of these widely-occurring special functions. For our purposes, the most important facts are the following asymptotic formulas as $m \to -\infty$:

$$K(m) = \frac{1}{2\sqrt{-m}}\left(\log(-m) + 2\log 4\right) + o(m^{-1})$$
$$E(m) = \sqrt{-m} + o(1),$$

which using (3.30) and $I_\lambda(a) = \lambda^2 I(\lambda^{-4}a)$ yield

$$I_\lambda(a) = \frac{1}{2}\sqrt{a}\left(\log a - 2 + 4\log 2 - 4\log\lambda\right) + \lambda^2 + o(1) \tag{3.31}$$

as $a \to \infty$ (the shifted argument of the complete elliptic integrals in (3.30) introduces only an $o(1)$ error). Furthermore, we have the expansions

$$\sqrt{a} = \frac{E}{2\pi} + o(1)$$
$$\log a = 2\log\left(\frac{E}{2\pi}\right) + o(1),$$

which together with (3.31) finally yield the formula (3.28). □

Coming back to identifying eigenfunctions with classical systems, restricting to even (respectively odd) eigenfunctions of W_{sa} amounts to identifying every orbit in the phase space with its reflection under $(q,p) \mapsto (-q,-p)$. In other words, one replaces the original phase space with its quotient by the transformation $(q,p) \mapsto (-q,-p)$. The phase space area of a subset of this quotient is half the area of its preimage in the original phase space.

The even (respectively odd) eigenfunctions with eigenvalues in $[-E^2, 0]$ thus correspond to that part of the quotient phase space which is the image of region (3.27) under the quotient map. By Weyl's law, the semiclassical approximation to the number of such eigenvalues is equal to the area of this image, which is $2\sigma(E,\lambda)$. Comparing (3.28) and (2.5), this means that the counting function of the negative eigenvalues which correspond to even (respectively odd) eigenfunctions is similar to that of the squares of the Riemann zeta zeroes (if $N(T)$ is the counting function of the Riemann zeta zeroes, then $N(\sqrt{T})$ that of their squares).

3.7 Dirac operator

The result of the previous subsection shows that the negative eigenvalues of W_{sa} corresponding to even eigenfunctions are similar to the squares of the Riemann zeta zeroes in terms of their counting function. Because these negative eigenvalues are solely due to W_2^+, we will restrict ourselves to this operator. We use this similarity to indicate in this section how an operator may be constructed whose eigenvalue counting function actually satisfies the same asymptotic formula (2.5) as the counting function of the Riemann zeta zeroes. Identifying the negative eigenvalues with the squares of the Riemann zeta zeroes, one is lead to the idea of obtaining such an approximate Hilbert-Pólya operator by constructing an operator which is in a certain sense the square root of W_2^+, because its eigenvalues will be the square roots of those of W_2^+. There are multiple ways of doing this, but the method used in [Connes and Moscovici, 2022] is directly inspired by physics, which will be explained first.

When trying to unify quantum mechanics, which describes the behaviour of particles on small scales, with Einstein's special theory of relativity, which drastically modifies the classical notions of space and time at higher velocities, one quickly encounters the Klein-Gordon equation

$$\left(\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right)\psi = \left(\frac{mc}{\hbar}\right)^2 \psi, \tag{3.32}$$

in which

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

is the Laplacian. The Klein-Gordon equation describes the time evolution of the wave function $\psi(x, y, z, t)$ of the particle in question, which essentially contains all the information about its state. As mentioned earlier in Subsection 3.6, the quantity $|\psi|^2$ is interpreted as a probability density for measurements of the particle described by ψ. However, the solutions of equation (3.32) in a certain sense have negative probabilities, which was interpreted as being unphysical. This lead Dirac to seek a first-order wave equation. His idea was to take a formal square root of the wave operator (so called because it appears in the wave equation)

$$\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}, \tag{3.33}$$

which appears on the left side of equation (3.32), by equating it to the factorisation

$$i\left(A\frac{\partial}{\partial x} + B\frac{\partial}{\partial y} + C\frac{\partial}{\partial z} + \frac{1}{c}D\frac{\partial}{\partial t}\right) \cdot i\left(A\frac{\partial}{\partial x} + B\frac{\partial}{\partial y} + C\frac{\partial}{\partial z} + \frac{1}{c}D\frac{\partial}{\partial t}\right),$$

expanding the product and equating terms on both sides. This lead him to the conclusion that the coefficients A, B, C, D satisfy relations such as $AB + BA = 0$, hence cannot be ordinary numbers, but must be matrices. Specifically, they are given by Dirac's gamma matrices $\gamma^1, \gamma^2, \gamma^3, \gamma^0$ respectively, which are defined as

$$\begin{aligned} \gamma^0 &= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \qquad \gamma^1 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix} \\ \gamma^2 &= \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & i & 0 & 0 \\ -i & 0 & 0 & 0 \end{pmatrix} \qquad \gamma^3 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}. \end{aligned} \tag{3.34}$$

Taking the square root of the right side of (3.32) and equating it to the derived square root of the left side, Dirac arrived at his famous first-order equation,

$$i\hbar\left(\frac{1}{c}\gamma^0\frac{\partial}{\partial t} + \gamma^1\frac{\partial}{\partial x} + \gamma^2\frac{\partial}{\partial y} + \gamma^3\frac{\partial}{\partial z}\right)\psi = mc\psi, \tag{3.35}$$

whose solutions do not exhibit negative probabilities. See [Talagrand, 2022] for more on the Dirac equation. Mathematicians would call the differential operator on the left side of (3.35) a Dirac operator.

The algebraic relations satisfied by the gamma matrices γ^μ define a mathematical structure called a Clifford algebra. In general, a Dirac operator is a linear combination of partial derivatives with coefficients in a Clifford algebra, like the left side of (3.35). However, using this general definition would lead us unnecessarily far into advanced algebra. A more pragmatic definition of a Dirac operator can be obtained as follows. The gamma matrices (3.34) may be written as 2×2 block matrices

$$\gamma^0 = \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix} \qquad \gamma^1 = \begin{pmatrix} 0 & \sigma_x \\ -\sigma_x & 0 \end{pmatrix}$$

$$\gamma^2 = \begin{pmatrix} 0 & \sigma_y \\ -\sigma_y & 0 \end{pmatrix} \qquad \gamma^3 = \begin{pmatrix} 0 & \sigma_z \\ -\sigma_z & 0 \end{pmatrix},$$

in which $\sigma_x, \sigma_y, \sigma_z$ are called the Pauli matrices. Using this representation, the Dirac operator on the left side of (3.35) may be written as a 2×2 matrix of operators

$$\begin{pmatrix} \frac{1}{c}\frac{\partial}{\partial t} I & \sigma_x \frac{\partial}{\partial x} + \sigma_y \frac{\partial}{\partial y} + \sigma_z \frac{\partial}{\partial z} \\ -\sigma_x \frac{\partial}{\partial x} - \sigma_y \frac{\partial}{\partial y} - \sigma_z \frac{\partial}{\partial z} & \frac{1}{c}\frac{\partial}{\partial t} I \end{pmatrix}$$

which squares to what is essentially the wave operator (3.33). It is in this sense that we define a Dirac operator, as a 2×2 matrix of operators which squares to second-order Laplacian-like operator.

Coming back to the construction of a Dirac square root of the prolate spheroidal operator, [Connes and Moscovici, 2022] likens W_2^+ to the wave operator (3.33) and proceeds to construct an analogous Dirac square root $\not{D}$ which squares to W_2^+. We will indicate informally in the rest of this subsection how this construction proceeds. We first factorise the prolate spheroidal differential expression W as a product of first-order differential operators in Proposition (3.36). This involves a Riccati differential equation, whose solutions form a one-parameter family, as described in Proposition (3.38). It will be useful to redefine the coefficient $p(x) = x^2 - \lambda^2$ so as to make it positive (λ, ∞). We will use this convention only throughout this subsection.

