

Behaviour of Eigenfunction Subsequences for Delta-Perturbed 2D Quantum Systems

by
Adam Newman

A Doctoral Thesis

Submitted in partial fulfillment of the requirements
for the award of
Doctor of Philosophy of Loughborough University

May 25, 2016

© by Adam Newman, 2016

Abstract

We consider a quantum system whose unperturbed form consists of a self-adjoint $-\Delta$ operator on a 2-dimensional compact Riemannian manifold, which may or may not have a boundary. Then as a perturbation, we add a delta potential / point scatterer at some select point p . The perturbed self-adjoint operator is constructed rigorously by means of self-adjoint extension theory. We also consider a corresponding classical dynamical system on the cotangent/cosphere bundle, consisting of geodesic flow on the manifold, with specular reflection if there is a boundary.

Chapter 2 describes the mathematics of the unperturbed and perturbed quantum systems, as well as outlining the classical dynamical system. Included in the discussion on the delta-perturbed quantum system is consideration concerning the strength of the delta potential. It is reckoned that the delta potential effectively has negative infinitesimal strength.

Chapter 3 continues on with investigations from [KMW10], concerned with perturbed eigenfunctions that approximate to a linear combination of only two “surrounding” unperturbed eigenfunctions. In Thm. 4.4 of [KMW10], conditions are derived under which a sequence of perturbed eigenfunctions exhibits this behaviour in the limit. The approximating pair linear combinations belong to a class of quasimodes constructed within [KMW10]. The aim of Chapter 3 in this thesis is to improve on the result in [KMW10].

In Chapter 3, preliminary results are first derived constituting a broad consideration of the question of when a perturbed eigenfunction subsequence approaches linear combinations of only two surrounding unperturbed eigenfunctions. Afterwards, the central result of this Chapter, namely Thm. 3.4.1, is derived, which serves as an improved version of Thm. 4.4 in [KMW10]. The conditions of this theorem are shown to be weaker than those in [KMW10]. At the same time though, the conclusion does not require the approximating pair linear combinations to be quasimodes contained in the domain of the perturbed operator. Cor. 3.5.2 allows for a transparent comparison between the results of this Chapter and [KMW10].

Chapter 4 deals with the construction of non-singular rank-one perturbations for which the eigenvalues and eigenfunctions approximate those of the delta-perturbed operator. This is approached by means of direct analysis of the construction and formulae for the rank-one-perturbed eigenvalues and eigenfunctions, by comparison that of the delta-perturbed eigenvalues and eigenfunctions. Successful results are derived to this end, the central result being Thm. 4.4.19. This provides conditions on a sequence of non-singular rank-one perturbations, under which all eigenvalues and eigenbasis members within an interval converge to those of the delta-perturbed operator.

Comparisons have also been drawn with previous literature such as [Zor80], [AK00] and [GN12]. These deal with rank-one perturbations approaching the delta potential within the setting of a whole Euclidean space \mathbb{R}^n , for example by strong resolvent convergence, and by limiting behaviour of generalised eigenfunctions associated with energies at every $E \in (0, \infty)$. Furthermore in Chapter 4, the suggestion from Chapter 2 that the delta potential has negative infinitesimal strength is further supported, due to the coefficients of the approximating rank-one perturbations being negative and tending to zero. This phenomenon is also in agreement with formulae from [Zor80], [AK00] and [GN12].

Chapter 5 first reviews the correspondence between certain classical dynamics and equidistribution in position space of almost all unperturbed quantum eigenfunctions, as demonstrated for example in [MR12]. Equidistribution in position space of almost all *perturbed* eigenfunctions, in the case of the 2D rectangular flat torus, is also reviewed. This result comes from [RU12], which is only stated in terms of the “new” perturbed eigenfunctions, which would only be a subset of the full perturbed eigenbasis. Nevertheless, in this Chapter it is explained how it follows that this position space equidistribution result also applies to a full-density subsequence of the full perturbed eigenbasis.

Finally three methods of approach are discussed for attempting to derive this position space equidistribution result in the case of a more general delta-perturbed system whose classical dynamics satisfies the particular key property.

Acknowledgements

I would like to express gratitude towards Prof. Jenya Ferapontov for his welcoming and encouraging dialogue with me during the time that I was enquiring about a doctoral research position at Loughborough University, and of course my supervisor, Dr. Brian Winn, who put forward a research topic which I am glad to say I accepted, and has helped to direct, shape and support my research throughout my time here at Loughborough University.

I would also like to express gratitude towards other academic staff who have been able to provide some of their expertise, such as Dr. Alex Strohmaier and Dr. Alexey Bolsinov. Furthermore I would like to express gratitude towards Dr. Thomas Bartsch for the advice that he has been providing concerning the organisation of my research and the content of what I write. It has also been a pleasant experience to meet academics from other institutions at conferences and events, such as Pär Kurlberg, Dmitry (Dima) Jakobson, Stéphane Nonnenmacher, Steve Zelditch and Sir Michael Berry.

I would like to express my appreciation towards my fellow colleagues (other doctoral researchers), having enjoyed both socialising with them and discussing mathematics with them.

I would like to express gratitude and appreciation towards my own family, for their continual love and support throughout.

Soli Deo gloria.

To God alone (Father, Son, Spirit) be the glory.

Contents

1	Introduction	7
1.1	Introduction to semiclassical analysis and quantum chaos	7
1.1.1	Classical mechanics	7
1.1.2	Quantum mechanics	10
1.1.3	Interface between quantum and classical mechanics	12
1.2	Preliminary facts and assumptions	14
1.3	Achievements in quantum chaos: eigenvalue statistics	16
1.3.1	Basic theory of eigenvalue statistics	16
1.3.2	Integrable dynamics, WKB quantisation and Poissonian statistics	18
1.3.3	Chaotic dynamics and random matrix statistics	24
1.4	Achievements in quantum chaos: behaviour of eigenfunctions	28
1.4.1	Quantisation of observables	28
1.4.2	Quantum ergodicity	31
1.4.3	Integrability and microlocalised WKB quasimodes	32
1.5	Addition of a Delta Scatterer	33
1.5.1	Localisation	34
1.5.2	Equidistribution	35
1.6	Overview of the Work in this Thesis	35
2	Specification of the Quantum and Classical Systems	38
2.1	The Unperturbed Quantum System	38
2.1.1	The Hilbert Space and the Self-Adjoint minus-Laplacian Operator	38
2.1.2	Eigenvalues and Eigenfunctions of the Self-Adjoint minus-Laplacian Operator	42
2.1.3	Resolvents of the Self-Adjoint minus-Laplacian Operator	44
2.1.4	Further Mathematical Tools	45
2.2	The Delta-Perturbed Quantum System	49

2.2.1	Introduction of the Delta Perturbation	49
2.2.2	Green's Functions	53
2.2.3	Action of the Delta-Perturbed Operators	56
2.2.4	Observations on the Strength of the Delta Potential	58
2.2.5	Eigenvalues and Eigenfunctions of the Delta-Perturbed Operators	61
2.3	The Classical System	62
2.3.1	The Unperturbed Classical System	62
2.3.2	The Perturbed Classical System	63
3	Approximation of Some Perturbed Eigenfunctions by a Combination of the Two Surrounding Unperturbed Eigenfunctions	64
3.1	Overview	64
3.2	Review of Work by Keating, Marklof and Winn	66
3.2.1	Quasimodes	66
3.2.2	Approximation of Perturbed Eigenfunctions by Two-Component Quasimodes	67
3.3	Further Work: Initial Observations on Conditions for Approximation . .	70
3.4	Derived Results	74
3.5	Analysis of Results: Comparison with Result by Keating, Marklof and Winn	79
4	Approximation of the Delta Potential by Non-Singular Rank-One Perturbations	83
4.1	Overview	83
4.2	Introducing Rank-One Perturbations and their Use as Approximations .	85
4.2.1	Review of Work by Zorbas on Whole Euclidean Space	85
4.2.2	Further Analysis of Result by Zorbas	88
4.2.3	Overview of Other Work on Operators Approaching the Delta Potential in Whole Euclidean Space	93
4.2.4	Rank-One Perturbations on the Compact Manifold	96
4.2.5	Consideration of Eigenvalues and Eigenfunctions	98
4.3	Eigenvalues and Eigenfunctions of the Rank-One Perturbed Operators . .	101
4.3.1	Construction of Eigenvalues and Eigenfunctions	101
4.3.2	Comparison with Eigenvalues and Eigenfunctions of the Delta Potential	106
4.4	Approximation of Eigenvalues and Eigenfunctions to those of the Delta Potential	108

4.4.1	Approximation of Eigenfunctions in common with the Unperturbed Operator	109
4.4.2	Approximation of New Eigenvalues	116
4.4.3	Approximation of New Eigenfunctions	128
4.4.4	Convergence of All Eigenvalues within an Interval and Corresponding Eigenfunctions	133
5	Equidistribution in Position Space	138
5.1	Systems where Work has Already Been Done	138
5.1.1	Classical Behaviour Leading to Position Space Equidistribution in the Unperturbed System	138
5.1.2	The Unperturbed and Delta-Perturbed Flat Torus	140
5.1.3	Methods of Arriving at Position Space Equidistribution	142
5.2	Pseudodifferential Operators on \mathbb{R}^n	143
5.2.1	Associating Ψ DOs with Symbols	143
5.2.2	Differential Operators and Polyhomogeneous Ψ DOs	144
5.3	Weyl's Law, Egorov's Theorem, Quantum Variance and Position Space Equidistribution	144
5.4	Potential Methods of Approach for the Delta-Perturbed System	150
5.4.1	Method 1: Computations using Formulae for Perturbed Eigenfunctions	150
5.4.2	Method 2: Approximation by Non-Singular Perturbations	152
5.4.3	Method 3: Theory Permitting Singular Behaviour	155
A	Further Material on Rank-One Perturbations	156
A.1	Construction of Resolvents	156
A.2	Further Observation of the Analogy between the Delta Potential and Rank-One Perturbations	160

Chapter 1

Introduction

1.1 Introduction to semiclassical analysis and quantum chaos

1.1.1 Classical mechanics

A physical particle, under classical mechanics, has a well-defined position at each moment in time. Thus under classical mechanics, the laws of physics can be expressed through equations governing the behaviour of the particle's position as a function of time. One such set of equations is **Hamilton's equations**:

$$\frac{dx_P}{dt} = \nabla_p H, \quad \frac{dp_P}{dt} = -\nabla_x H. \quad (1.1)$$

Here x_P is the (possibly generalised) position of the particle P , p_P is its (possibly generalised) momentum, t is time, and H is the *Hamiltonian*, which is the energy of the particle as a real-valued function of position and momentum. Assume position here to be defined on n -dimensional Euclidean space. The Hamiltonian H is then a function on $2n$ -dimensional position-momentum *phase space*, with position coordinates $x = (x_1, \dots, x_n)$ and momentum coordinates $p = (p_1, \dots, p_n)$, and $\nabla_x H := \left(\frac{\partial H}{\partial x_1}, \dots, \frac{\partial H}{\partial x_n} \right)$, $\nabla_p H := \left(\frac{\partial H}{\partial p_1}, \dots, \frac{\partial H}{\partial p_n} \right)$.

Assume this system to be autonomous, meaning that the function $(x, p) \mapsto H(x, p)$ does not vary with time. Given any (smooth enough) real function f on the phase space (such is referred to as an *observable*), let f_P be the value of f at the position and momentum of P . It then follows that

$$\frac{df_P}{dt} = \nabla_x f \cdot \frac{dx_P}{dt} + \nabla_p f \cdot \frac{dp_P}{dt} = \nabla_x f \cdot \nabla_p H - \nabla_p f \cdot \nabla_x H =: \{f, H\}. \quad (1.2)$$

It then follows in particular that the energy H_P of the particle does not vary with time. The binary operation $\{\cdot, \cdot\}$ here is referred to as the *Poisson bracket*, and is defined more generally (assuming Euclidean space) as follows:

$$\{f, g\} := \nabla_x f \cdot \nabla_p g - \nabla_p f \cdot \nabla_x g = \sum_{j=1}^n \left(\frac{\partial f}{\partial x_j} \frac{\partial g}{\partial p_j} - \frac{\partial f}{\partial p_j} \frac{\partial g}{\partial x_j} \right). \quad (1.3)$$

As a basic example of a Hamiltonian system, consider the simple case of a non-relativistic system involving a single particle P of mass m within a scalar potential $V(x)$. Here

$$p_P = m \frac{dx_P}{dt}, \quad \frac{dp_P}{dt} = -\nabla V(x), \quad H = \frac{\|p\|^2}{2m} + V(x). \quad (1.4)$$

It is easy to check that (1.4) is consistent with (1.1).