Proposition 3.36. Suppose w is a solution of the Riccati equation

$$\sqrt{p(x)}w'(x) + w(x)^2 = -q(x) + \left(\frac{p''(x)}{4} - \frac{p'(x)^2}{16p(x)}\right) \tag{3.36}$$

for $x \in (\lambda, \infty)$. Defining the first-order differential operator ∇ with action $\xi \mapsto p^{\frac{1}{4}}(\xi p^{\frac{1}{4}})'$, we have the factorisation

$$W = (\nabla + w)(\nabla - w). \tag{3.37}$$

Proof. We denote the first derivative operator by ∂, with action $\xi \mapsto \xi'$. Furthermore, let f be some (sufficiently regular) function. We denote the operator $\xi \mapsto f\xi$ simply by f. We now define by composition the differential operators

$$T_1 = f\partial f$$
$$T_2 = \partial f^4 \partial.$$

The commutator of ∂ and f has action $[\partial, f]\xi = (\partial f - f\partial)\xi = (f\xi)' - f\xi' = f'\xi$, meaning $[\partial, f] = f'$. Using this relation, one obtains

$$\begin{aligned} T_1^2 = f\partial f^2 \partial f &= \partial f^3 \partial f - f' f^2 \partial f \\ \partial f^3 \partial f &= \partial f^4 \partial + \partial f^3 f' \\ f' f^2 \partial f &= f' f^3 \partial + (f f')^2, \end{aligned}$$

which implies that $T_1^2 - T_2 = 2(ff')^2 + f^3 f''$. Setting $f = p^{\frac{1}{4}}$ gives $T_1 = \nabla$ and yields

$$\nabla^2 - \partial p \partial = \frac{p''}{4} - \frac{(p')^2}{16p}. \tag{3.38}$$

The commutator $[\nabla, w]$ is multiplication by the function $\sqrt{p}w'$, as may be easily checked. Using this, the identity (3.38) and the differential equation (3.36), we get

$$\begin{aligned} (\nabla + w)(\nabla - w) &= \nabla^2 + w\nabla - \nabla w - w^2 \\ &= \nabla^2 - w^2 - [\nabla, w] \\ &= \nabla^2 - w^2 - \sqrt{p}w' \\ &= \partial p \partial + \frac{p''}{4} - \frac{(p')^2}{16p} - w^2 - \sqrt{p}w' \\ &= \partial p \partial + q, \end{aligned}$$

which proves (3.38), because the last operator is precisely W (recall that we have redefined p). □

Lemma 3.37. Let u_1, u_2 be a basis of solutions for the differential equation $Wu = 0$ on (λ, ∞). For $z \in \mathbb{C}$, define the solution $u = u_1 + zu_2$. If $z \notin \mathbb{R}$, then u will not have any zeroes.

Proof. If u has zero, say $u(x) = 0$, then it will follow that $u_1(x), u_2(x) = 0$ separately, because $z \notin \mathbb{R}$. This means that the Wronskian $p(u_1' u_2 - u_1 u_2')$ has a zero and consequently u_1, u_2 are linearly dependent, by a standard result of the theory of linear differential equations (see for example [Braun, 1992]). But this is a contradiction, as u_1, u_2 are assumed to be linearly independent. Hence, u cannot have a zero. □

Proposition 3.38. Defining $u = u_1 + zu_2$ as in Lemma (3.37) with $z \notin \mathbb{R}$ and the differential operator ∇ as in Proposition (3.36), all solutions of the Riccati equation (3.36) are given by

$$w_z = \frac{\nabla u}{u}. \tag{3.39}$$

Proof. The function $w_z = \nabla u / u$ is well-defined by Lemma (3.37). Direct calculation verifies that it satisfies (3.36). Now suppose w is an arbitrary solution of (3.36). Using the particular solution w_i, the function $v = w - w_i$ satisfies the Bernoulli differential equation

$$\sqrt{p}v' + 2w_i v + v^2 = 0. \tag{3.40}$$

By the standard method of solving Bernoulli equations (see for example [Braun, 1992]), the substitution $y = v^{-1}$ reduces (3.40) to a linear differential equation. Using particular solutions w_α, w_β of (3.36), we form particular solutions

$$v_1 = w_\alpha - w_i$$
$$v_2 = w_\beta - w_i$$

of (3.40), in which α, β are distinct complex numbers both unequal to i. The functions v_1^{-1}, v_2^{-1} are solutions of (3.40), hence for any $t \in \mathbb{C}$ we can combine them into a solution

$$\left(\frac{t}{v_1} + \frac{1-t}{v_2}\right)^{-1} = \frac{v_1 v_2}{t v_1 + (1-t) v_2} \tag{3.41}$$

We show that v is of this form for some choice of t. First, notice that (3.40) satisfies the hypotheses of the existence and uniqueness theorem for first order differential equations. This means that solutions which coincide somewhere are identically equal. Because 0 is a solution of (3.40) and v is not identically zero due to the linear independence of u_1, u_2, it follows that v has no zeroes. Similarly, v_1 and v_2 coincide nowhere, as w_α and w_β are not identically equal. If they were equal, it would follow that the Wronskian of $u_1 + \alpha u_2$ and $u_1 + \beta u_2$ is zero, meaning these solutions are linearly dependent. This is a contradiction if $\alpha \neq \beta$. Similarly, v_2 does not have any zeroes and v_1 because $\beta \neq i$. Choosing any $x \in (\lambda, \infty)$ and setting

$$t = \frac{v_2(x)(v_1(x) - v(x))}{v(x)(v_1(x) - v_2(x))},$$

it follows that v coincides with (3.41) at x, meaning they are identically equal:

$$v = \frac{v_1 v_2}{t v_1 + (1-t) v_2}.$$

Consequently, we have

$$w = w_i + \frac{(w_\alpha - w_i)(w_\beta - w_i)}{t(w_\alpha - w_i) + (1-t)(w_\beta - w_i)}$$

which, as one may verify, becomes equal to w_z upon setting $\alpha = -i$ and

$$z = \frac{i(i(t-1) + \beta(t+1))}{i(t+1) + \beta(t-1)} \notin \mathbb{R}.$$

□

We now come to the definition of the Dirac operator $\not{D}$. We remember the reader that we do not give a rigorous description of the construction in [Connes and Moscovici, 2022]. The reasoning there is non-detailed, to the point of being non-rigorous. We mostly reproduce this reasoning, being a bit more detailed and indicating what needs to be done to make the reasoning rigorous.

We denote throughout this subsection the Hilbert space $L^2((\lambda, \infty))$, on which W_2^+ is an operator, by $\mathcal{H}$. Choosing a function w such that we have a decomposition $W = (\nabla + w)(\nabla - w)$, as may be done according to Propositions 3.36 and 3.38, we formally define

$$\not{D} = \begin{pmatrix} 0 & \nabla + w \\ \nabla - w & 0 \end{pmatrix} \tag{3.42}$$

on the Hilbert space $\mathcal{H} \oplus \tilde{\mathcal{H}}$, in which $\tilde{\mathcal{H}}$ is another copy of $L^2((\lambda, \infty))$ which will be given a different inner product later. The square of $\not{D}$ is given by

$$\not{D}^2 = \begin{pmatrix} (\nabla + w)(\nabla - w) & 0 \\ 0 & (\nabla - w)(\nabla + w). \end{pmatrix}$$

The first operator on the diagonal is equal to the prolate spheroidal operator, by the factorisation $W = (\nabla + w)(\nabla - w)$. The second operator on the diagonal can be expressed as

$$(\nabla - w)(\nabla + w) = W + 2\sqrt{p}w'.$$

It is claimed by [Connes and Moscovici, 2022] that these operators on the diagonal are isospectral, meaning $\not{D}^2$ has the same spectrum as W, barring questions of domain. It is in this sense that $\not{D}$ is a Dirac square root of W_2^+. If this construction were rigorous, one could apply the spectral mapping theorem (see Theorem 10.55 in [van Neerven, 2022]) to show that the spectrum of $\not{D}$ consists of the square roots of the spectrum of W. A different approach is taken by [Connes and Moscovici, 2022], in which the spectrum of $\not{D}$ is determined without reference to $\not{D}^2$. They give the operator $\not{D}$ the domain

$$\left\{(\xi, \tilde{\xi}) \mid \xi \in D(W_2^+),\, (\nabla + w)\tilde{\xi} \in D(W_2^+)\right\}. \tag{3.43}$$

Expressions such as $(\nabla + w)\tilde{\xi}$, may not be pointwise defined or fail to be square-integrable. Hence, these expressions should be interpreted in the weak sense[9]. That is to say, one can define a distributional version of the operator $\nabla + w$ and we want this distribution to be given by a square-integrable function when acting on $\tilde{\xi}$. Not only that, we want this 'weak' $(\nabla + w)\tilde{\xi}$ to even belong to the domain $D(W_2^+)$. Using a formal integration parts, we see that the definition of a weak $\nabla \pm w$ should be the following.