One can also study Hamiltonian systems in which the position of the particle is confined to some subset of the Euclidean space. There would then be some rule as to what happens when the particle hits a wall of this region that it is confined to (unless $H(x, p)$ is chosen in such a way that the particle cannot reach the boundary).

One may consider, for example, a system given by (1.4), with position confined to some compact region, together with the additional rule that when the particle hits the boundary, it reflects with specular reflection (like light off a mirror), with no discontinuous change in the particle's *speed* (magnitude of the velocity vector). In other words, all components of the velocity vector tangential to the wall at that point do not change discontinuously upon reflection, but the normal component switches sign, without a discontinuous change in its magnitude. In this instance, when the particle hits the boundary, the particle's position as a function of time remains continuous, but there is a discontinuity in the particle's momentum. Such systems are commonly studied with $V(x)$ simply set to zero, so between bounces the particle simply moves in constant velocity motion. The *shape* of the confining region is sufficient to provide interesting dynamics to the system.

Systems like this, involving a confined particle bouncing between walls, are commonly referred to as *billiards*.

For a Hamiltonian system involving such discontinuities in the particle's trajectory in phase space, such a discontinuity can in general result in a discontinuous change in the value of an observable f along the particle's trajectory, even if $\{f, H\} = 0$. However, the value of the Hamiltonian along the particle's trajectory must remain constant over time, even when such a discontinuity in the trajectory occurs. Indeed, for a system satisfying (1.4), together with specular reflection and no discontinuous change in speed when the

particle hits a wall, it is easy to see that there is no discontinuous change in the value of the Hamiltonian when the particle reflects.

In a well-defined Hamiltonian system, for “almost every” possible *initial state* (that is, the position and momentum of the particle at time $t = 0$), the resulting trajectory of the particle is then fully determined, both forwards and backwards in time. Some trajectories may “go wrong”, typically if

- (i) the particle hits the wall at a corner point, i.e. point on the wall where there is no well-defined tangent line/plane,
- (ii) the particle hits the wall tangentially – especially an issue if the particle hits the wall at e.g. an *inflection point* tangentially, unless one allows for the particle to glide along the wall,
- (iii) the particle ends up hitting the wall infinitely many times within a finite time period.

However, in a well-defined Hamiltonian system, only a “negligible” set of points in the phase space would result in such “bad trajectories”.

The collection of all possible well-defined trajectories is then referred to as the *flow* or *dynamical system*. More precisely, one can define the flow Φ^t as follows: $\Phi^t(x_0, p_0) = (x_P(t), p_P(t))$ if the initial state $(x_P(0), p_P(0)) = (x_0, p_0)$.

Since the Hamiltonian is conserved under the flow (meaning that H is constant along all trajectories), one can also study the flow on individual energy shells - an “energy shell” meaning a (generically $(2n - 1)$ -dimensional) surface in phase space consisting of all points at which the Hamiltonian takes a particular specified value. In the simple case of a Euclidean billiard (position confined to $\Omega \subset \mathbb{R}^n$) following (1.4) with $V(x) = 0$ and specular reflection at the boundary, the energy shell \mathcal{E}_E with energy $H = E > 0$ is simply given by:

$$\mathcal{E}_E = \Omega \times \sqrt{2mE} \mathcal{S}_p^{n-1}, \quad (1.5)$$

where $\sqrt{2mE} \mathcal{S}_p^{n-1}$ is the sphere of radius $\sqrt{2mE}$ in momentum space. For such a system, the dynamics on one energy shell is identical to that on any other energy shell, except for some trivial linear rescalings.

The concepts of Hamiltonian mechanics, which have been described above for Euclidean space, can then be generalised to Riemannian manifolds. In this case, with the position space being a Riemannian manifold (with or without boundary), the phase space is the corresponding cotangent bundle. In the generalisation of (1.4) to a Riemannian manifold \mathcal{M} , setting $V(x) = 0$, the motion of the particle is constant speed geodesic

motion, and the equations

$$p_P = m \frac{dx_P}{dt}, \quad H = \frac{||p||^2}{2m} \quad (1.6)$$

still hold, with $p_P \in T_{x_P}^* \mathcal{M}$, *except* replacing $\frac{dx_P}{dt}$ with the covector that is matched onto the particle's velocity vector by the Riemannian metric.

1.1.2 Quantum mechanics

In quantum mechanics, the physical state of a particle at a given moment in time is typically specified by the particle's *wavefunction* ψ , which is a normalised member of some Hilbert space (assuming a single-particle system). Typically this Hilbert space would be $L^2(\mathbb{R}^n)$, or the L^2 space of whatever region the particle is confined to, and the wavefunction in general can be complex-valued. There would then be a probability distribution for the particle's position, given by $|\psi(x)|^2$. If the position space is Euclidean, there is also a probability distribution for the particle's momentum, obtained via the Fourier transform of the wavefunction.

In some cases, the wavefunction is not scalar-valued, but is given by a multi-entry column vector referred to as a *spinor*. This would be used when accounting for a property of quantum particles known as *spin*.

Whereas in classical mechanics, observables are given by scalar functions on position-momentum phase space, in quantum mechanics, observables are specified by linear operators acting within the quantum Hilbert space. For a given observable, there would typically be a probability distribution for the value of the quantity represented by this observable. Letting A be the linear operator representing an observable, the expectation value of this observable is given by:

$$\langle A \rangle = \langle A\psi, \psi \rangle, \quad (1.7)$$

where $\langle \cdot, \cdot \rangle$ is the inner product, linear in the left entry and conjugate-linear in the right entry, and ψ again is the wavefunction.

There is also a correspondence between classical observables and quantum observables. Very loosely speaking, assuming for the moment Euclidean space, and selecting an origin about which to define position vectors, one would define the *position operator* \hat{x} and *momentum operator* \hat{p} as follows:

$$(\hat{x}\psi)(x) = x\psi(x), \quad \hat{p}\psi = -i\hbar\nabla\psi. \quad (1.8)$$

Then for a classical observable $f(x, p)$, the corresponding quantum observable would be an operator formally expressible as $f(\hat{x}, \hat{p})$. Here \hbar is the *reduced Planck constant*,

a constant of nature with value $\approx 1.055 \times 10^{-34} \text{ kg m}^2 \text{ s}^{-1}$. This concept, namely the quantisation of an observable, can be formulated rigorously, and it can also be extended to quantum systems on Riemannian manifolds.

Note that although *individual scalar quantities* would have probability distributions determined by the corresponding quantum operators and by the system's wavefunction, in general there would not necessarily exist a well-defined probability distribution for the simultaneous values of several scalar quantities together. However, one can still consider for example, a probability distribution for the particle's position (despite being given by the simultaneous values of the particle's n coordinates), and in the case of Euclidean space, one can likewise consider a probability distribution for the particle's momentum (despite again being a vector specified by n scalar values).

A vital operator in a quantum system is the *Hamiltonian operator*. This is a self-adjoint operator acting within the quantum Hilbert space, representing the energy of the system. In general there would be a probability distribution for the energy of the system, but the energy takes value E with full probability if and only if the wavefunction ψ is an eigenfunction of the Hamiltonian operator H and the corresponding eigenvalue is E , i.e. $H\psi = E\psi$.

In the quantum analogue of a classical system satisfying (1.4), the Hamiltonian operator is given by:

$$H\psi = -\frac{\hbar^2}{2m}\Delta\psi + V\psi, \quad (1.9)$$

where Δ is the Laplacian derivative:

$$\Delta\psi := \frac{\partial^2\psi}{\partial x_1^2} + \dots + \frac{\partial^2\psi}{\partial x_n^2}. \quad (1.10)$$

In the case where the particle is confined to a region with walls, there would then be *boundary conditions* imposed - that is, a restriction on the domain of the Hamiltonian operator to functions satisfying certain specified rules at the boundary (on top of the general "well-behavedness" of the function required for an operator of the form (1.9) to be able to act upon that function). The most commonly studied boundary conditions are *Dirichlet* (loosely speaking, functions are zero at the boundary), and *Neumann* (loosely speaking, the normal directional derivative at the boundary is zero).

The Laplacian derivative also has a generalisation to Riemannian manifolds, known as the *Laplace-Beltrami* operator. Thus (1.9) can be extended to Riemannian manifolds.

The time-evolution of the wavefunction in a quantum system is given by the **Schrödinger equation**:

$$H\psi = i\hbar\frac{\partial\psi}{\partial t}. \quad (1.11)$$

As a result, there is also an equation for the time-derivative of the expectation of an observable (analogous to (1.2)), given by *Ehrenfest's theorem*. Letting A be the quantum operator for some observable, assuming A is defined independently of time, the time-derivative of its expectation is:

$$\frac{d}{dt} \langle A \rangle = \frac{1}{i\hbar} \langle [A, H] \rangle := \frac{1}{i\hbar} \langle AH\psi - HA\psi, \psi \rangle. \quad (1.12)$$

Note that if the wavefunction at time $t = 0$ is an eigenfunction of the Hamiltonian with eigenvalue E , then assuming the system is autonomous, the time-evolution of the wavefunction is simply:

$$\psi(t) = e^{-\frac{iEt}{\hbar}} \psi(0). \quad (1.13)$$

Multiplication of the wavefunction by a spatially constant phase factor makes no physical difference to the system, and so eigenstates of the Hamiltonian operator are *stationary*. In a Hamiltonian eigenstate there is no time-variation in any physical properties of the system.

1.1.3 Interface between quantum and classical mechanics

Physical objects in the macroscopic world essentially follow classical mechanics, while the behaviour of particles on subatomic scale has been found to be accurately described by quantum mechanics. It is thus understood that the laws of physics are more fundamentally described by quantum mechanics, but that in the macroscopic world, these laws of physics amount to something extremely approximate to classical mechanics. It is thus of significant interest to physicists to try and understand the interface between quantum and classical mechanics. Unlike the interface between non-relativistic classical mechanics and special relativity, which is very well understood, the interface between classical and quantum mechanics is still an active area of research.

One particular “puzzle” is this: a well-established phenomenon occurring in many dynamical systems governed by classical mechanics is **chaos**. Loosely speaking, this is an effective long-term unpredictability of trajectories in deterministic systems due to extreme sensitivity to initial conditions. However, time-evolution in quantum mechanics is governed entirely by *linear* equations, which cannot produce chaotic dynamics. How then can these chaotic systems arise in a universe governed by quantum mechanics?

There is also however, a strong interest in correlations between dynamical properties of classical systems, and properties of *stationary states* in the corresponding quantum systems. This thesis shall mainly be concerned with this area of study.

One major technique in studying the interface between quantum and classical mechanics is to take the **semiclassical limit**. Although in reality, \hbar is a constant of nature, the fact that we don't observe quantum behaviour on the macroscopic scale can be related to the fact that \hbar is so small. Thus it is expected that if we take a quantum system, and then theoretically send \hbar to zero while keeping all other relevant quantities fixed, this quantum system should then bear resemblance to the corresponding classical system as \hbar tends to zero. This limit as $\hbar \rightarrow 0$ is commonly referred to as the semiclassical limit.

When for example, studying the behaviour of the spectrum of the quantum Hamiltonian operator and corresponding eigenstates in the semiclassical limit, one could while sending $\hbar \rightarrow 0$, fix a particular energy value E , and then study the behaviour of the Hamiltonian spectrum in the “immediate vicinity” of this value E . One could likewise study the corresponding eigenfunctions thereof. Alternatively, as \hbar is varied, one could consider each value of \hbar for which there is a Hamiltonian eigenvalue precisely coinciding with E , and consider the corresponding eigenfunction. One could then study the sequence of eigenstates formed by doing this as \hbar is decreased down to zero (see e.g. [Ber85, Ber87, Non13]).

Quantum chaos, broadly speaking, is the study of how properties of a quantum system, particularly in the high-energy or $\hbar \rightarrow 0$ semiclassical limit, relate to dynamical properties of the corresponding classical system, particularly dynamics that relate in some way to chaos or a lack of chaos. If for example, the quantum system is described by (1.9) with Dirichlet conditions wherever there is a boundary, then the corresponding classical system is described by (1.4), with the same region on which the particle is confined, the same potential $V(x)$, and specular reflection whenever the particle hits the boundary. The study of quantum chaos has involved a mix of numerical findings, heuristic arguments, rigorous proofs and also physical experiments.

Many studies in the area of quantum chaos have involved, rather than sending $\hbar \rightarrow 0$, instead treating \hbar as a constant and exploring behaviour of eigenstates and spectrum as one goes further up the spectrum. This high-energy limit is another form of semiclassical limit, alongside $\hbar \rightarrow 0$. It is this latter approach that shall be used in the main part of the thesis. In this Introduction chapter though, both approaches shall be discussed.

Consider for example, a quantum system confined to a compact region with connected interior, following (1.9) with $V = 0$ and Dirichlet or Neumann boundary conditions if the region has a boundary (compact manifolds do not necessarily have a boundary, e.g. a sphere or flat torus). In this case the Hamiltonian operator has a countable orthonormal

eigenbasis $(\phi_n)_{n \in \mathbb{N}}$ with corresponding eigenvalues $E_1 < E_2 \leq E_3 \leq E_4 \leq E_5 \leq \dots \rightarrow \infty$ (all eigenvalues are real and non-negative). Now considering the plain $-\Delta$ operator, keeping the same boundary conditions as the Hamiltonian if there is a boundary, and considering its eigenvalue-eigenfunction equation:

$$-\Delta \phi_j = \lambda_j \phi_j, \quad (1.14)$$

the j^{th} eigenfunction of the Hamiltonian is then simply the same ϕ_j as in (1.14), and the corresponding Hamiltonian eigenvalue is simply:

$$E_j = \frac{\hbar^2}{2m} \lambda_j. \quad (1.15)$$

Hence in this case, taking a fixed energy value E' and examining the Hamiltonian eigenstates in the vicinity $E \approx E'$, while sending \hbar to zero, is equivalent to keeping \hbar fixed and examining the Hamiltonian eigenstates in a corresponding vicinity of E' while sending E' to infinity.

If however, a potential $V(x)$ is then added, the eigenvalue-eigenfunction equation $H\psi = E\psi$ can then be written in the form:

$$-\Delta \psi + \frac{2m}{\hbar^2} V \psi = \lambda \psi, \quad E = \frac{\hbar^2}{2m} \lambda. \quad (1.16)$$

Thus varying \hbar here would have the effect of varying the strength of the perturbation being added to the $-\Delta$ operator, as well as rescaling the Hamiltonian eigenvalues. Note though that if V is a constant potential of value V_0 then the effect of varying \hbar is just a linear rescaling of the Hamiltonian eigenvalues, like (1.15), *except* this rescaling is centred about V_0 rather than 0.

Beside from Hamiltonian systems where the position space is some Euclidean domain or Riemannian manifold and the classical phase space is the cotangent bundle, other systems on which quantum chaos has been studied include *quantum graphs* (e.g. [Win03, BKW04, BKS07]), and systems for which the ‘‘classical dynamical system’’ constitutes a map on the flat torus (e.g. [HB80, BB96, ENW06]).

1.2 Preliminary facts and assumptions

Given a Hamiltonian system on an n -dimensional position space \mathcal{M} (assume $n \geq 2$), and thus $2n$ -dimensional phase space $T^*\mathcal{M}$, the standard $2n$ -dimensional volume measure $\mu_{T^*\mathcal{M}}$ is preserved under the flow Φ^t , i.e. for every measurable $V \subset T^*\mathcal{M}$ (for which

all points in V give rise to fully determined trajectories both forwards and backwards in time):

$$\mu_{T^*\mathcal{M}}(\Phi^t(V)) = \mu_{T^*\mathcal{M}}(V) \quad \forall t \in \mathbb{R}. \quad (1.17)$$

With the phase space being $2n$ -dimensional, each generic energy shell is $(2n-1)$ -dimensional (an example of an exception being the zero-energy shell in a system satisfying (1.4) with $V = 0$, which is only n -dimensional). Letting σ_E be the standard $(2n-1)$ -dimensional volume measure on a generic energy shell \mathcal{E}_E , it can be derived from the invariance of the standard measure on the phase space under the flow, combined with the invariance of the Hamiltonian under the flow, that the following measure $\tilde{\mu}_E$ on \mathcal{E}_E is invariant under the flow:

$$d\tilde{\mu}_E = \frac{d\sigma_E}{\|\nabla H\|}. \quad (1.18)$$

Here $d\tilde{\mu}_E$ and $d\sigma_E$ are the respective measures of an infinitesimal element at a point on the energy shell, ∇H is the (phase space) gradient covector of H at this point (in Euclidean space, $\nabla H := \left(\frac{\partial H}{\partial x_1}, \dots, \frac{\partial H}{\partial x_n}, \frac{\partial H}{\partial p_1}, \dots, \frac{\partial H}{\partial p_n}\right)$), and $\|\nabla H\|$ is the norm of ∇H under the standard metric on $T^*\mathcal{M}$. See e.g. §4.1.3 of [DT09] for justification of (1.18).

For the following two sections of this Introduction chapter, assume that for the classical system, we are interested in the dynamics on some open set $\Omega := \{(x, p) \in T^*\mathcal{M} : H(x, p) \in I_\Omega\}$, where I_Ω is some open interval, which could be bounded or unbounded. (If $T^*\mathcal{M}$ has a boundary then an “open” subset of $T^*\mathcal{M}$ may in this context include boundary points). Assume H to be C^∞ -smooth on Ω , possibly except at some “singular points” (but this singular set shouldn’t be “too bad”), and assume each energy shell \mathcal{E}_E in Ω ($E \in I_\Omega$) satisfies some basic requirements, in particular:

- (i) $\mu_{T^*\mathcal{M}}(\Omega_E)$ is strictly positive and finite, where $\Omega_E := \{(x, p) \in T^*\mathcal{M} : H(x, p) \leq E\}$,
- (ii) \mathcal{E}_E is a $(2n-1)$ -dimensional surface on which both σ and $\tilde{\mu}$ are well-defined (completed) Borel measures that are absolutely continuous with respect to each other (meaning that they agree on which Borel sets have zero measure and which have strictly positive measure),
- (iii) $\tilde{\mu}_E(\mathcal{E}_E)$ is strictly positive and finite,
- (iv) the set of points on \mathcal{E}_E that fail to give rise to fully determined trajectories, if there are any such points, has zero (complete) $\tilde{\mu}_E$ -measure.

In this case, one can define on each energy shell, the *normalised Liouville measure* $\mu_E := \frac{\tilde{\mu}_E}{\tilde{\mu}_E(\mathcal{E}_E)}$, so $\mu_E(\mathcal{E}_E) = 1$. In the particular case of a system satisfying (1.4) with $V = 0$ on

a compact Euclidean position space $\mathcal{M} \subset \mathbb{R}^n$, the normalised Liouville measure on an energy shell $\mathcal{E}_E = \mathcal{M} \times \sqrt{2mE} \mathcal{S}_p^{n-1}$ is simply the standard $(2n - 1)$ -dimensional volume measure normalised.

1.3 Achievements in quantum chaos: eigenvalue statistics

As a general reference for this section, see e.g. [Ber87].

1.3.1 Basic theory of eigenvalue statistics

Taking some $E \in I_\Omega$, assuming \hbar to be small, the quantum Hamiltonian eigenvalues in close proximity to the value E form a discrete set of energy levels, with mean density:

$$\langle \rho(E) \rangle \rightarrow \frac{1}{(2\pi\hbar)^n} \frac{d}{dE} \mu_{T^*\mathcal{M}}(\Omega_E) \quad (1.19)$$

as $\hbar \rightarrow 0$. This result is an example of a so-called *Weyl law*.

One can then study statistical properties of the energy level spacings, in the immediate vicinity of the value E , or perhaps over the whole range I_Ω , as $\hbar \rightarrow 0$. In some cases, one would instead work with a fixed \hbar , and study statistical properties of the discrete energy levels of the Hamiltonian spectrum, where the role of decreasing \hbar is replaced with increasing energy.

For a system satisfying (1.9) with $V = 0$ on a compact position space with connected interior (and appropriate boundary conditions if there is a boundary), again there is a discrete set of eigenvalues $E_1 < E_2 \leq E_3 \leq E_4 \leq E_5 \leq \dots \rightarrow \infty$, and defining the *spectral counting function* $\mathcal{N}(E) := \#\{j : E_j \leq E\}$, there is then a Weyl law stating:

$$\mathcal{N}(E) \sim \frac{\text{vol}(\mathcal{M}) \text{vol}(B_1^n) m^{\frac{n}{2}}}{2^{\frac{n}{2}} (\pi\hbar)^n} E^{\frac{n}{2}} \quad (1.20)$$

as $E \rightarrow \infty$, where vol is volume (i.e. standard measure), B_1^n is the unit ball in \mathbb{R}^n (so for example, $\text{vol}(B_1^2) = \pi$, $\text{vol}(B_1^3) = \frac{4\pi}{3}$), and ‘‘LHS \sim RHS’’ in some limit means $\frac{\text{LHS}}{\text{RHS}} \rightarrow 1$ in that limit (assuming RHS is nonzero everywhere sufficiently close to the limit).

When analysing spectral statistics (either with or without an interest in sending $\hbar \rightarrow 0$), typically one would first rescale the energy levels so as to make the mean spacing = 1 (sometimes this would involve a nonlinear rescaling). When defining the energy level sequence on which to analyse the spacing statistics, in some cases one would simply take this sequence to be the non-decreasing sequence of all (rescaled) energy levels (within the

range of interest), with degenerate eigenvalues of multiplicity k appearing k consecutive times in the sequence.

In some cases though, it would be appropriate to make further adjustments when defining this sequence. For example, if there is a basic feature of the system that would involve the eigenvalues having a certain degeneracy (e.g. the $-\frac{\hbar^2}{2m}\Delta$ operator on a flat torus), then it may be appropriate to have distinct eigenvalues appearing only once in the sequence, or if an eigenvalue has further degeneracy beyond this “basic degeneracy”, then the eigenvalue would be repeated only a number of times in accordance with this “further degeneracy”.

As another example, symmetries in the system could cause each eigenfunction (or each member of the eigenbasis if the eigenbasis is so chosen) to belong to one out of a finite number of symmetry classes (e.g. even and odd, about a line of symmetry). In this case it could be appropriate to split the spectrum into subspectra corresponding to each of these symmetry classes, and then consider statistical properties of each of these subspectra.

Once one has a sequence of levels (rescaled appropriately) with which to study spacing statistics, one common statistic to consider is the *level spacings probability distribution* $P(s)$. Loosely speaking, $P(s) : [0, \infty) \rightarrow [0, \infty)$, (if it exists) is a function (or distribution) whereby the proportion of nearest neighbour spacings whose value belongs to some interval I is given by $\int_I P(s) ds$. In the case where this sequence $(x_j)_{j \in \mathbb{N}}$ is infinite, $P(s)$ can be defined as follows [Mar01]:

$$\begin{aligned} \int_0^\infty P(s)\phi(s) ds &= \lim_{N \rightarrow \infty} \int_0^\infty \left(\frac{1}{N} \sum_{j=1}^N \delta(s - x_{j+1} + x_j) \right) \phi(s) ds \\ &= \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{j=1}^N \phi(x_{j+1} - x_j) \end{aligned} \quad (1.21)$$

for all “sufficiently nice” test functions ϕ . Here δ is the Dirac delta function.

Notice that if $P \in L^1[0, \infty)$, and if in place of ϕ , the characteristic function of some interval I is inserted, i.e. $\chi_I(x) = \{1 \text{ if } x \in I; 0 \text{ if } x \notin I\}$, then (1.21) gives $\int_I P(s) ds$ being the density of the subsequence of the level spacings sequence $(x_{j+1} - x_j)_{j \in \mathbb{N}}$ consisting of all terms with value belonging to I . Given a sequence $(a_j)_{j \in \mathbb{N}}$ and subsequence $(a_{j_k})_{k \in \mathbb{N}}$ ((k_j) being a strictly increasing sequence of positive integers), the density of this subsequence is defined to be $\lim_{N \rightarrow \infty} \#\{k : j_k \leq N\}/N$ ($\#$ here denoting number of elements in a set).

In the case where the limit $\hbar \rightarrow 0$ is considered, one can consider the corresponding limiting $P(s)$ distribution. $P(s)$ can be understood to be a short-range statistic. An

example of a long-range statistic is the *spectral rigidity*. See for example, [Ber85] for a definition of spectral rigidity. A fundamental set of statistics by which the statistical behaviour of these energy levels (rescaled to have mean spacing =1) may be defined is the collection of *N-point correlation functions*, $N \in \mathbb{N} \setminus \{1\}$ (the 1-point correlation function is just the mean spacing).