Definition 3.39. A function $\xi \in \mathcal{H}$ is said to possess a weak $\nabla \pm w$, which we denote by $(\nabla \pm w)\xi \in \mathcal{H}$, if for all $\varphi \in \mathcal{D}(\mathbb{R})$ (on which we may obviously apply $\nabla \pm w$ pointwise) we have

$$\int_\lambda^\infty \varphi(x)(\nabla \pm w)\xi(x)\, dx = -\int_\lambda^\infty (\nabla \mp w)\varphi(x)\xi(x)\, dx.$$

Taking the previous remarks into account, the action of $\not{D}$ consists of applying weak versions of the differential operators $\nabla \pm w$ and its domain should really include the condition that $(\nabla - w)\xi$ and $(\nabla + w)\tilde{\xi}$ exist as elements of $\mathcal{H}$, in addition to the two conditions in (3.43). With the operator $\not{D}$ thus defined, the following reasoning is used to show that its spectrum consists precisely of the square roots of eigenvalues of W_2^+. One takes an orthonormal basis of $\mathcal{H}$ consisting of eigenfunctions (ξ_μ) of W_2^+, parameterised by eigenvalue μ. Defining the functions $\tilde{\xi}_\mu = (\nabla - w)\xi$, again in the weak sense, we choose an inner product on $\tilde{\mathcal{H}}$ which makes $(\tilde{\xi}_\mu)$ an orthonormal basis. We denote the inner product on $\mathcal{H}$ by $\langle \cdot, \cdot \rangle_1$ and the inner product on $\tilde{\mathcal{H}}$ by $\langle \cdot, \cdot \rangle_2$. Letting

$$\xi = \sum_\mu \langle \xi_\mu, \xi \rangle_1 \xi_\mu$$
$$\tilde{\xi} = \sum_\mu \langle \tilde{\xi}_\mu, \tilde{\xi} \rangle_2 \tilde{\xi}_\mu,$$

[9]The situation is similar to that of Proposition 3.9, in which $D(W_{\max})$ is seen to be equal to the set of functions in $L^2(\mathbb{R})$ which have a 'weak W' in $L^2(\mathbb{R})$.

and ignoring questions of convergence, the action of $\not{D}$ on $(\xi, \tilde{\xi})$ can be formally expressed as

$$\not{D}(\xi, \tilde{\xi}) = \sum_{\mu} \mu \langle \tilde{\xi}_\mu, \tilde{\xi} \rangle_2 (\xi_\mu, 0) + \langle \xi_\mu, \xi \rangle_1 (0, \tilde{\xi}_\mu), \tag{3.44}$$

in which we have used the plausible equality $(\nabla + w)\tilde{\xi}_\mu = W\xi_\mu$, which follows from the factorisation $W = (\nabla + w)(\nabla - w)$. We actually prove this equality in the following lemma.

Lemma 3.40. Suppose $\xi \in \mathcal{H}$ is a function possessing a weak $\nabla - w$, say $\tilde{\xi} = (\nabla - w)\xi \in \mathcal{H}$. Then $\tilde{\xi}$ has a weak $\nabla + w$, equal to $W\xi$ in weak sense.

Proof. The factorisation (3.37) holds for sufficiently regular functions, in particular for compactly supported smooth functions $\varphi \in \mathcal{D}(\mathbb{R})$. Furthermore, $\mathcal{D}(\mathbb{R})$ is obviously closed under the operators $\nabla \pm w$. Hence, we have

$$\begin{aligned}
\int_\lambda^\infty (W\varphi)(x)\xi(x)\,dx &= \int_\lambda^\infty (\nabla + w)(\nabla - w)\varphi(x)\xi(x)\,dx \\
&= -\int_\lambda^\infty (\nabla - w)\varphi(x)(\nabla - w)\xi(x)\,dx \\
&= -\int_\lambda^\infty (\nabla - w)\varphi(x)\tilde{\xi}(x)\,dx \\
&= \int_\lambda^\infty \varphi(x)\xi(x)\,dx.
\end{aligned}$$

□

The formal equation (3.44) means that we can view $\not{D}$ as being an infinite direct sum of the finite-rank operators $(\xi, \tilde{\xi}) \mapsto \mu\langle \tilde{\xi}_\mu, \tilde{\xi} \rangle_2 (\xi_\mu, 0) + \langle \xi_\mu, \xi \rangle_1 (0, \tilde{\xi}_\mu)$. On the subspaces spanned by the basis vectors $(\xi_\mu, 0)$ and $(0, \tilde{\xi_\mu})$, these maps have matrix representations

$$\begin{pmatrix} 0 & \mu \\ 1 & 0 \end{pmatrix},$$

meaning they have as eigenvalues $\pm\sqrt{\mu}$. Using a version of Lemma A.1 for infinite direct sums, we would then conclude that the spectrum of $\not{D}$ is given by $\{\pm\sqrt{\mu} \mid \mu \in \sigma(W_2^+)\}$.

Proposition 3.41. The spectrum of $2\not{D}$ is discrete and simple, consisting precisely of the numbers $\pm 2\sqrt{\mu}$ with $\mu \in \sigma(W_2^+)$. Its imaginary eigenvalues are symmetric under conjugation. With $\lambda = \sqrt{2}$, the counting function $N(E)$ of those eigenvalues with positive imaginary part satisfies the same asymptotic formula (2.5) as that of the Riemann zeta zeroes,

$$N(E) = \frac{E}{2\pi}\left(\log\left(\frac{E}{2\pi}\right) - 1\right) + O(1). \tag{3.45}$$

Proof. The above presentation makes it plausible that the spectrum of $\not{D}$ consists of the square roots of the eigenvalues belonging to W_2^+, though we stress this is not proven rigorously here. Because W_2^+ has discrete and simple spectrum by Proposition 3.31, $2\not{D}$ also has discrete and simple spectrum, with its eigenvalues being precisely the numbers $\pm 2\sqrt{\mu}$ for $\mu \in \sigma(W_2^+)$. The negative eigenvalues μ, which

correspond to the squares of the Riemann zeta zeroes, yield imaginary eigenvalues of $\not{D}$ which come in conjugate pairs. The number of eigenvalues with imaginary part in $[0, E]$ is equal to the number of eigenvalues $\mu \in \sigma(W_2^+)$ in the range $[-(E/2)^2, 0]$. By the results of Subsection 3.6, this number is approximately $2\sigma(E/2, \sqrt{2})$, which is asymptotically equal to (3.45) according to Proposition 3.28 with $\lambda = \sqrt{2}$. □

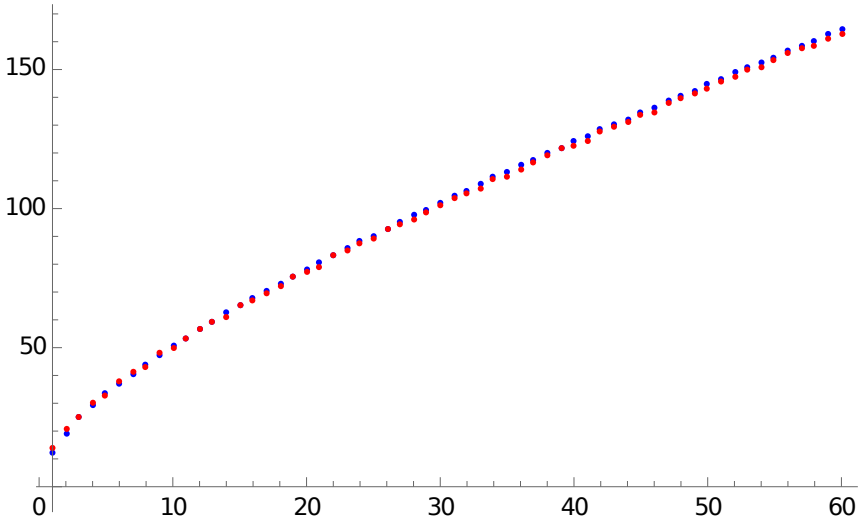

Figure 2: The (positive) imaginary parts of eigenvalues of $\not{D}$ (in blue), as calculated by Connes, and of the non-trivial Riemann zeta zeroes (in red) for first sixty eigenvalues and zeroes. The numerical calculation of the eigenvalues is explained in more detail in Appendix D. Figure taken from [Connes and Moscovici, 2022].

In the sense of Proposition (3.41), the operator $2\not{D}$ is an approximate Hilbert-Pólya operator. Its imaginary eigenvalues may be computed numerically and plotted against the imaginary parts of the non-trivial Riemann zeta zeroes, to visually demonstrate this property (see Fig. 2). The numerical calculations are presented in more detail in Appendix D. We note that the asymptotic relation (3.28), on which (3.45) is based, can actually be rigorously derived, as shown in [Connes and Moscovici, 2022]. Finally, we indicate what needs to be formulated exactly and proven in the discussion above Proposition 3.41 to make the presentation rigorous.

1. It needs to be proven that there exists an orthonormal basis of $L^2((\lambda, \infty))$ consisting of eigenfunctions of W_2^+. That is to say, the eigenfunctions of W_2^+ are complete. The proof of the corresponding fact for regular Sturm-Liouville problems, meaning the coefficient $p(x)$ has no zeroes, is not difficult, and may for example be found in [Al-Gwaiz, 2008]. The case of a singular problem is more complicated and is treated in [Titchmarsh, 1946].

2. It need to be proven that eigenfunctions ξ_μ possess weak a $\nabla - w$, so that one may define $\tilde{\xi} = (\nabla - w)\xi_\mu$. It follows from Lemma 3.30 that ξ_μ is differentiable, meaning $(\nabla - w)\xi_\mu$ is

pointwise defined. One only needs to show that this function is square-integrable.