For an infinite sequence of levels $(x_j)_{j \in \mathbb{N}}$, the pair (2-point) correlation function $R_2(s)$ is a distribution on \mathbb{R} defined as follows [Mar01]:

$$\begin{aligned} \int_{-\infty}^{\infty} R_2(s) \phi(s) \, ds &= \lim_{N \rightarrow \infty} \int_{-\infty}^{\infty} \left(\frac{1}{N} \sum_{j=1}^N \sum_{k=1}^N \delta(s - x_j + x_k) \right) \phi(s) \, ds \\ &= \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{j=1}^N \sum_{k=1}^N \phi(x_j - x_k) \end{aligned} \quad (1.22)$$

for all “sufficiently nice” test functions ϕ . Notice that in this equation, the $j = k$ terms add up to $\phi(0)$ (for every N , and hence also in the limit $N \rightarrow \infty$), thus corresponding to a $\delta(s)$ part in the $R_2(s)$ distribution. Sometimes $R_2(s)$ is defined so as to exclude the $j = k$ terms.

The $P(s)$ distribution is fully determined by the full collection of correlation functions (provided all of these are indeed well-defined). Spectral rigidity can also be determined from just the pair correlation function.

It has been found that the spectral statistics of many quantum systems display universal features, which largely depend on some characteristic features of the corresponding classical systems.

1.3.2 Integrable dynamics, WKB quantisation and Poissonian statistics

One feature that the classical dynamical system may or may not possess is *integrability* (more precisely, *Liouville integrability*). In this case, a mathematical technique known as the *WKB method* (Wentzel-Kramers-Brillouin) yields an approximate determination of the positioning (on the real line) of the corresponding quantum Hamiltonian eigenvalues in the semiclassical limit [Per77, BT77]. The *Berry-Tabor conjecture* then asserts that *generically*, if the classical system is integrable then the quantum eigenvalues behave statistically like the output of a Poisson process [BT77].

The classical dynamics on the phase space region Ω (as defined in §1.2) is said to be *integrable* (in the Liouville sense) if there exists a set of n real scalar functions f_1, \dots, f_n on Ω (n being the dimension of the position space), which are C^∞ -smooth except possibly

at some “singular points” (but this singular set shouldn’t be “too bad”), and satisfy the following conditions:

- (i) f_1, \dots, f_n are *functionally independent* - meaning that at each generic point on Ω (i.e. every point except for those on some “singular set”), the gradients $\nabla f_1, \dots, \nabla f_n$ are linearly independent covectors in the $2n$ -dimensional cotangent space at that point (one may perhaps be more generous here as to what kinds of singular set are permissible with regards to independent gradients, compared to say, what kinds of singular set are permissible for there to be a discontinuity in one or more of these functions). This can equivalently be reformulated as follows (understanding the phase space to be a smooth manifold): for each generic point on Ω there is a coordinate chart on a neighbourhood of the point for which the values of f_1, \dots, f_n form n of the $2n$ coordinates.
- (ii) These functions are all *constants of motion* - meaning that the value of each of these functions is constant along each (generic) trajectory. In particular, it must hold (by equation (1.2)) that $\{f_j, H\} = 0 \ \forall j$, but this is not necessarily sufficient by itself in the case where there are discontinuous trajectories (e.g. specular reflection at a boundary).
- (iii) They are *Poisson-commuting*: $\{f_j, f_k\} = 0 \ \forall j, k$ (equivalently $\{f_j, f_k\} = \{f_k, f_j\}$).

The Poisson bracket $\{\cdot, \cdot\}$ again is given by equation (1.3) in the case where the position space is Euclidean, and has a generalisation to the case where the position space is a Riemannian manifold (in fact it can even be defined independently of metric, provided it is indeed the cotangent bundle, not the tangent bundle, being taken as the phase space).

For a general Hamiltonian system, a set of functions satisfying these above conditions can be *at most* n in number, and the system is integrable if there exists a set of *precisely* n such functions. In fact, in a general Hamiltonian system, at each generic point on the phase space there will exist a neighbourhood of the point, on which there exists a set of precisely n functions satisfying these conditions (in place of (ii), simply having $\{f_j, H\} = 0 \ \forall j$). Thus since Hamiltonian systems are always “locally integrable”, when meaningfully defining integrability of a system, it is important that these n functions are *globally* defined on the phase space, or on the invariant region of phase space that is of interest (see e.g. Lec. 1 in [Dei96]), (*invariant* meaning that all trajectories that start in the region remain in this region, both forwards and backwards in time).

Whereas in a general Hamiltonian system, each generic trajectory is confined to a $(2n - 1)$ -dimensional energy shell, in the case of an integrable Hamiltonian system, it is

furthermore the case that each generic trajectory is confined to an n -dimensional region of phase space where the values of f_1, \dots, f_n are all constant on this region. If the system is integrable, there will always exist a selection of such functions f_1, \dots, f_n for which one of these functions is the Hamiltonian itself.

Typically f_1, \dots, f_n are chosen in such a way that the Hamiltonian is at least expressible as a smooth function of the values of f_1, \dots, f_n , so the Hamiltonian is constant on every region for which the values of all these functions are constant. In particular, if the inverse image of $(f_1, \dots, f_n) : \Omega \rightarrow \mathbb{R}^n$ on some open $X \subset \mathbb{R}^n$ is open in Ω (call this inverse image Y), (again, an “open” set in Ω may contain boundary points of $T^*\mathcal{M}$), if Y contains no points at which any of the functions f_1, \dots, f_n nor H fail to be smooth (thus also f_1, \dots, f_n, H are pairwise Poisson-commuting at all points on Y), nor any points at which the gradient covectors $\nabla f_1, \dots, \nabla f_n$ fail to be linearly independent, and if the inverse image of $(f_1, \dots, f_n) : \Omega \rightarrow \mathbb{R}^n$ on each singleton $\{x\} \subset X$ is non-empty and connected, then the Hamiltonian on Y can also be expressed as a smooth function on X in \mathbf{f} -space (\mathbf{f} -space being \mathbb{R}^n used as a grid on which to represent the values of f_1, \dots, f_n).

Example (i). *The rectangular billiard* - Consider a system satisfying (1.4) with $V = 0$ on a 2D rectangular box (that is, the *position space* is this 2D rectangular box), and with specular reflection at the boundary, so the particle moves in constant velocity straight line motion between reflections, and maintains the same speed of motion when it reflects. Assume the sides of the rectangle to be parallel to the coordinate axes. It is easy to see then that p_1^2 and p_2^2 (p_1, p_2 being momentum coordinates) are both preserved along every well-defined trajectory (an ill-defined trajectory would occur if the particle hits directly at a corner point). Defining $\nabla := \left(\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \frac{\partial}{\partial p_1}, \frac{\partial}{\partial p_2} \right)$, we have

$$\nabla H = \left(0, 0, \frac{p_1}{m}, \frac{p_2}{m} \right), \quad \nabla(p_1^2) = (0, 0, 2p_1, 0), \quad \nabla(p_2^2) = (0, 0, 0, 2p_2). \quad (1.23)$$

It then follows that $\{p_1^2, p_2^2\} = \{H, p_1^2\} = \{H, p_2^2\} = 0$, and that ∇H , $\nabla(p_1^2)$ and $\nabla(p_2^2)$ are *pairwise* linearly dependent at each point where either $p_1 = 0$ or $p_2 = 0$, and pairwise linearly independent at all other points (but the three gradients together are linearly dependent everywhere).

The set of points where either $p_1 = 0$ or $p_2 = 0$ should not be deemed to be “too bad” a singular set where linear independence of gradients fails, and on each positive energy shell only a measure zero set of points would yield ill-defined trajectories. Hence this system is an integrable system, where examples of a pair of functionally independent, Poisson-commuting constants of motion include: (p_1^2, p_2^2) , (H, p_1^2) and (H, p_2^2) . Notice that since p_1^2 and p_2^2 are both conserved, each trajectory is therefore confined to a phase space

region given by the Cartesian product of this 2D rectangular box with a set of at most four individual points in momentum space.

Example (ii). *The circle billiard* - Consider now a system like the previous one except this time the position space being a 2D disc. Assume the origin of the position coordinate system to coincide with the centre of the disc. Define *angular momentum* L as follows:

$$L := x \cdot R_{\perp} p = x_1 p_2 - x_2 p_1, \quad (1.24)$$

where R_{\perp} is the $\frac{\pi}{2}$ rotation given by the matrix $\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$. In straight line constant velocity motion, $R_{\perp} p$ is perpendicular to the line along which the particle moves, and so $x \cdot R_{\perp} p$ is constant over all x on this line. Thus angular momentum is conserved in constant velocity motion (constant speed and direction of motion).

Then at a point of reflection, using subscripts $-$ and $+$ to represent states before and after reflection respectively, and letting \mathbf{n} be the unit outward normal vector to the wall at the point of reflection, we have

$$p_+ - p_- = -2(p_- \cdot \mathbf{n})\mathbf{n}, \quad (1.25)$$

and so

$$L_+ - L_- = x \cdot R_{\perp}(p_+ - p_-) = -2(p_- \cdot \mathbf{n})(x \cdot R_{\perp} \mathbf{n}), \quad (1.26)$$

but since the boundary is a circle centred at the origin, it follows that x and \mathbf{n} are parallel at all points of the boundary, so $x \cdot R_{\perp} \mathbf{n} = 0$. Hence angular momentum is a constant of motion for this circle billiard.

$$\nabla H = \left(0, 0, \frac{p_1}{m}, \frac{p_2}{m}\right), \quad \nabla L = (p_2, -p_1, -x_2, x_1). \quad (1.27)$$

$\{H, L\} = 0$ (consistent with the fact already stated that L is conserved in constant velocity motion), and ∇H and ∇L are linearly dependent only at points where $p_1 = p_2 = 0$. At all points in phase space where the momentum vector is nonzero, ∇H and ∇L are linearly independent. Hence this circle billiard is an integrable system.

Other examples of integrable systems include geodesic flow (generalisation of (1.4) with $V = 0$ to Riemannian manifolds) on the 2-sphere (that is, the sphere in 3D Euclidean space taken as a 2D manifold) and geodesic flow on the 2D rectangular flat torus. This flat torus can be constructed by taking a 2D rectangular lattice $\mathcal{L} = \begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix} \mathbb{Z}^2$, then taking the quotient \mathbb{R}^2/\mathcal{L} (that is, a partition on \mathbb{R}^2 where two points belong

to the same equivalence class if the difference between their position vectors is an element of \mathcal{L} , and then \mathbb{R}^2/\mathcal{L} is this set of equivalence classes), and then making \mathbb{R}^2/\mathcal{L} into a locally Euclidean, 2D compact Riemannian manifold without boundary, whereby given a sufficiently small open neighbourhood $X \subset \mathbb{R}^2$ of any point $x \in \mathbb{R}^2$, defining $[X] := \{[x] : x \in X\} \subset \mathbb{R}^2/\mathcal{L}$, the map $x \mapsto [x]$ from X to $[X]$ preserves the Riemannian manifold structure (which in this case is Euclidean). The “flat torus” is topologically equivalent to the “ring torus” (that is, the surface of a ring doughnut shape).

Note that on the sphere, the geodesics are simply the great circles, so every trajectory is periodic. Geodesic flow on the sphere is an example of a so-called *superintegrable* system.

Now in an integrable system there is a particular type of selection of n functionally independent, Poisson-commuting constants of motion, in which these n functions are referred to as *actions* (although singular sets may in some cases be worse here than permissible when *defining* integrability in terms of *existence* of n functionally independent, Poisson-commuting constants of motion). See e.g. Ch. 5 of [AKKN07] for details concerning how these “actions” are defined.

Label these actions I_1, \dots, I_n , and let \mathbf{I} denote the collection of these, so $\mathbf{I} = (I_1, \dots, I_n)$. Assuming there is no feature of the system that would cause H (on Ω) to fail to be expressible as a function of \mathbf{I} (on the region of \mathbf{I} -space relevant to Ω), one could consider a square lattice $a\mathbb{Z}^n + \mathbf{b}$ in \mathbf{I} -space, and for each lattice point in the region of \mathbf{I} -space relevant to Ω , one could take the value of H at that point, and doing this over all such lattice points, obtain a discrete set of energy values in I_Ω . The *WKB method* yields the result that in the semiclassical limit, the Hamiltonian eigenvalues approximately coincide with the energy values obtained by considering an appropriate square lattice in \mathbf{I} -space, with lattice point spacing decreasing in direct proportion to \hbar as \hbar is decreased down to zero [BT77].