3. It must be shown how to choose an inner product on $\tilde{\mathcal{H}}$ which makes the functions $\tilde{\xi}_\mu$ an orthonormal basis. In [Connes and Moscovici, 2022] it is actually stated that the inner product should be chosen such that the scaled functions $\mu^{-\frac{1}{2}}\tilde{\xi}_\mu$ become an orthonormal basis, though the reason for the scaling is unclear.

4. The decomposition of $\not{D}$ as an infinite direct sum of finite-rank operators needs to be made rigorous. Specifically, one needs to first define what an infinite direct sum of operators means. Then, the domain of $\not{D}$ and the finite-rank operators needs to be chosen so that the equality between $\not{D}$ and the direct sum rigorously holds. Finally, a version of Lemma A.1 needs to be proven for infinite direct sums. A useful reference might be [Çevik and Ismailov, 2012].

4 Conclusion

The subject of this thesis was the article [Connes and Moscovici, 2022], in which it was discovered that the spectrum of a suitable uniquely defined self-adjoint realisation of the prolate spheroidal operator on $(-\infty, \infty)$ has a discrete spectrum that is asymptotically similar to the squares of the Riemann zeta zeroes. To make the reasoning and results of [Connes and Moscovici, 2022] more understandable, the objective of this thesis was to provide context and motivation and to fill in missing details, which were omitted from the article.

Section 2 provided both mathematical and physical context. We first introduced in general terms the Riemann hypothesis and presented the Hilbert-Pólya conjecture as a possible, operator theoretic way of proving it. Using the physical interpretation of self-adjoint operators as observables, we also discussed three indications of the Hilbert-Pólya conjecture being true. These included Montgomery's pair conjecture and the classical Hamiltonian proposed by Berry and Keating.

Section 3 set out to provide details to [Connes and Moscovici, 2022]. We first gave a brief overview of the theory of self-adjoint extensions. We then followed [Connes and Moscovici, 2022] but gave more detail. This consisted of applying the presented extension theory to the prolate spheroidal differential expression and finally arriving at the self-adjoint realisation of the prolate spheroidal operator of [Connes and Moscovici, 2022]. Using a non-rigorous semiclassical approximation, its spectral similarity to the squares of the Riemann zeta zeroes was shown. Finally, we indicated how one might go about constructing a Dirac square root of the previous operator, whose imaginary spectrum is asymptotically similar to the non-trivial Riemann zeta zeroes. We did not give a fully rigorous presentation of this part of [Connes and Moscovici, 2022], but did indicate what needs to be done to make it rigorous.

The link between the prolate spheroidal operator and the Riemann zeta zeroes was already present in Connes' earlier work [Connes, 1997] on an operator theoretic proof of the Riemann hypothesis. The result of [Connes and Moscovici, 2022] has strengthened this link, but at the same time has made it even more mysterious. It is not clear why the Riemann zeta zeroes should have anything to do with the seemingly unrelated prolate spheroidal operator, which finds its main use in mathematical physics and signal analysis. Combined with the already serendipitous results obtained by Slepian (see [Slepian, 1983]) on the use of the prolate spheroidal operator in signal analysis, it seems clear that the effort to understand the prolate spheroidal operator and its marvelous properties will remain an interesting and exciting area of research.

5 References

[Akhiezer and Glazman, 1981a] Akhiezer, N. I. and Glazman, I. M. (1981a). *Theory of Linear Operators in Hilbert Space. Vol I.* Pitman.

[Akhiezer and Glazman, 1981b] Akhiezer, N. I. and Glazman, I. M. (1981b). *Theory of Linear Operators in Hilbert Space. Vol II.* Pitman.

[Al-Gwaiz, 2008] Al-Gwaiz, M. (2008). *Sturm-Liouville Theory and its Applications.* Springer.

[Bender et al., 2017] Bender, C. M., Brody, D. C., and Müller, M. P. (2017). Hamiltonian for the zeros of the riemann zeta function. *Phys. Rev. Lett.*, 118:130201.

[Berry, 1986] Berry, M. V. (1986). Riemann's zeta function: A model for quantum chaos? In *Quantum Chaos and Statistical Nuclear Physics*, pages 1–17. Springer.

[Berry and Keating, 1999a] Berry, M. V. and Keating, J. P. (1999a). *H=xp and the Riemann Zeros*, pages 355–367. Springer US, Boston, MA.

[Berry and Keating, 1999b] Berry, M. V. and Keating, J. P. (1999b). The Riemann Zeros and Eigenvalue Asymptotics. *SIAM Review*, 41(2):236–266.

[Braun, 1992] Braun, M. (1992). *Differential Equations and Their Applications, Fourth Edition.* Springer.

[Brezis, 2010] Brezis, H. (2010). *Functional Analysis, Sobolev Spaces and Partial Differential Equations.* Universitext. Springer.

[Burden and Faires, 2001] Burden, R. and Faires, J. (2001). *Numerical Analysis, 7th Edition.* Brooks/Cole.

[Byrd and Friedman, 1971] Byrd, P. F. and Friedman, M. D. (1971). *Handbook of Elliptic Integrals for Engineers and Scientists.* Springer.

[Connes, 1997] Connes, A. (1997). Trace formula in noncommutative Geometry and the zeros of the Riemann zeta function. *Journées équations aux dérivées partielles.*

[Connes and Moscovici, 2022] Connes, A. and Moscovici, H. (2022). The UV prolate spectrum matches the zeros of zeta. *Proceedings of the National Academy of Sciences*, 119(22):e2123174119.

[Edwards, 1974] Edwards, H. (1974). *Riemann's Zeta Function.* Pure and Applied Mathematics. Academic Press.

[Erdelyi, 1956] Erdelyi, A. (1956). *Asymptotic Expansions.* Dover Publications.

[Goldstein et al., 2001] Goldstein, H., Poole, C., and Safko, J. L. (2001). *Classical Mechanics, Third Edition.* Addison-Wesley.

[Griffiths and Schroeter, 2018] Griffiths, D. and Schroeter, D. (2018). *Introduction to Quantum Mechanics, Third Edition.* Pearson Education.

[Hörmander, 1989] Hörmander, L. (1989). *The Analysis of Linear Partial Differential Operators I (2nd edition).* Grundlehren der mathematische Wissenschaften. Springer-Verlag.

[Katsnelson, 2018] Katsnelson, V. (2018). *Self-adjoint Boundary Conditions for the Prolate Spheroid Differential Operator*, pages 357–386. Springer International Publishing, Cham.

[Kolmogorov and Fomin, 1970] Kolmogorov, A. and Fomin, S. (1970). *Introductory Real Analysis*. Dover Publications.

[Kota, 2012] Kota, V. (2012). Random matrix theory in nuclear structure: Past, present and future. In *Proceedings of the DAE Symp. on Nucl. Phys.*, volume 57.

[Mehta, 1967] Mehta, M. (1967). *Random Matrices and the Statistical Theory of Energy Levels*. Academic Press.

[Montgomery, 1973] Montgomery, H. L. (1973). The pair correlation of zeros of the zeta function. *Analytic number theory*, 24:181–193.

[Naimark, 1967] Naimark, M. (1967). *Linear Differential Operators Part II*. Frederick Ungar Publishing.

[Odlyzko, 1987] Odlyzko, A. M. (1987). On the distribution of spacings between zeros of the zeta function. *Mathematics of Computation*, 48(177):273–308.

[Richard-Jung et al., 2017] Richard-Jung, F., Ramis, J.-P., Thomann, J., and Fauvet, F. (2017). New characterizations for the eigenvalues of the prolate spheroidal wave equation. *Studies in Applied Mathematics*, 138(1):3–42.

[Riemann, 1859] Riemann, B. (1859). Ueber die Anzahl der Primzahlen unter einer gegebenen Grosse. *Monatsberichte der Berliner Akademie*.

[Rudin, 1986] Rudin, W. (1986). *Real and Complex Analysis, Third Edition*. McGraw-Hill.

[Rudin, 1991] Rudin, W. (1991). *Functional Analysis*. Mc-Graw-Hill.

[Sierra and Rodríguez-Laguna, 2011] Sierra, G. and Rodríguez-Laguna, J. (2011). $h = xp$ model revisited and the riemann zeros. *Phys. Rev. Lett.*, 106:200201.

[Slepian, 1983] Slepian, D. (1983). Some comments on fourier analysis, uncertainty and modeling. *SIAM Review*, 25(3):379–393.

[Slepian and Pollak, 1961] Slepian, D. and Pollak, H. O. (1961). Prolate spheroidal wave functions, fourier analysis and uncertainty I. *The Bell System Technical Journal*, 40(1):43–63.

[Stein and Shakarchi, 2003] Stein, E. and Shakarchi, R. (2003). *Complex Analysis*. Princeton University Press.

[Stone, 2005] Stone, A. (2005). Einstein's Unknown Insight and the Problem of Quantizing Chaos. *Physics Today*, 58(8):37–43.

[Subramanyan et al., 2021] Subramanyan, V., Hegde, S. S., Vishveshwara, S., and Bradlyn, B. (2021). Physics of the inverted harmonic oscillator: From the lowest landau level to event horizons. *Annals of Physics*, 435:168470.

[Talagrand, 2022] Talagrand, M. (2022). *What Is a Quantum Field Theory?* Cambridge University Press.

[Titchmarsh, 1946] Titchmarsh, E. (1946). *Eigenfunction Expansions Associated with Second-Order Differential Equations. Part I.* Oxford University Press.

[Titchmarsh, 1986] Titchmarsh, E. (1986). *The Theory of The Riemann Zeta-Function.* Clarendon Press.

[van Neerven, 2022] van Neerven, J. (2022). *Functional Analysis.* Cambridge Studies in Advanced Mathematics. Cambridge University Press.

[Victor, 2019] Victor, I. (2019). *100 years of Weyl's Law*, pages 641–729. Springer International Publishing, Cham.

[Weidenmüller and Mitchell, 2009] Weidenmüller, H. A. and Mitchell, G. E. (2009). Random matrices and chaos in nuclear physics: Nuclear structure. *Rev. Mod. Phys.*, 81:539–589.

[Weidmann, 1987] Weidmann, J. (1987). *Spectral Theory of Ordinary Differential Operators.* Springer-Verlag Berlin.

[Yakaboylu, 2022] Yakaboylu, E. (2022). Formally Self-Adjoint Hamiltonian for the Hilbert-Pólya Conjecture.

[Zettl, 2005] Zettl, A. (2005). *Sturm-Liouville Theory*, volume 121 of *Mathematical Surveys and Monographs.* American Mathematical Society.

[Zettl et al., 1977] Zettl, A., Kauffman, R. M., and Read, T. T. (1977). *The Deficiency Index Problem for Powers of Ordinary Differential Expressions.* Springer-Verlag Berlin.

[Çevik and Ismailov, 2012] Çevik, E. and Ismailov, Z. (2012). Spectrum of the direct sum of operators. *Electronic Journal of Differential Equations.*

A Operator Decomposition

We present in this appendix some standard results on orthogonal decompositions of operators which are used in the thesis. For more details, one can consult textbooks on functional analysis, such as [van Neerven, 2022]. However, the results stated and proven in this appendix cannot always be found in the literature.

Suppose $A : D(A) \subseteq \mathcal{H} \to \mathcal{H}$ is an operator on some Hilbert space $\mathcal{H}$. Given an orthogonal decomposition $\mathcal{H} = U \oplus V$, in which $V = U^\perp$, we say that A is orthogonally decomposable along this decomposition if A commutes with the orthogonal projection P onto U. Recall that this means that $D(A)$ is invariant under P and that $PAx = APx$ for all $x \in D(A)$. It follows that A also commutes with the orthogonal projection Q onto V and that U, V are invariant under A, meaning we may define restriction operators

$$A_1 : D(A_1) \subseteq U \to U$$
$$A_2 : D(A_2) \subseteq V \to V$$

defined by $D(A_1) = D(A) \cap U$, $A_1 x = Ax$ and similarly for A_2. These operators on U, V are unique, in the sense that they are the only operators such that $Ax = A_1 Px + A_2 Qx$ for all $x \in D(A)$.

Lemma A.1. If an operator $A : D(A) \subseteq \mathcal{H} \to \mathcal{H}$ is orthogonally decomposable along $\mathcal{H} = U \oplus V$, then its spectrum is related to the spectra of its restriction operators by

$$\sigma(A) = \sigma(A_1) \cup \sigma(A_2).$$

Proof. It is obviously equivalent to prove the relation

$$\rho(A) = \rho(A_1) \cap \rho(A_2)$$

for the resolvent sets. Let $\mu \in \rho(A_1) \cap \rho(A_2)$. Then the operators $A_1 - \mu$ and $A_2 - \mu$ have bounded inverses $B_1 : U \to D(A_1)$ and $B_2 : V \to D(A_2)$ respectively. Defining $B = B_1 \oplus B_2$, it is not hard to verify that B is bounded and is an inverse to $A - \mu$, hence $\mu \in \rho(A)$. Conversely, given $\mu \in \rho(A)$, there exist a bounded inverse $B : \mathcal{H} \to D(A)$ to $A - \mu$. We prove that it leaves U invariant, the proof being similar for V. Suppose $u \in U$ and orthogonally decompose $Bu = u' + v'$. Applying $A - \mu$ yields

$$u = (A - \mu)u' + (A - \mu)v'.$$

Because U and V are invariant under A, the summands are elements of U and V respectively. From the uniqueness of orthogonal decomposition, it follows that $(A - \mu)v' = 0$. Applying B gives $v' = 0$, meaning $Bu = u' \in U$. We can now define restriction operators B_1, B_2 on U, V respectively and easily show that they are bounded inverses to $A_1 - \mu$ and $A_2 - \mu$, giving us $\mu \in \rho(A_1) \cap \rho(A_2)$. □

Lemma A.2. If a self-adjoint operator $A : D(A) \subseteq \mathcal{H} \to \mathcal{H}$ can be orthogonally decomposed a decomposition $\mathcal{H} = U \oplus V$, then its restriction operators A_1, A_2 are self-adjoint as well.

Proof. We prove only that A_1 is self-adjoint, the proof for A_2 being similar. Because A is self-adjoint, it is in particular symmetric and this property is easily seen to be inherited by A_1. Thus, it suffices to prove that $D(A_1^*) \subseteq D(A_1)$. Let $y \in D(A_1^*)$. Because A_1 is an operator on U, this

means that $y \in U$ and $\langle A_1 u, y\rangle = \langle u, A_1^* y\rangle$ for all $u \in U$. For any $x \in D(A)$, we have an orthogonal decomposition $x = u + v$ with $u, v \in D(A)$. Using orthogonality, we have $\langle Ax, y\rangle = \langle Au, y\rangle$. Hence, $\langle Ax, y\rangle = \langle u, A_1^* y\rangle = \langle x, A_1^* y\rangle$, in which we have used orthogonality once more. We conclude that $y \in D(A^*)$. Using the self-adjointness of A, this means $y \in D(A)$, which shows that $y \in D(A_1)$ when combined with $y \in U$. $\square$

B Integration

We assume the reader is familiar with measure-theoretic integration, especially with L^p spaces. A good reference on these topics is [Rudin, 1986]. In this thesis, we are primarily interested in the spaces $L^2(I)$ of complex valued square-integrable functions for open intervals $I \subseteq \mathbb{R}$, as these form Hilbert spaces suitable for the analysis of differential operators over $\mathbb{R}$. In this appendix, we prove some facts about integration which are needed throughout this thesis, beginning with the continuity of the Lebesgue integral.

Proposition B.1. Suppose f is integrable over $(a, b) \subseteq \mathbb{R}$. For any $\varepsilon > 0$, there exists a $\delta > 0$ such that for any measurable set $A \subseteq (a, b)$ with Lebesgue measure $\lambda(A) < \delta$ we have

$$\int_A |f(t)|\,dt < \varepsilon.$$

Proof. First suppose f is bounded, say $|f| \leq M$. The proposition then easily follows from the bound

$$\int_A |f(t)|\,dt \leq M\lambda(A).$$

If f is not bounded, one uses the definition of the Lebesgue integral to find a simple function $g \leq |f|$, which is bounded, such that

$$\int_a^b |f(t)|\,dt - \int_a^b g(t)\,dt < \frac{1}{2}\varepsilon.$$

Choose δ such that $\int_A g(t)\,dt < \varepsilon/2$ whenever $\lambda(A) < \delta$, we get

$$\begin{aligned}\int_A |f(t)|\,dt &= \int_A |f(t)|\,dt - \int_A g(t)\,dt + \int_A g(t)\,dt \\ &\leq \int_a^b |f(t)|\,dt - \int_a^b g(t)\,dt + \int_A g(t)\,dt \\ &< \varepsilon.\end{aligned}$$

□

Proposition B.2. Let $(a, b) \subseteq \mathbb{R}$ be a finite or infinite interval and suppose f is integrable over (a, b). Then we have

$$\lim_{x \to a^+} \int_x^b f(t)\,dt = \int_a^b f(t)\,dt$$
$$\lim_{x \to b^-} \int_a^x f(t)\,dt = \int_a^b f(t)\,dt.$$

Proof. For finite a, the limit follows from the equality

$$\int_a^b f(t)\,dt - \int_x^b f(t)\,dt = \int_a^x f(t)\,dt$$

and Proposition B.1, which shows that

$$\left|\int_a^x f(t)\,dt\right| \leq \int_a^x |f(t)|\,dt < \varepsilon$$

for x sufficiently close to a. For infinite b, one makes use of the dominated convergence theorem. Specifically, we define the sequence of functions $f_n = f\mathbf{1}_{(a,a+n)}$ for $n > 1$, which converges pointwise to f and is dominated by f. Hence, we get

$$\begin{aligned} &\lim_{n\to\infty} \int_a^\infty |f_n(t) - f(t)|\,dt = 0 \\ \iff &\lim_{n\to\infty} \int_{a+n}^\infty |f(t)|\,dt = 0. \end{aligned}$$

Because the function $x \mapsto \int_x^b |f(t)|\,dt$ is non-increasing, it follows that

$$\lim_{x\to\infty} \int_x^\infty |f(t)|\,dt = 0,$$

from which the desired limit follows easily. The cases in which a is infinite and b is finite are proven completely similarly. □

Recall that functions $f \in L^2(I)$ are defined up to sets of measure zero. This means that it is not possible in general to speak of function values $f(x)$, as these are not uniquely defined. It is possible to speak, however, of function values of continuous functions in $L^2(I)$. For this, we first need to know how to define continuity of almost everywhere defined functions, as continuity is normally defined pointwise. The following pair of definition and proposition show how to do so in a well-defined manner.