Example. For the rectangle billiard, with the side parallel to the x_1 -axis having length a and the side parallel to the x_2 -axis having length b , the quantum eigenvalues for the Dirichlet Hamiltonian (1.9) with $V = 0$ are given by:

$$E_{kl} = \frac{\pi^2 \hbar^2}{2m} \left(\frac{k^2}{a^2} + \frac{l^2}{b^2} \right), \quad (1.28)$$

where $k, l \in \mathbb{N}$. For the classical flow, the actions are [LZS06]:

$$I_1 = \frac{a}{\pi} |p_1|, \quad I_2 = \frac{b}{\pi} |p_2|. \quad (1.29)$$

Thus for each $k, l \in \mathbb{N}$:

$$\begin{aligned} H(\mathbf{I} = (k\hbar, l\hbar)) &= \frac{p_1^2 + p_2^2}{2m} \Big|_{\mathbf{I}=(k\hbar, l\hbar)} = \frac{1}{2m} \left(\left(\frac{\pi}{a} k\hbar \right)^2 + \left(\frac{\pi}{b} l\hbar \right)^2 \right) \\ &= \frac{\pi^2 \hbar^2}{2m} \left(\frac{k^2}{a^2} + \frac{l^2}{b^2} \right) = E_{kl}. \end{aligned} \quad (1.30)$$

Hence the Hamiltonian eigenvalues in this case are precisely the energies at the points on the (quadrant) lattice $\hbar \mathbb{N}^2$ in \mathbf{I} -space.

Another question of interest is then the statistical behaviour of eigenvalue spacings. Even the simple formula (1.28) yields highly non-trivial statistics. Berry and Tabor [BT77] argue that for a generic classically integrable system, the quantum eigenvalues behave statistically like the output of a Poisson process (upon appropriate rescaling), at least in the semiclassical limit. A Poisson process is a process that outputs a random sequence of event times $0 < T_1 < T_2 < T_3 < \dots \rightarrow \infty$, whereby given any $T' > 0$, the probability distribution for $\{T_k - T' : k \in \mathbb{N}, T_k > T'\}$ is equal to the probability distribution for $\{T_j : j \in \mathbb{N}\}$, and the random process $\{T_k - T' : k \in \mathbb{N}, T_k > T'\}$ is independent of the random process $\{T_j : j \in \mathbb{N}, T_j \leq T'\}$. For a Poisson process with unit mean spacing:

$$P(s) = e^{-s}. \quad (1.31)$$

The work in [BT77] involves both heuristic (non-rigorous) theoretical arguments and numerical findings. Numerical support for this conjecture is also provided in [MK79], looking at eigenvalues of the circle billiard corresponding to eigenfunctions with odd-odd parity. There is furthermore heuristic discussion on spectral rigidity for classically integrable systems in [Ber85], together with numerical discussion, with numerics coming from [CCG85].

Note that this conjecture, namely the *Berry-Tabor conjecture*, applies to *generic* classically integrable systems. It certainly is not true of all classically integrable systems. Consider for example, the eigenvalues for the rectangle billiard given in (1.28). For a generic side length ratio, Poissonian eigenvalue statistics are evident. If however, the ratio b^2/a^2 is rational then it is easily shown that all eigenvalues are integer multiples of some fixed value, which is not at all resemblant of the output of a (continuous time) Poisson process. However, in [BT77] statistical behaviour analogous to Poissonian statistics is postulated for this (effectively discrete time) case.

For the rectangle billiard, an eigenvalue E has multiplicity given by $\#\{(k, l) \in \mathbb{N} \times \mathbb{N} : E_{kl} = E\}$. In particular, if b^2/a^2 is irrational then every eigenvalue is simple (multiplicity

= 1). However, for a 2D rectangular flat torus for which the “periodic rectangle” has side lengths a and b , the eigenvalues of the Hamiltonian given by (1.9) with $V = 0$ are:

$$E_{kl} = \frac{2\pi^2\hbar^2}{m} \left(\frac{k^2}{a^2} + \frac{l^2}{b^2} \right), \quad (1.32)$$

this time with $k, l \in \mathbb{Z}$, so the multiplicity of an eigenvalue E is $\#\{(k, l) \in \mathbb{Z} \times \mathbb{Z} : E_{kl} = E\}$. If b^2/a^2 is irrational then generic eigenvalues have multiplicity 4 ($k^2, l^2 > 0$), and the others have multiplicity 2 (either $k^2 > 0, l^2 = 0$ or $k^2 = 0, l^2 > 0$), except the zero eigenvalue which is simple. These multiplicities are certainly uncharacteristic of a Poisson process, but if these multiplicities are “put aside”, then the eigenvalues may yield Poissonian statistics for appropriate side length ratios.

Another counterexample to the Berry-Tabor conjecture is the harmonic oscillator - position space is the whole of \mathbb{R}^n , but there is a potential of the form $V(x) = a_1x_1^2 + \dots + a_nx_n^2$ with $a_1, \dots, a_n > 0$ (thus still confining each trajectory to a bounded region in phase space). In [BT77] is contained theoretical discussion as to why the case of the harmonic oscillator fails. Finally, a most stark counterexample to the Berry-Tabor conjecture is the sphere. The self-adjoint $-\Delta$ operator on the 2-sphere of unit radius has eigenvalues $l(l+1)$ with multiplicity $2l+1$ for $l \in \{0\} \cup \mathbb{N}$.

In the general statement of the Berry-Tabor conjecture, there is not currently a mathematically precise definition of the term “generic”. However, the notion of Poissonian statistics can be defined rigorously, by stating that the statistical behaviour of the eigenvalue spacings is Poissonian if all correlation functions match those that the event times of a Poisson process would have with full probability. The pair correlation function for a Poisson process of unit mean spacing is [Mar01]:

$$R_2(s) = \delta(s) + 1, \quad (1.33)$$

(or simply $R_2(s) = 1$ if the $j = k$ terms in (1.22) are excluded).

It has been proven *rigorously* that for various classically integrable systems, the pair correlation function matches that of a Poisson process. Work towards this has been carried out in [CLM94], [Sar97], [Mar03] and [EMM05], and also reviewed in [Mar01]. An example of such a system is the 2D rectangular flat torus whose square of side length ratio is *diophantine* (this is, loosely speaking, a particular “strong version” of irrationality; see [Mar01] for a definition).

1.3.3 Chaotic dynamics and random matrix statistics

On the opposite extreme of integrable dynamics would be *chaotic* dynamics. Again, this is loosely speaking an effective long-term unpredictability of trajectories due to

extreme sensitivity to initial conditions. It is conjectured that for generic classically chaotic systems the eigenvalue spacing statistics of the corresponding quantum system resembles eigenvalue spacings from certain ensembles in random matrix theory.

Now in general there has been more than one different way in which the term “chaos”, in the context of the theory of dynamical systems, has been defined. For the case of this conjecture, namely the *BGS* (Bohigas-Giannoni-Schmit) or *random matrix* conjecture, concerning eigenvalue spacing statistics for classically chaotic systems, it is reasonable to take “chaotic” systems more precisely to be *K-systems*, as is done in [BGS84b]. See for example §3.9.5 of [Wim14] for a definition of a K-system.

A particular feature of K-systems is that they are always *ergodic*. The classical dynamical system is ergodic on an energy shell \mathcal{E}_E if under the normalised Liouville measure, every invariant measurable set has either zero measure or full measure, where again a set is invariant if every trajectory that begins in that set remains in that set for all time (both forwards and backwards). When focussing on a particular phase space region Ω following the specifications given in §1.2, the system can be said to be ergodic if the flow on each energy shell in Ω is ergodic under the normalised Liouville measure (note though that this does *not* mean that the flow on Ω is ergodic in the sense of every invariant measurable subset of Ω having either zero or full measure with respect to the measure $\mu_{T^*\mathcal{M}}$ on Ω).

Ergodicity and integrability are mutually exclusive. To see this, suppose the system is integrable. Then one can take two disjoint open sets A and B on some energy shell \mathcal{E}_E , whose images under $\mathbf{f}_{2,n} := (f_2, \dots, f_n)$ (as defined in §1.3.2; letting $f_1 = H$) are also disjoint open sets in \mathbb{R}^{n-1} (to help see this, it could be useful to have A and B being subsets of some open $X \subset \Omega$ for which there is a coordinate chart with f_1, \dots, f_n forming n of the $2n$ coordinates). Now A and B are positive measure sets under the normalised Liouville measure, and so $\mathcal{E}_E \cap \mathbf{f}_{2,n}^{-1}\mathbf{f}_{2,n}(A) \supset A$ and $\mathcal{E}_E \cap \mathbf{f}_{2,n}^{-1}\mathbf{f}_{2,n}(B) \supset B$ are also positive measure sets. But then $\mathcal{E}_E \cap \mathbf{f}_{2,n}^{-1}\mathbf{f}_{2,n}(A)$ and $\mathcal{E}_E \cap \mathbf{f}_{2,n}^{-1}\mathbf{f}_{2,n}(B)$ (possibly wishing to exclude zero measure subsets that give rise to ill-defined trajectories) are also invariant and disjoint. Hence the flow on \mathcal{E}_E is not ergodic.

Examples of 2D Euclidean billiards (consisting of constant velocity motion between strikes upon the wall and specular reflection when striking the wall) that possess the K-property are the *Sinai billiard* (a circle within a rectangle - the particle is confined outside the circle but inside the rectangle) and the *Bunimovich stadium billiard* (shaped like a stadium, with a rectangular part in the middle and a semicircular part on either side). Another example of a K-system is geodesic flow on a negatively curved compact

Riemannian manifold (see e.g. §1 of [AKN09]). This example satisfies a particularly strong form of chaos known as the *Anosov* property (see e.g. §2.4.2 of [Non13] for a definition).

Now there are three random matrix ensembles that are relevant to the theory of quantum eigenvalue statistics for classically chaotic systems, namely the *Gaussian Orthogonal Ensemble* (GOE), *Gaussian Unitary Ensemble* (GUE) and *Gaussian Symplectic Ensemble* (GSE). However, the third of these (GSE) is only of relevance when incorporating the quantum property known as *spin*.

For each $N \in \mathbb{N}$, the $N \times N$ Gaussian Orthogonal Ensemble consists of a probability distribution on the space of $N \times N$ real symmetric matrices ($M = M^T$). This probability distribution can be constructed as follows:

- (i) The $\frac{1}{2}N(N+1)$ entries in the upper triangle are independent random variables,
- (ii) the probability distribution for each off-diagonal entry is the Gaussian normal distribution with mean 0 and variance 1,
- (iii) the probability distribution for each diagonal entry is the Gaussian normal distribution with mean 0 and variance 2.

One particular feature of the Gaussian Orthogonal Ensemble is that it is invariant under orthogonal conjugation, meaning that if M is an $N \times N$ matrix-valued random variable with the GOE probability distribution, and P is an $N \times N$ real orthogonal matrix ($P^{-1} = P^T$), then the resulting random matrix PMP^{-1} also has the GOE probability distribution. The $N \times N$ Gaussian Unitary Ensemble likewise consists of a probability distribution on the space of $N \times N$ complex Hermitian matrices ($M = \overline{M^T}$), which is invariant under unitary ($P^{-1} = \overline{P^T}$) conjugation.

Remembering that real symmetric and complex Hermitian matrices always have real eigenvalues, one can consider spacing statistics for the eigenvalues of a GOE or GUE random matrix. Now in the same way that the output of a Poisson process would, with almost-certainty (i.e. probability 1), have certain statistical properties (e.g. $P(s) = e^{-s}$), so likewise concerning the limiting behaviour of $N \times N$ GOE and GUE eigenvalue statistics as $N \rightarrow \infty$. In particular, for both GOE and GUE eigenvalue statistics in the $N \rightarrow \infty$ limit, the level spacings probability distribution is given by a well-defined $P(s)$ function, which is well approximated by for example, the $P(s)$ function in the 2×2 case (see e.g. [Bog00]):

$$P_{\text{GOE}}^{2 \times 2}(s) = \frac{\pi}{2} s e^{-\frac{\pi}{4} s^2}, \quad P_{\text{GUE}}^{2 \times 2}(s) = \frac{32}{\pi^2} s^2 e^{-\frac{4}{\pi} s^2}. \quad (1.34)$$

For both GOE and GUE, $P(0) = 0$ (so $P(s) \rightarrow 0$ as $s \rightarrow 0^+$), indicating that for “small” L , the proportion of consecutive eigenvalue spacings that are smaller than L is “very small”. This is referred to as *level repulsion*, and clearly does not hold in the case of a Poisson process. For large s , the decay of $P(s)$ is approximately the decay of a Gaussian function, and thus is faster than the decay of $P(s)$ for a Poisson process.

Focussing on quantum systems without spin incorporated, it is conjectured that for a generic classically chaotic system, if this classical system possesses time-reversal symmetry then the eigenvalue statistics for the corresponding quantum system resembles GOE eigenvalue statistics (in the $N \rightarrow \infty$ limit), and if there is not time-reversal symmetry then the eigenvalue statistics resembles GUE eigenvalue statistics.