Definition B.3. A function $f \in L^2(I)$ is said to be continuous if it is almost everywhere equal to a continuous function. Said differently, the equivalence class $[f]$ has a continuous representative.

Proposition B.4. Suppose that $f, g : I \subseteq \mathbb{R} \to \mathbb{C}$ are continuous and almost everywhere equal to each other. Then f and g are everywhere equal on I.

Proof. Defining the continuous function $h = f - g$, we prove that $h(x) = 0$ for any $x \in I$. Suppose that $h(x) \neq 0$. Without loss of generality, we assume $h(x) > 0$. By continuity, there is a $\delta > 0$ such that $h(t) > 0$ for all $t \in (x - \delta, x + \delta)$. But this would mean that the set of points for which f and g differ has positive measure, which is a contradiction. □

We can similarly define for almost everywhere defined functions any property which implies continuity, such as differentiability. Another such property is absolute continuity, which is of importance in this thesis. Essentially, the class of absolutely continuous functions on a compact interval $[a, b]$ is the largest class of functions on $[a, b]$ for which the fundamental theorem calculus holds when using the Lebesgue integral. We use this characterisation to define absolute continuity and local absolute continuity.

Definition B.5. A function $f : [a, b] \to \mathbb{C}$ is absolutely continuous if there is some integrable function $g : [a, b] \to \mathbb{C}$ such that

$$f(x) = f(a) + \int_a^x g(t)\,dt$$

for all $x \in [a, b]$. Given an open interval $I \subseteq \mathbb{R}$, a function $f : I \to \mathbb{C}$ is said to be locally absolutely continuous if it is absolutely continuous on each compact interval $[a, b] \subseteq I$.

Combining this definition with Proposition B.1, it is clear that (locally) absolutely continuous functions are continuous. This is not the definition which one usually encounters in textbooks, but is equivalent to it. For a good treatment of absolute continuity and related concepts, the reader may for example consult [Kolmogorov and Fomin, 1970]. The following propositions, stated without proof, express properties of absolutely continuous functions which are needed in this thesis.

Proposition B.6. Suppose f and g are absolutely continuous on $[a, b]$. Then $f + g$ and fg are as well. Furthermore, if there is a $C > 0$ such that $|g| \geq C$ on $[a, b]$, then f/g is also absolutely continuous.

Proposition B.7. If f is absolutely continuous, say

$$f(x) = f(a) + \int_a^x g(t)\, dt,$$

then f is almost everywhere differentiable and its almost everywhere defined derivative f' is almost everywhere equal to g. This uniquely identifies g up to a set of measure zero.

Proposition B.8. If f is absolutely continuous on $[a, b]$ and has continuous almost-everywhere defined derivative f', then f is continuously differentiable on $[a, b]$.

Proof. If f' is continuous, its Lebesgue integral over a compact interval coincides with its Riemann integral. Hence, we may apply the standard fundamental theorem of calculus to conclude that

$$f(x) = f(a) + \int_a^x f'(t)\, dt$$

is differentiable with continuous derivative f', meaning it is continuously differentiable. □

Proposition B.9. Let $x_0 \in \mathbb{R}$ and suppose f is continuous at x_0 and locally absolutely continuous on $(x_0 - r, x_0)$ and $(x_0, x_0 + r)$ for some $r > 0$. If f' is integrable on $(x_0 - r, x_0 + r)$, then f will be locally absolutely continuous on $(x_0 - r, x_0 + r)$.

Proof. It suffices to proof the absolute continuity of f on compact intervals $[a, b]$ which have $x_0 \in (a, b)$. Using the integrability of f' and the local absolute continuity of f, we have

$$\begin{aligned}\int_a^x f'(t)\, dt &= \int_a^{x_0-\varepsilon} f'(t)\, dt + \int_{x_0+\varepsilon}^x f'(t)\, dt + \int_{x_0-\varepsilon}^{x_0+\varepsilon} f'(t)\, dt \\ &= f(x_0 - \varepsilon) - f(a) + f(x) - f(x_0 + \varepsilon) + \int_{x_0-\varepsilon}^{x_0+\varepsilon} f'(t)\, dt\end{aligned}$$

for $x \in (x_0, b]$ and $\varepsilon > 0$ small enough. Continuity of f at x_0 and Proposition B.1 imply

$$\begin{aligned}\lim_{\varepsilon \to 0^+} (f(x_0 - \varepsilon) - f(x_0 + \varepsilon)) &= 0 \\ \lim_{\varepsilon \to 0^+} \int_{x_0-\varepsilon}^{x_0+\varepsilon} f'(t)\, dt &= 0,\end{aligned}$$

which yield

$$\int_a^x f'(t)\,dt = f(x) - f(a).$$

□

C Distributions

Distributions are generalisations of functions. They are particularly useful for differential equations, in which they and related concepts (such as weak derivatives and weak solutions) form a good framework for the study of differential equations, which is why they appear in [Connes and Moscovici, 2022]. The reader is referred to [Rudin, 1991] for a detailed introduction to distributions and some of their applications to differential equations. In this appendix we state and prove some facts related to distributions that are used throughout the thesis.

Definition C.1. Let $\mathcal{D}(\mathbb{R})$ denote the set of compactly supported smooth (complex-valued) functions on $\mathbb{R}$. A distribution (on $\mathbb{R}$) is a linear map $\Lambda : \mathcal{D}(\mathbb{R}) \to \mathbb{C}$ satisfying a continuity condition. We denote the set of distributions by $\mathcal{D}'(\mathbb{R})$.

We do not go into the details of what the continuity condition precisely entails. One can consult the literature for this. Given a locally integrable function[10] $f \in L^1_{\text{loc}}(\mathbb{R})$, the map

$$\varphi \mapsto \int_{\mathbb{R}} \varphi(x) f(x)\, dx \tag{C.1}$$

defines a distribution. This is the distribution associated to the function f, and is uniquely determined by f, in the sense of the following proposition, which we state without proof.

Proposition C.2. Suppose that $f, g \in L^1_{\text{loc}}(\mathbb{R})$. If for all $\varphi \in \mathcal{D}(\mathbb{R})$ we have

$$\int_{\mathbb{R}} \varphi(x) f(x)\, dx = \int_{\mathbb{R}} \varphi(x) g(x)\, dx,$$

then f and g are almost everywhere equal.

The specific distributions (C.1) show us how to define a notion of derivative for distributions. One would like to say that

$$\varphi \mapsto \int_{\mathbb{R}} \varphi(x) f'(x)\, dx$$

is the derivative of the distribution (C.1). However, this definition does not make sense if f is not differentiable. Using a formal integration by parts, this distribution should be the same as

$$\varphi \mapsto -\int_{\mathbb{R}} \varphi'(x) f(x)\, dx,$$

which is well-defined and defined in terms of the distribution (C.1). Generalising, this leads to the following definition of the derivative of a distribution (higher order derivatives are defined similarly, taking appropriate care of the minus sign).

Definition C.3. The distributional derivative of $\Lambda \in \mathcal{D}'(\mathbb{R})$ is the distribution Λ' defined by the action $\Lambda'(\varphi) = -\Lambda(\varphi')$. One can indeed show that this map is linear and continuous.

A more specialized class of distributions is obtained by replacing $\mathcal{D}(\mathbb{R})$ by the larger class of Schwartz functions $\mathcal{S}(\mathbb{R})$. A Schwartz function is by definition a smooth function $\varphi : \mathbb{R} \to \mathbb{C}$ such that

$$\sup_{x \in \mathbb{R}} \left| x^n \varphi^{(m)}(x) \right| < \infty$$

[10] That is, a function which is integrable over each compact interval $[a, b] \subseteq \mathbb{R}$.

for all $n, m \geq 0$. That is, φ and all its derivatives decay faster to zero at $\pm\infty$ than any polynomial. We gather some elementary properties of $\mathcal{S}(\mathbb{R})$ in the following proposition.

Proposition C.4. The Schwartz space $\mathcal{S}(\mathbb{R})$ is closed under sums, products, differentiation and multiplication by polynomials[11].

Definition C.5. A tempered distribution (on $\mathbb{R}$) is a linear map $\Lambda : \mathcal{S}(\mathbb{R}) \to \mathbb{C}$ satisfying a continuity condition. We denote the set of tempered distributions by $\mathcal{S}'(\mathbb{R})$.

Schwartz functions form a class for which the Fourier inversion theorem holds, which makes them useful in the study of the Fourier transform. That is, restricting the Fourier transform F to $\mathcal{S}(\mathbb{R})$ yields a map $F : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R})$ whose inverse is given by the inverse Fourier transform. A similar fact holds for tempered distributions, upon defining a Fourier transform for tempered distributions.

The rest of this appendix is devoted to proving some facts about the distributions which we use in the text. First, in Proposition 3.9, we claim that the map on $\mathcal{S}(\mathbb{R})$ defined by

$$\varphi \mapsto \int_{\mathbb{R}} (W\varphi)(x)\xi(x)\,dx \tag{C.2}$$

is a tempered distribution, in which $\xi \in L^2(\mathbb{R})$. We will indicate how this is proven to be true. It follows from Proposition C.4 that $W\varphi \in \mathcal{S}(\mathbb{R})$. One can show that $\mathcal{S}(\mathbb{R}) \subseteq L^2(\mathbb{R})$, thus Hölder's inequality gives that (C.2) is finite, hence well-defined. Given a tempered distribution Λ and a polynomial p, one can define the maps

$$\Lambda' : \varphi \mapsto -\Lambda(\varphi')$$
$$p\Lambda : \varphi \mapsto \Lambda(p\varphi)$$

and show that these are tempered distributions as well. The map (C.2) is built up of these two operations on tempered distributions, starting with the tempered distribution $\varphi \mapsto \int_{\mathbb{R}} \varphi(x)\xi(x)\,dx$, which shows that it is a tempered distribution as well.

Proposition C.6. If $\varphi, \psi \in \mathcal{S}(\mathbb{R})$, then we have the integration by parts formula

$$\int_{\mathbb{R}} \varphi'(x)\psi(x)\,dx = -\int_{\mathbb{R}} \varphi(x)\psi'(x)\,dx.$$

Proof. Because $\mathcal{S}(\mathbb{R})$ is closed under multiplication, it suffices to prove

$$\int_{\mathbb{R}} \varphi'(x)\,dx = 0$$

for all $\varphi \in \mathcal{S}(\mathbb{R})$, as one can then use the product rule to derive the integration by parts formula. To do so, we define the sequence $\psi_n = \varphi' \mathbf{1}_{[-n,n]}$ and apply the dominated convergence theorem. We have pointwise convergence $\psi_n \to \varphi'$ and (ψ_n) is dominated by φ', which is integrable as an element of $\mathcal{S}(\mathbb{R})$. Hence

$$\int_{\mathbb{R}} \varphi'(x)\,dx = \lim_{n\to\infty} \int_{\mathbb{R}} \psi_n(x)\,dx.$$

[11] that is, $p\varphi \in \mathcal{S}(\mathbb{R})$ if p is a polynomial and $\varphi \in \mathcal{S}(\mathbb{R})$

Because φ' is continuous, we may replace the Lebesgue integral by the Riemann integral and use the standard fundamental theorem of calculus to get

$$\begin{aligned}\int_{\mathbb{R}} \psi_n(x)\,dx &= \int_{-n}^{n} \varphi'(x)\,dx \\ &= \varphi(n) - \varphi(-n) \to 0\end{aligned}$$

as $n \to \infty$, because φ is a Schwartz function. This proves the assertion. □

Proposition C.7. Suppose $\Lambda \in \mathcal{D}'(\mathbb{R})$ is a distribution such that $\Lambda'' = 0$, that is, for each $\varphi \in \mathcal{D}(\mathbb{R})$ we have $\Lambda(\varphi'') = 0$. Then there exist unique complex numbers a, b such that

$$\Lambda(\varphi) = \int_{\mathbb{R}} \varphi(x)(ax + b)\,dx$$

for all $\varphi \in \mathcal{D}(\mathbb{R})$. In other words, Λ is the distribution corresponding to the degree-one polynomial $ax + b$.

Proof. One easily finds in the literature (for example, theorem 3.1.4 in [Hörmander, 1989]) the theorem that $\Lambda' = 0$ implies that Λ is the distribution corresponding to a constant function, in the sense of (C.1). We use this fact to prove the proposition. Because $(\Lambda')' = 0$, there is some $a \in \mathbb{C}$ such that

$$\Lambda'(\varphi) = \int_{\mathbb{R}} \varphi(x) a\,dx.$$

The distributional derivative of $\varphi \mapsto \int_{\mathbb{R}} \varphi(x) ax\,dx$ is given by $\varphi \mapsto \int_{\mathbb{R}} \varphi(x) a\,dx$. This means that the distributional derivative of

$$\varphi \mapsto \Lambda(\varphi) - \int_{\mathbb{R}} \varphi(x) ax\,dx$$

is zero, from which the desired conclusion follows when applying the theorem mentioned at the beginning of the proof once again. □

Proposition C.8. If $f \in L^1_{\mathrm{loc}}(\mathbb{R})$ and $\varphi \in \mathcal{D}(\mathbb{R})$, define for some arbitrary x_0 the function

$$F(x) = \int_{x_0}^{x} f(t)\,dt.$$

Then we have the equality

$$\int_{\mathbb{R}} \varphi(t) F(t)\,dt = -\int_{\mathbb{R}} \varphi'(t) f(t)\,dt.$$

Proof. See Lemma 8.2 in [Brezis, 2010]. □

D Numerical Calculation

The imaginary eigenvalues of the Dirac operator $2\not{D}$, which are plotted in Fig. 2 together with the imaginary parts of the non-trivial Riemann zeta zeroes, are not actually calculated using $\not{D}$ directly. Instead, one calculates the negative eigenvalues μ of W_2^+ and then uses the fact that the imaginary eigenvalues of $2\not{D}$ are given by $\pm 2i\sqrt{-\mu}$. These eigenvalues are those of the singular Sturm-Liouville boundary-value problem on (λ, ∞) (the parameter λ is given the value $\sqrt{2}$, as in Proposition 3.41, but we will keep writing λ) given by

$$\begin{cases} W\xi = \mu\xi \\ \lim_{x\to\lambda^+} p(x)\xi'(x) = 0 \\ \lim_{x\to\infty} \left(x\sin(2\pi\lambda x)\xi'(x) - (2\pi\lambda x\cos(2\pi\lambda x) - \sin(2\pi\lambda x))\xi(x)\right) = 0. \end{cases} \tag{D.1}$$

We will indicate in this appendix how one may numerically solve this problem, to obtain a figure like Fig. 2. We use a numerical method for boundary value problems called the 'shooting method' (see for example [Burden and Faires, 2001]). To do so, we first recall some theoretical facts which we derived about the differential equation $W\xi = \mu\xi$. Using the Frobenius method, we found in Subsection 3.3 that near λ there is a basis of consisting of two solutions of the form

$$f(x)$$
$$f(x)\log(x-\lambda) + g(x),$$

in which f, g are analytic functions which may be chosen such that $f(0) = 1$. As was pointed out in the proof of Proposition 3.31, the boundary condition

$$\lim_{x\to\lambda^+} p(x)\xi'(x) = 0$$

forces the logarithmic term to vanish. This means that the solution should be finite at λ. Conversely, the boundary condition is automatically satisfied when assuming the solution is finite at λ, as it is then a multiple of the solution f, which is analytic at λ. This means that to solve (D.1), we seek solutions ξ which are finite at λ and satisfy

$$\lim_{x\to\infty} \left(x\sin(2\pi\lambda x)\xi'(x) - (2\pi\lambda x\cos(2\pi\lambda x) - \sin(2\pi\lambda x))\xi(x)\right) = 0. \tag{D.2}$$

The shooting methods consists of numerically solving the differential equation $W\xi = \mu\xi$ with initial conditions $\xi(0) = 1, \xi'(0) = 0$ for each μ of interest and checking whether this solution satisfies (D.2). If it does, then we have found an eigenvalue. There are two problems with this approach. First, the differential equation is singular at λ, which can be problematic for numerical integrators. Second, we cannot numerically integrate over the entire interval (λ, ∞), meaning we cannot check the condition (D.2). We take care of these problems by numerically integrating over the interval $(\lambda+\varepsilon, N)$, for some small $\varepsilon > 0$ and some large N. As an example, the numerical integration corresponding to $\mu = 0$ is plotted in Fig. 3. We have plotted $C(x) = x\sin(2\pi\lambda x)\xi'(x) - (2\pi\lambda x\cos(2\pi\lambda x) - \sin(2\pi\lambda x))\xi(x)$ for values of x near N in Fig. 4. As $x \to \infty$, it seems to settle down to sinusoidal behaviour (though it seems to decay at a later point). Hence, we propose to check the condition D.2 by computing the average of C over a number of periods near N. This average is a function of μ, which we denote by $s(\mu)$.