Note that any classical system given by (1.4), with specular reflection if there is a boundary, possesses time-reversal symmetry. Thus generically, if such a system is chaotic, the corresponding quantum system, given by (1.9) (taking complex scalar-valued wavefunctions, as opposed to complex multi-entry column vector-valued wavefunctions), with appropriate boundary conditions (e.g. Dirichlet) if there is a boundary, is conjectured to have GOE eigenvalue statistics (this quantum system does not involve spin). Time-reversal symmetry can be broken, for example by involving a magnetic field.

Early work involving heuristic arguments suggesting random matrix quantum eigenvalue statistics for classically chaotic systems includes [ZF74] and [Zas77]. In fact, this random matrix theory was originally developed (mainly by Wigner, Dyson and Mehta) in order to describe proposed statistical behaviour of spectra of heavy nuclei (see [Por65] and [Meh67]). Numerical findings supporting GOE eigenvalue statistics for the stadium billiard can be found in [MK79], [CVG80] and [BGS84a], and for the Sinai billiard, [BGS84b].

In [BR86] is contained both theoretical predictions and numerical findings in favour of GUE eigenvalue statistics for planar chaotic *Aharonov-Bohm* billiards - billiards with a single magnetic flux line whose magnetic vector potential is given by a delta function with direction orthogonal to the plane of the billiard. Although “almost all” classical trajectories avoid the point of magnetic flux, and so the classical flow is regarded to be unaffected by it, it still affects the corresponding quantum system, and being a *magnetic* field, it still results in GUE eigenvalue statistics as predicted for classically chaotic systems without time-reversal symmetry (except at one particular special nonzero value for the strength of this magnetic delta potential, for which it is GOE eigenvalue statistics that is predicted).

Discussion, involving heuristic arguments, on random matrix eigenvalue statistics for

classically chaotic systems (both with and without time-reversal symmetry), as reflected specifically in spectral rigidity, can be found in [Ber85], as well as Poissonian spectral rigidity in the case of classically integrable systems.

1.4 Achievements in quantum chaos: behaviour of eigenfunctions

As a general reference for this section, see e.g. [Non13].

1.4.1 Quantisation of observables

Given a (well-behaved) function $f(x, p)$ on classical phase space $T^*\mathcal{M}$, a corresponding operator \hat{f}_\hbar acting on the quantum Hilbert space can be obtained through an appropriate *quantisation procedure*, typically *Weyl quantisation* (in the Euclidean case). If \mathcal{M} is Euclidean, this operator can be expressed formally as $\hat{f}_\hbar = f(\hat{x}, \hat{p})$, where \hat{x} and \hat{p} are given by (1.8). Note that the operator \hat{f}_\hbar is in general dependent on \hbar , when treating \hbar as a variable, with an interest in the limit $\hbar \rightarrow 0$. If however, f is dependent only on position (i.e. $f(x, p) = f(x, p') \forall x \in \mathcal{M} \forall p, p' \in T_x^*\mathcal{M}$ at which f has a well-defined value), then \hat{f}_\hbar is just the operation of multiplication by $f(x)$, and so in this case is independent of \hbar .

Again, for a given wavefunction ψ , the quantum expectation value of the observable given classically by $f(x, p)$ is $\langle f \rangle = \langle \hat{f}_\hbar \psi, \psi \rangle$. Given the wavefunction ψ and a given value of \hbar , there is a corresponding distribution $W_{\psi, \hbar}$ on $T^*\mathcal{M}$ called the *Wigner function*, satisfying the following:

$$\int_{T^*\mathcal{M}} f(x, p) W_{\psi, \hbar}(x, p) dx dp = \langle \hat{f}_\hbar \psi, \psi \rangle \quad (1.35)$$

for all “well-behaved” test functions f . The Wigner function can be interpreted as a quasi-probability density on phase space under which the classical expectation of f is equal to its quantum expectation, only the Wigner function can be negative in some regions (but still must be real). For more details on quantisation of observables and Wigner functions, see e.g. [ZFC05]. In the Euclidean case, an example of a non-negative phase space density associated with the wavefunction is the *Husimi* function/measure (see [Non13] for a definition).

A foundational result in semiclassical analysis and quantum chaos is one known as *quantum-classical correspondence*, or *Egorov’s theorem*. This is a result that relates quantum evolution with classical evolution. Note first that the time-evolution of the

wavefunction solving (1.11) can be expressed in the following form:

$$\psi(t) = \exp\left(-\frac{iHt}{\hbar}\right) \psi(0), \quad (1.36)$$

with $\exp(-iHt/\hbar)$, for each $t \in \mathbb{R}$, being a unitary operator in the quantum Hilbert space.

Given some $f \in C_0^\infty(T^*\mathcal{M}^\circ)$ (C_0^∞ being the space of C^∞ -smooth compactly supported functions; assume if necessary that the classical Hamiltonian is C^∞ -smooth everywhere on phase space, or that $\text{supp} f$ is bounded away from all points where the Hamiltonian fails to be smooth if there are any), defining $f_t := f \circ \Phi^t$ for each $t \in \mathbb{R}$ (Φ^t being the classical flow), Egorov's theorem (or one form of it) states that in the limit $\hbar \rightarrow 0$:

$$\exp\left(\frac{i\hat{H}_\hbar t}{\hbar}\right) \hat{f}_\hbar \exp\left(-\frac{i\hat{H}_\hbar t}{\hbar}\right) = \hat{f}_{t,\hbar} + \mathcal{O}(e^{\Gamma|t|\hbar}) \quad \forall t \in \mathbb{R}, \quad (1.37)$$

where \hat{H}_\hbar is still the quantum Hamiltonian (just represented in such a way as to show dependence on \hbar), $\Gamma > 0$ is some value that depends on the flow and on the observable f but not on t , and the notation $\mathcal{O}(e^{\Gamma|t|\hbar})$ is used to represent a ‘‘remainder’’ operator which, for each $t \in \mathbb{R}$, has operator norm $\leq Ce^{\Gamma|t|\hbar}$ for all sufficiently small \hbar , where C is some t -independent positive constant.

Another significant result is the *generalised Weyl law*, which shall be stated here in the case of a system satisfying (1.9) with $V = 0$ on a compact position space (with connected interior), and with Dirichlet boundary conditions if there is a boundary. Let $\{k_j^2\}_{j \in \mathbb{N}}$ be the eigenvalues of the self-adjoint $-\Delta$ operator (k_j then being the positive square root), so with $H = -\frac{\hbar^2}{2m}\Delta$ having eigenvalues $\{E_j\}_{j \in \mathbb{N}}$, it follows that $E_j = \frac{\hbar^2}{2m}k_j^2$. Let $\{\psi_j\}_{j \in \mathbb{N}}$ be a corresponding orthonormal eigenbasis. Copying [Non13], allow quantities to be expressible as dimensionless values (i.e. select units of quantities to set to 1), and in particular set mass $m = 1$. For each $j \in \mathbb{N}$ with $k_j > 0$, define \hbar_j to be the value of \hbar for which $E_j = \frac{1}{2}$, so $\hbar_j = 1/k_j$. Let $\mathcal{E}_{1/2}$ be the energy shell in phase space of energy $\frac{1}{2}$, and let $\mu_{1/2}$ be the normalised Liouville measure on this energy shell. The generalised Weyl law then states:

$$\sum_{j:0 < k_j \leq K} \left\langle \hat{f}_{\hbar_j} \psi_j, \psi_j \right\rangle \sim \frac{\text{vol}(\mathcal{M})\text{vol}(B_1^n)}{(2\pi)^n} K^n \int_{\mathcal{E}_{1/2}} f \, d\mu_{1/2} \quad (1.38)$$

as $K \rightarrow \infty$, for all suitable phase space functions f .

Observe that if $f = 1$ is plugged into (1.38), so \hat{f}_{\hbar_j} is just the identity map for all j , then we obtain:

$$\#\{j : 0 < k_j \leq K\} \sim \frac{\text{vol}(\mathcal{M})\text{vol}(B_1^n)}{(2\pi)^n} K^n \quad (1.39)$$

as $K \rightarrow \infty$. This is consistent with (1.20). Then dividing (1.38) by (1.39) gives:

$$\frac{1}{\#\{j : 0 < k_j \leq K\}} \sum_{j:0 < k_j \leq K} \langle \hat{f}_{\hbar_j} \psi_j, \psi_j \rangle \sim \int_{\mathcal{E}_{1/2}} f \, d\mu_{1/2} \quad (1.40)$$

as $K \rightarrow \infty$.

Often in quantum chaos studies for which \hbar is treated as a constant, the formulation of quantisation of observables is somewhat different. Typically an operator in the quantum system would be a *polyhomogeneous pseudodifferential operator*, and at least in the case where the position space is a region in Euclidean space, associated to this pseudodifferential operator (abbreviated Ψ DO) would be a corresponding function on the phase space (cotangent bundle) known as its *symbol* (or at least this symbol would be defined modulo symbols of order $-\infty$, see §3.2 in Ch. I of [Shu01]). Furthermore, this symbol (being polyhomogeneous) would have an *asymptotic expansion*, whose leading term is referred to as the *principal symbol*. The principal symbol of a polyhomogeneous Ψ DO is also well-defined when the position space more generally is a manifold, due to certain invariant behaviour under coordinate transformations (see e.g. §4 in Ch. I of [Shu01]).

Like differential operators, one can speak of the *order* m of a pseudodifferential operator (only now, m can take any real value; an order m Ψ DO is also order \tilde{m} for each $\tilde{m} > m$; furthermore an order m polyhomogeneous Ψ DO is also order $m + l$ for each $l \in \mathbb{N}$, with zero $(m+l)$ -order principal symbol). The principal symbol of an order m polyhomogeneous Ψ DO, being a function on the cotangent bundle, is positively homogeneous of order m in covector p , meaning that, if we call this principal symbol a_m , we have $a_m(x, rp) = r^m a_m(x, p) \, \forall x \in \mathcal{M}^\circ, p \in T_x^* \mathcal{M}^\circ \setminus \{0\}, r \in (0, \infty)$. It obviously follows then that in order to determine the function a_m on the whole cotangent bundle $T^* \mathcal{M}^\circ$ (excluding points where the covector is zero), it is sufficient to specify a_m on the unit cotangent bundle (also known as the cosphere bundle) $S^* \mathcal{M}^\circ := \{(x, p) \in T^* \mathcal{M}^\circ : \|p\| = 1\}$.

Commonly, definitions and theorems relating quantum and classical observables would be stated in terms of polyhomogeneous Ψ DOs of certain order and their *principal* symbols (see e.g. [ZZ96] or [Sch01]). In this case one would obviously not be working with $C_0^\infty(T^* \mathcal{M}^\circ)$ as the space of classical observables. When integration of a principal symbol is involved, it would not be over the whole cotangent bundle, but over a more appropriate surface within the cotangent bundle, typically the cosphere bundle, or the surface on which the principal symbol of the quantum Hamiltonian is 1 (and these two would be the same when the Hamiltonian operator is $-\Delta$).

1.4.2 Quantum ergodicity

As stated in §1.3.3, the classical dynamical system is ergodic on an energy shell \mathcal{E}_E if under the normalised Liouville measure, every invariant measurable set has either zero measure or full measure, where again a set is invariant if every trajectory that begins in that set remains in that set for all time (both forwards and backwards).

Birkhoff’s Ergodic Theorem: If the classical flow Φ^t on a shell \mathcal{E}_E is ergodic, then for each $f \in L^1(\mathcal{E}_E)$ it holds that

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T f \circ \Phi^t(x, p) dt = \int_{\mathcal{E}_E} f d\mu_E \quad (1.41)$$

for almost all $(x, p) \in \mathcal{E}_E$ (where “almost all” means “for a full measure set”).

Since time-reversal does not affect whether a set is invariant, and thus does not affect ergodicity, the above statement also holds true if in LHS(1.41), \int_0^T is replaced with \int_{-T}^0 . It also then follows that this statement holds true if in LHS(1.41), $\frac{1}{T} \int_0^T$ is replaced with $\frac{1}{2T} \int_{-T}^T$.

This ergodic theorem essentially equates temporal averages of observables with spatial averages if the flow on the shell \mathcal{E}_E is ergodic. Observe also that for any measurable set $S \subset \mathcal{E}_E$, taking f to be the characteristic function of S (i.e. $f = 1$ on S and 0 everywhere else on \mathcal{E}_E), this ergodic theorem yields that for almost all starting points in \mathcal{E}_E , the overall proportion of time that the trajectory spends within S is equal to the measure of S (under the normalised Liouville measure).

Von Neumann’s Ergodic Theorem: If the classical flow Φ^t on a shell \mathcal{E}_E is ergodic, then for each $f \in L^2(\mathcal{E}_E)$ it holds that

$$\frac{1}{T} \int_0^T f \circ \Phi^t dt \xrightarrow[L^2]{T \rightarrow \infty} \int_{\mathcal{E}_E} f d\mu_E. \quad (1.42)$$

Again, this also holds if \int_0^T is replaced with \int_{-T}^0 , and likewise if $\frac{1}{T} \int_0^T$ is replaced with $\frac{1}{2T} \int_{-T}^T$.

The **quantum ergodicity theorem** gives us a certain limiting behaviour of quantum eigenfunctions in the semiclassical or high-energy limit, namely *equidistribution* of a full-density subsequence of eigenfunctions (in which case the system is said to possess *quantum ergodicity*), when the corresponding classical dynamics is ergodic. Work towards this theorem, under various settings, has been carried out in e.g. [Sni74], [Ver85], [Zel87], [HMR87], [GL93] and [ZZ96].

To state the quantum ergodicity theorem in the case of a system whose quantum Hamiltonian operator is a self-adjoint $-\Delta$ (with Dirichlet boundary conditions if there is

a boundary), and whose classical flow on each energy shell (being a shell in the cotangent bundle of constant $\|p\|$) is geodesic flow (with specular reflection if there is a boundary), working with zero-order Ψ DOs and their principal symbols, and taking the high-energy limit (see e.g. [Zel87] and [ZZ96]):

If the classical flow is ergodic then there exists a full-density subsequence $(\Psi_{j_n})_{n \in \mathbb{N}}$ of orthonormal eigenbasis $(\Psi_j)_{j \in \mathbb{N}}$ such that for every zero-order polyhomogeneous Ψ DO A with compactly supported Schwartz kernel in $\mathcal{M}^\circ \times \mathcal{M}^\circ$ (see §5.3 for a definition of the Schwartz kernel), we have

$$\langle A\Psi_{j_n}, \Psi_{j_n} \rangle \xrightarrow{n \rightarrow \infty} \int_{S^*\mathcal{M}} \sigma_0(A), \quad (1.43)$$

where $\sigma_0(A)$ is the zero-order principal symbol of A .

This subsequence $(\Psi_{j_n})_{n \in \mathbb{N}}$ is said to *equidistribute* in phase space. Equidistribution in phase space is stronger than equidistribution in position space, which can be defined as follows: for every measurable subset $X \subset \mathcal{M}$ whose boundary has zero measure (d -dimensional volume measure for \mathcal{M} being d -dimensional) [MR12],

$$\lim_{n \rightarrow \infty} \int_X |\Psi_{j_n}(x)|^2 dx = \frac{\text{vol}(X)}{\text{vol}(\mathcal{M})}. \quad (1.44)$$

In essence, this says that in the high-energy limit, the probability of the particle in a stationary state being found within X is equal to the measure of X as a fraction of the total measure of \mathcal{M} .

In [MR12], it is shown that for *rational polygon* billiards, though they are not ergodic (rational polygon billiards are neither ergodic nor integrable except for rectangles and certain specific triangles, which are integrable), they do still satisfy position space equidistribution of a full-density subsequence of eigenfunctions. The key property of the classical system here is that (1.42) (with $\frac{1}{T} \int_0^T$ is replaced with $\frac{1}{2T} \int_{-T}^T$) holds for all smooth f depending *only on position* (i.e. $f(x, p) = f(x, p') \forall p, p' \in T_x^*\mathcal{M}$). It is also remarked in [MR12] that this result holds with Neumann as well as Dirichlet boundary conditions, and furthermore holds for an arbitrary *translation surface*.

1.4.3 Integrability and microlocalised WKB quasimodes

Included in §1.3.2 is discussion on the principle that if the classical system is integrable, then the energies of lattice points, for a certain \hbar -dependent square lattice in \mathbf{I} -space, approximate the quantum Hamiltonian eigenvalues as $\hbar \rightarrow 0$.

It is furthermore the case that associated with these lattice points in \mathbf{I} -space are corresponding *quasimodes* (approximate quantum eigenfunctions), which approximate

the quantum Hamiltonian eigenfunctions as $\hbar \rightarrow 0$. Furthermore, these quasimodes are *microlocalised* (loosely speaking, their Wigner functions become highly concentrated as $\hbar \rightarrow 0$ - focussing not on lattice points of fixed $\mathbb{N} \times \mathbb{N}$ specification while they approach zero as $\hbar \rightarrow 0$, but rather, while \hbar is being decreased down to zero, considering the lattice points that intersect the vicinity of a fixed \hbar -independent point in \mathbf{I} -space) on the region of phase space of their corresponding \mathbf{I} -value.

Taking then the example of the rectangular billiard discussed in §1.3.2, for a generic fixed \mathbf{I} -value, the corresponding region in phase space is the Cartesian product of the 2D rectangle with a set of four points in momentum space (if one of the two I -coordinates is zero then it is two points in momentum space; if both coordinates are zero then it is just the origin in momentum space). As a result, in the semiclassical or high-energy limit, quantum eigenfunctions of the rectangle billiard would have their momentum probability distribution (obtained via the Fourier transform of the eigenfunction) concentrated on four (or for some of them, two) points in momentum space. Observe that this resembles the fact that all classical orbits are confined to four (or for some of them, two) points in momentum space.

1.5 Addition of a Delta Scatterer

For a quantum system of sufficiently low dimension, one can consider perturbing the system by placing a *point scatterer / delta potential* at some select point $p \in \mathcal{M}^\circ$. The perturbed Hamiltonian operator would then be a select operator from a family of *self-adjoint extensions* of the restriction of the original unperturbed operator to functions vanishing at p .

For eigenvalues and eigenfunctions, one would start with an orthonormal eigenbasis of the unperturbed operator whereby for each distinct eigenvalue, *at most one* of the corresponding eigenfunctions in the eigenbasis would be non-vanishing at p . One would then delete the eigenfunctions that are nonvanishing at p . Next, one would insert the “new eigenfunctions”, whereby the eigenvalues would be the solutions to a particular equation, and then there would be a formula for the corresponding eigenfunctions in terms of these eigenvalues and the unperturbed eigenbasis. The eigenvalues corresponding to these “new eigenfunctions” form an interlacing between the unperturbed eigenvalues for which there are functions in the corresponding eigenspace that do not vanish at p (*interlacing* meaning one between each consecutive pair).

The eigenvalue interlacing given by any one of these self-adjoint extensions (other

than the unperturbed operator itself) is sometimes referred to as the *weak coupling limit*. There is also a modification of this interlacing that has been studied, referred to as the *strong coupling limit*.

For an overview of some current conjectural theory and rigorous results concerning eigenvalue and eigenfunction statistics in the case of a delta potential on a 2D and a 3D flat torus, considering both the weak coupling and strong coupling regimes, see [Ueb14].

Work carried out so far on behaviour of eigenfunction subsequences (taking the high-energy limit rather than sending $\hbar \rightarrow 0$) for systems with a delta potential includes [KMW10], [RU12], [Yes13], [KU14], [Yes15] and [KU(Pr15)].

1.5.1 Localisation

In [KMW10], working with the addition of a delta potential to a self-adjoint $-\Delta$ operator on a 2-dimensional compact Riemannian manifold with or without boundary, a class of quasimodes for the delta-perturbed operator is constructed. Analysis is then performed on how well these quasimodes can be used to approximate eigenfunctions of the delta-perturbed operator.

Included in this work is a theorem, namely Thm. 4.4, of the following form, working specifically with the “ H_π ” self-adjoint extension: for a subsequence of the sequence of new eigenfunctions, suppose the surrounding unperturbed eigenvalues and corresponding eigenfunctions which do not vanish at p satisfy certain specified requirements. Then the members of this subsequence approximate in the limit to quasimodes which are linear combinations of just two unperturbed eigenfunctions non-vanishing at p . These two eigenfunctions correspond to surrounding unperturbed eigenvalues.

This theorem is then applied (heuristically) to the case of the Dirichlet $-\Delta$ on a rectangle billiard of generic side length ratio, perturbed with a delta potential placed at the centre of the rectangle. This delta-perturbed billiard is known as the *Šeba billiard*. It is argued that there is a subsequence of the sequence of new eigenfunctions for which, for each eigenfunction high up in this subsequence, the momentum distribution is concentrated around eight points. This is because the eigenfunction is approximately a linear combination of just two unperturbed eigenfunctions, each having their momentum distribution concentrated around four points. Numerical support for this can be found in [BKW03].

One of the aims of the work carried out for this thesis is to weaken the conditions of Thm. 4.4 in [KMW10]. This work is documented in Chapter 3.

More recent work has been carried out in [KU(Pr15)], working on a 2D delta-perturbed

flat torus of diophantine square of side length ratio, demonstrating through *rigorous* means the phenomenon of new eigenfunction subsequences localising around a set of four points in momentum space. The strong coupling limit is also investigated. Furthermore, discussion is included on how the work can be modified to the case of a delta-perturbed Dirichlet rectangle.

1.5.2 Equidistribution

In [RU12] it is proved that for a 2-dimensional delta-perturbed flat torus, the sequence of new eigenfunctions has a full-density subsequence that equidistributes in position space. As discussed in §5.1.2 of this thesis, the classical flow on the flat torus satisfies the dynamical property sufficient for the *unperturbed* quantum system to have a full-density subsequence of eigenfunctions in the eigenbasis that equidistributes in position space. Combining these two facts, it follows that the whole eigenbasis of the perturbed system has a full-density subsequence that equidistributes in position space.

In Chapter 5 of this thesis, interest is then expressed in deriving a more general result, namely that for a more general system given by a delta-perturbed $-\Delta$ on a compact manifold (with Dirichlet boundary conditions if there is a boundary), if the classical system satisfies the relevant dynamical property, then not only will the unperturbed quantum system have a full-density subsequence of eigenfunctions that equidistributes in position space, but so will the delta-perturbed system.

Further developments after [RU12], concerning position space and phase space equidistribution for a delta-perturbed flat torus (both 2D and 3D), can be found in [Yes13], [KU14] and [Yes15].

1.6 Overview of the Work in this Thesis

The setting within which the work in this thesis is carried out is the following: the position space \mathcal{M} is a two-dimensional compact Riemannian manifold, with connected interior \mathcal{M}° , and either no boundary or piecewise smooth and Lipschitz boundary $\partial\mathcal{M}$. The quantum Hilbert space is then $L^2(\mathcal{M})$. The *unperturbed* quantum Hamiltonian operator is the self-adjoint $-\Delta$ (minus Laplacian), with Dirichlet boundary conditions if $\partial\mathcal{M} \neq \emptyset$. The *perturbed* quantum Hamiltonian operator consists of the addition of a delta potential, at a select point $p \in \mathcal{M}^\circ$. This is constructed rigorously via means of self-adjoint extension theory. A substantial description of the system, including discussion of the eigenvalues and eigenfunctions of the unperturbed and perturbed systems, is given

in Chapter 2.

Again, §1.5.1 and 1.5.2 provide background from which Chapters 3 and 5 stem. Theorem 4.4 in [KMW10] derives a set of conditions under which a subsequence of the sequence of new perturbed eigenfunctions approaches linear combinations of only two surrounding unperturbed eigenfunctions. More precisely, these pair linear combinations belong to a class of quasimodes (i.e. approximate eigenfunctions) constructed within [KMW10]. Again, this result was used to infer localisation of perturbed eigenfunction subsequences around eight points in momentum space, due to composite unperturbed eigenfunctions localising around four points.

In Chapter 3 of this thesis, firstly basic results are derived, giving broadened consideration of the question of when a new perturbed eigenfunction subsequence approaches linear combinations of the two surrounding unperturbed eigenfunctions. This is particularly as opposed to focussing purely on the quasimodes given in [KMW10]. Later on, results are derived which would serve as an improvement on Thm. 4.4 in [KMW10]. In particular, a weakening of the conditions stated in Thm. 4.4 of [KMW10] has been demonstrated.

Chapter 5 of this thesis addresses the question of equidistribution in position space of a full-density subsequence of eigenfunctions of the delta-perturbed operator. For the unperturbed system, equidistribution in position space of a full-density subsequence of eigenfunctions follows if the classical dynamics satisfies the condition that (1.42) (with $\frac{1}{T} \int_0^T$ is replaced with $\frac{1}{2T} \int_{-T}^T$) holds for all smooth f depending only on position. This again is demonstrated in [MR12], which deals with rational polygon billiards. It is then of interest to extend this result to the delta-perturbed system.

This full-density position space equidistribution has already been proven in [RU12] for the case of a 2D delta-perturbed rectangular flat torus. [RU12] only focusses explicitly on the sequence of *new* perturbed eigenfunctions. However, within §5.1.2 in this thesis, an explanation is given on how it follows, in the case of the flat torus, that this position space equidistribution extends to a full-density subsequence of the *full eigenbasis* of the delta-perturbed operator.