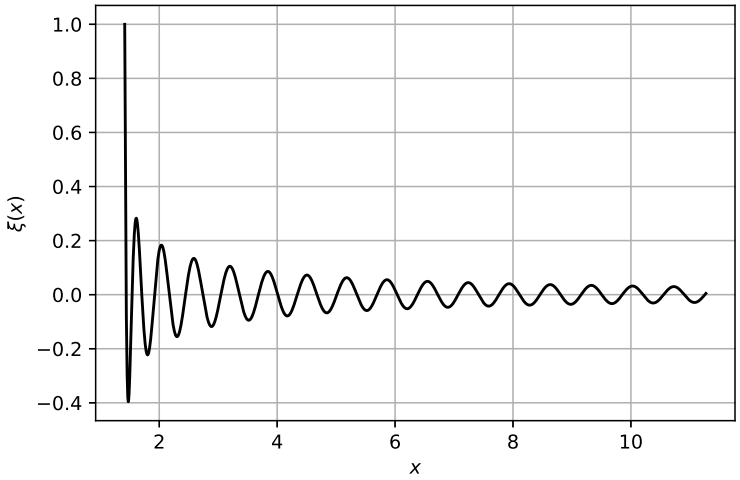

Figure 3: Numerical solution of $W\xi = \mu\xi$ with initial conditions $\xi(0) = 1, \xi'(0) = 0$. The numerical parameters used in this integration are $N = 100$, $\varepsilon = 10^{-5}$ and step size $\Delta x = 10^{-4}$.

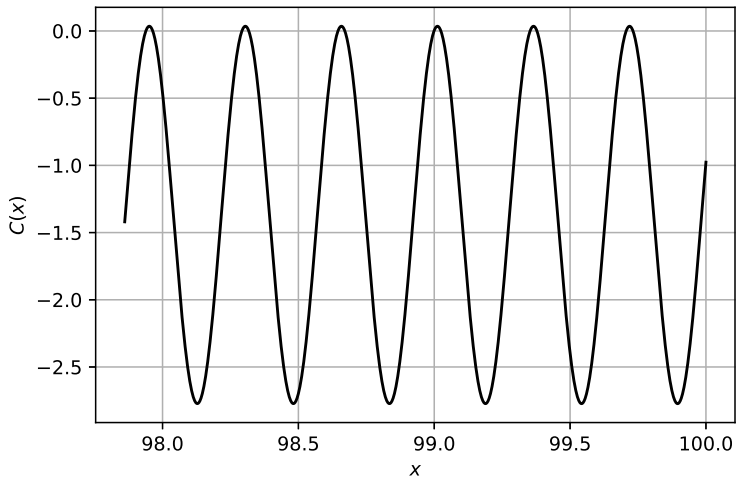

Figure 4: The function $C(x)$ for values of x near N, calculated for the solution in Fig. 3. In general, C seems to behave sinusoidally for large x.

To illustrate the numerical method, we calculate $s(\mu)$ for 2000 discrete values μ_n in the range $(-1300, 0)$. We implement it in Python, with the code provided at the end of this appendix. The results of these calculations are given by the curve in Fig. 5. Where this curve crosses the horizontal axis, there is an eigenvalue. We find these crossings by looking for n such that $s(\mu_{n+1})$ and $s(\mu_n)$ differ in sign and estimate the crossing by the midpoint $(\mu_{n+1} + \mu_n)/2$. The resulting estimates for the eigenvalues are then converted into imaginary eigenvalues of $2\not{D}$ by the rule $\mu \mapsto 2i\sqrt{-\mu}$ and these have been plotted in Fig. 6 together with the imaginary parts of the non-trivial Riemann zeta zeroes. These results approximately agree with those of Fig. 2.

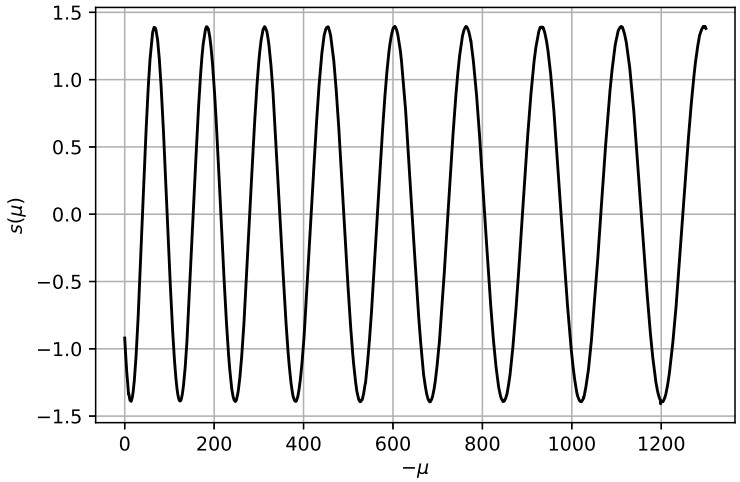

Figure 5: The values of $s(\mu)$, for 2000 discrete values μ_n in the range $(-1300, 0)$, resulting from a numerical calculation with parameters $N = 400$, $\varepsilon = 10^{-6}$ and step size $\Delta x = 4 \cdot 10^{-4}$. The average of C was taken over the interval $[390, 400]$. The eigenvalues are the points for which $s(\mu) = 0$ holds.

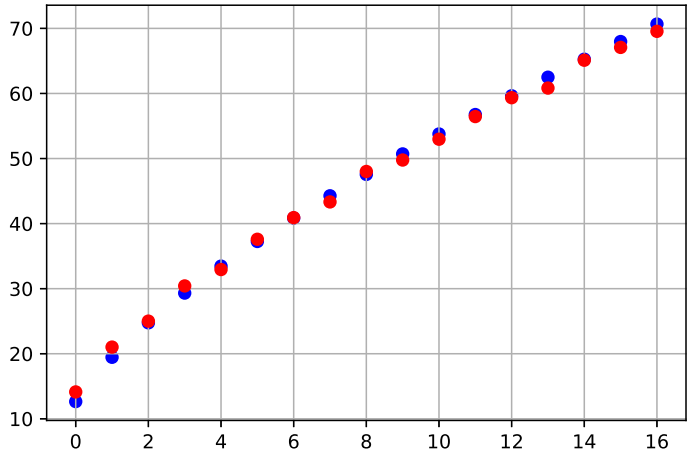

Figure 6: Eigenvalues (in blue) of $2\not{D}$ as calculated from the results shown in Fig. 5. The imaginary parts of the non-trivial Riemann zeta zeroes are plotted as well (in red). These numerical results seem to approximately agree with those of [Connes and Moscovici, 2022], shown in Fig. 2.

```
# Code for numerical calculation of eigenvalues
# of the prolate spheroidal operator and the
# associated Dirac square root

# Import necessary packages
# odeint used to solve initial value problems

import numpy as np
from scipy.integrate import odeint
from matplotlib import pyplot as plt

# Set parameters

a = np.sqrt(2)
eps = 0.000001
N = 400
N_t = 1000000

# Define domain of integration
# and set initial values

t_span = np.linspace(a + eps , N, N_t)
z0 = [1,0]

# This function calculates the derivative
# of z = [xi, xi_dot]

def derive(z,t):

    xi, xi_dot = z

    return [xi_dot, (mu*xi - (2*np.pi*a*t)**2*xi - 2*t*xi_dot)/(t**2 - a**2)]

# Perform the numerical integration for
# some values of mu

mu_list = np.linspace(-1300,0,2000)
results_list = []

for mu in mu_list:

    # Numerical integration

    z = odeint(derive, z0, t_span)

    # Extract components
```

```
    xi = z[:,0]
    xi_dot = z[:,1]

    # Calculate boundary condition by avering
    # over the interval [390, 400]

    test = t_span*np.sin(2*np.pi*a*t_span)*xi_dot - (2*np.pi*a*np.cos(2*np.pi*a*t_span) -
    results_list.append(np.average(test[-10*(N_t/N):]))


# Estimate eigenvalues as midpoints of crossings
# and convert them to eigenvalues of Dirac operator

eigenvalues = []

for i in range(0,len(results_list) - 1):

    # Check whether sign changes

    if results_list[i + 1]*results_list[i] < 0:

        eigenvalues.append(2*np.sqrt(-1*(mu_list[i + 1] + mu_list[i])/2))
```