It is still of interest to derive a result that applies to more general delta-perturbed systems. Successful arrival at such a result is not achieved within Chapter 5. Nevertheless, in §5.4, three methods are discussed for approaching this task. Method 1 is to make use of the formulae for the perturbed eigenvalues and eigenfunctions in terms of those of the unperturbed operator. Method 2 is to consider a sequence of non-singular perturbations that approach the delta potential. Standard results in semiclassical analysis leading to

position space (and phase space) equidistribution should be applicable to the non-singular perturbations, particularly given the results in [Sch01]. Method 3 is to develop or work with a semiclassical theory which, at a more fundamental level, permits a certain extent of singular behaviour. To this end, adaptation of the work in [JSSV15] may be a reasonable way forward.

Regarding non-singular perturbations which approach the delta potential, this is the subject of Chapter 4. More precisely, Chapter 4 deals with non-singular *rank-one* perturbations of the self-adjoint $-\Delta$, approaching the delta potential. Examples of literature dealing with this are [BF61], [Zor80], [AGHHE88], [AK00] and [GN12]. These however deal mostly in the setting of a whole Euclidean space, whereas Chapter 4 here works in the setting of the compact manifold \mathcal{M} .

In Chapter 4, a construction is given for an orthonormal eigenbasis and corresponding eigenvalues of a rank-one perturbation, which parallels that in the case of the delta potential. Based on the analogous features in eigenvalues and eigenfunctions between rank-one perturbations and the delta potential, conditions are then derived on a sequence of rank-one perturbations under which (some of) their eigenvalues and eigenfunctions are found to approach those of the delta potential.

Chapter 2

Specification of the Quantum and Classical Systems

We shall work on a 2-dimensional compact Riemannian manifold \mathcal{M} , with connected interior \mathcal{M}° , which may either be without boundary (i.e. $\mathcal{M} = \mathcal{M}^\circ$), or with Lipschitz, piecewise C^∞ -smooth boundary $\partial\mathcal{M}$. “Lipschitz” here would rule out corner points on the boundary of zero or 2π angle.

We shall consider an unperturbed quantum system, a perturbed quantum system and a corresponding classical system, describing a particle confined to \mathcal{M} . The quantum system is described by a self-adjoint operator, namely the *Hamiltonian* operator, on the Hilbert space $L^2(\mathcal{M})$, and the classical system is described by a flow on the unit cotangent bundle $S^*\mathcal{M}$.

2.1 The Unperturbed Quantum System

2.1.1 The Hilbert Space and the Self-Adjoint minus-Laplacian Operator

Given the 2D compact Riemannian manifold \mathcal{M} , we have the associated Hilbert space $L^2(\mathcal{M})$, endowed with the inner product:

$$\langle f, g \rangle = \int_{\mathcal{M}} f(x) \overline{g(x)} dx, \quad (2.1)$$

and induced norm:

$$\|f\| = \sqrt{\langle f, f \rangle} = \sqrt{\int_{\mathcal{M}} |f(x)|^2 dx}. \quad (2.2)$$

$L^2(\mathcal{M})$ is a *separable* Hilbert space. One meaning of this is that it has a countable orthonormal basis.

The state of a quantum particle confined within \mathcal{M} , at any moment in time, is specified by a normalised member of $L^2(\mathcal{M})$ (ignoring spin), referred to as the *wavefunction*. If $\psi(x)$ is the wavefunction, then $|\psi(x)|^2$ is the probability density for the particle's position on \mathcal{M} .

For the *unperturbed* quantum system, the Hamiltonian operator H shall be taken to be a self-adjoint $-\Delta$ operator. This means that H is a self-adjoint extension of the operator $-\Delta : C_0^\infty(\mathcal{M}^\circ) \rightarrow C_0^\infty(\mathcal{M}^\circ)$, where Δ is the Laplacian derivative and $C_0^\infty(\mathcal{M}^\circ)$ is the space of C^∞ -smooth complex-valued functions on \mathcal{M} with compact support within \mathcal{M}° . $\Delta = \partial_x^2 + \partial_y^2$ if \mathcal{M} is flat, but it also has a generalisation to Riemannian manifolds known as the *Laplace-Beltrami* operator. Note that $C_0^\infty(\mathcal{M}^\circ)$ is dense in $L^2(\mathcal{M})$.

The Laplace-Beltrami operator in local coordinates, in n dimensions (so in our case $n = 2$), is given by

$$\Delta\phi = \frac{1}{\sqrt{\det(g_{\mu\nu})}} \sum_{i=1}^n \sum_{j=1}^n \frac{\partial}{\partial x_i} \left(g^{ij} \sqrt{\det(g_{\mu\nu})} \frac{\partial\phi}{\partial x_j} \right), \quad (2.3)$$

where $(g_{\mu\nu})_{\mu,\nu=1}^n$ is the *covariant metric tensor* and $(g^{\mu\nu})_{\mu,\nu=1}^n$ is the *contravariant metric tensor*. Given any two tangent vectors $X = (X^\mu)_{\mu=1}^n, Y = (Y^\nu)_{\nu=1}^n \in T_x\mathcal{M}$ at a point $x \in \mathcal{M}$, letting $g(\cdot, \cdot)$ be the Riemannian metric, one has

$$g(X, Y) = \sum_{\mu=1}^n \sum_{\nu=1}^n g_{\mu\nu} X^\mu Y^\nu. \quad (2.4)$$

Given any two cotangent vectors $\xi = (\xi_\mu)_{\mu=1}^n, \omega = (\omega_\nu)_{\nu=1}^n \in T_x^*\mathcal{M}$ we have

$$g(\xi, \omega) = \sum_{\mu=1}^n \sum_{\nu=1}^n g^{\mu\nu} \xi_\mu \omega_\nu. \quad (2.5)$$

The contravariant metric tensor is the inverse matrix of the covariant metric tensor.

By H being *self-adjoint*, this means that the operator H , which has dense domain in $L^2(\mathcal{M})$, is equal to its adjoint operator H^* , whose graph is:

$$\{(v, w) \in L^2(\mathcal{M}) \times L^2(\mathcal{M}) : \langle Hu, v \rangle = \langle u, w \rangle \ \forall u \in \text{Dom}(H)\}. \quad (2.6)$$

Note that being a self-adjoint operator, H is in particular a *symmetric/Hermitian* operator, that is:

$$\langle Hu, v \rangle = \langle u, Hv \rangle \ \forall u, v \in \text{Dom}(H). \quad (2.7)$$

Now there is a particular class of linear functionals (forming a vector space) on $C_0^\infty(\mathcal{M}^\circ)$ referred to as *distributions*. Let $\mathcal{D}'(\mathcal{M}^\circ)$ denote the space of distributions on \mathcal{M}° . $\mathcal{D}'(\mathcal{M}^\circ)$ includes all functionals on $C_0^\infty(\mathcal{M}^\circ)$ of the form $\phi \mapsto \int_{\mathcal{M}} \phi(x)u(x) dx =: \langle \phi, u \rangle_{ll}$, where $u \in L_{loc}^1(\mathcal{M}^\circ) \supset L^2(\mathcal{M})$, and the subscript ll here means linearity in both arguments, rather than conjugate-linearity in one of the two arguments. By identifying each $u \in L_{loc}^1(\mathcal{M}^\circ)$ with $\langle \cdot, u \rangle_{ll} \in \mathcal{D}'(\mathcal{M}^\circ)$, $L_{loc}^1(\mathcal{M}^\circ)$ can be considered to be a subspace of $\mathcal{D}'(\mathcal{M}^\circ)$. Note in particular that for any $u, v \in L_{loc}^1(\mathcal{M}^\circ)$, if the functionals $\langle \cdot, u \rangle_{ll}$ and $\langle \cdot, v \rangle_{ll}$ are equal then $u = v$. For further discussion on the theory of distributions, see for example §V of [RS80], §1 of [Sai91], §3.4 of [Tay96a] or [FJ98].

For each $u \in \mathcal{D}'(\mathcal{M}^\circ)$ the *distributional Laplacian* $\Delta u \in \mathcal{D}'(\mathcal{M}^\circ)$ is defined as follows:

$$\langle \phi, \Delta u \rangle_{ll} := \langle \Delta \phi, u \rangle_{ll} \quad \forall \phi \in C_0^\infty(\mathcal{M}^\circ). \quad (2.8)$$

Note that under this definition, the distributional Laplacian coincides with the usual Laplacian derivative on $C^2(\mathcal{M}^\circ)$. Furthermore, given any $v, w \in L^2(\mathcal{M})$, if $-\Delta v = w$ then

$$\begin{aligned} \langle -\Delta u, v \rangle &= \langle -\Delta u, \bar{v} \rangle_{ll} = \overline{\langle -\Delta u, v \rangle_{ll}} = \overline{\langle -\Delta \bar{u}, v \rangle_{ll}} = \overline{\langle \bar{u}, w \rangle_{ll}} = \langle u, \bar{w} \rangle_{ll} \\ &= \langle u, w \rangle \quad \forall u \in C_0^\infty(\mathcal{M}^\circ), \end{aligned} \quad (2.9)$$

and so $(-\Delta \upharpoonright_{C_0^\infty(\mathcal{M}^\circ)})^* v = w$. Conversely, if $(-\Delta \upharpoonright_{C_0^\infty(\mathcal{M}^\circ)})^* v = w$ then

$$\begin{aligned} \langle -\Delta u, v \rangle_{ll} &= \langle -\Delta u, \bar{v} \rangle = \overline{\langle -\Delta u, v \rangle} = \overline{\langle -\Delta \bar{u}, v \rangle} = \overline{\langle \bar{u}, w \rangle} = \langle u, \bar{w} \rangle \\ &= \langle u, w \rangle_{ll} \\ \Rightarrow \langle \Delta u, v \rangle_{ll} &= \langle u, -w \rangle_{ll} \quad \forall u \in C_0^\infty(\mathcal{M}^\circ), \end{aligned} \quad (2.10)$$

and so $-\Delta v = w$. Hence the adjoint of the operator $-\Delta : C_0^\infty(\mathcal{M}^\circ) \rightarrow C_0^\infty(\mathcal{M}^\circ)$ is the restriction of the distributional $-\Delta$ operator to all $v \in L^2(\mathcal{M})$ for which $-\Delta v \in L^2(\mathcal{M})$ also.

Note also that for each $v \in \text{Dom}(H)$,

$$\langle -\Delta u, v \rangle = \langle Hu, v \rangle = \langle u, Hv \rangle \quad \forall u \in C_0^\infty(\mathcal{M}^\circ), \quad (2.11)$$

and so H is a restriction of the adjoint of $-\Delta : C_0^\infty(\mathcal{M}^\circ) \rightarrow C_0^\infty(\mathcal{M}^\circ)$. Hence $Hv = -\Delta v \quad \forall v \in \text{Dom}(H)$ in the distributional sense. Likewise if \tilde{H} is any self-adjoint operator satisfying $\tilde{H}v = -\Delta v \quad \forall v \in \text{Dom}(\tilde{H})$ then it is a self-adjoint extension of $-\Delta : C_0^\infty(\mathcal{M}^\circ) \rightarrow C_0^\infty(\mathcal{M}^\circ)$. This is because $(-\Delta \upharpoonright_{C_0^\infty(\mathcal{M}^\circ)})^{**}$ is the closure of $-\Delta \upharpoonright_{C_0^\infty(\mathcal{M}^\circ)}$, with *closure* here meaning the operator formed by taking the closure of the graph in $L^2(\mathcal{M}) \times L^2(\mathcal{M})$, if indeed this does give the graph of an operator, which in this case

it does (see Thm. VIII.1 in §VIII.1 of [RS80]). Thus for any restriction of the operator $(-\Delta|_{C_0^\infty(\mathcal{M}^o)})^*$ whose domain is dense, the graph of the adjoint of this restriction will include all members of the graph of the closure of $-\Delta|_{C_0^\infty(\mathcal{M}^o)}$. Hence if this restriction is self-adjoint, then it is an extension of the closure of $-\Delta|_{C_0^\infty(\mathcal{M}^o)}$.

The topology on $L^2(\mathcal{M}) \times L^2(\mathcal{M})$ here is that induced by e.g. the norm

$$\|(u, v)\| = \sqrt{\|u\|^2 + \|v\|^2}. \quad (2.12)$$

If \mathcal{M} is without boundary, there is precisely one self-adjoint $-\Delta$ operator, whose domain is all $v \in L^2(\mathcal{M})$ for which $-\Delta v \in L^2(\mathcal{M})$ also. This domain is the *Sobolev space* $H^2(\mathcal{M})$ (the “ H ” here being different from H as in the Hamiltonian operator).

While for each $k \in \mathbb{N}$ (still assuming \mathcal{M} is without boundary), $C^k(\mathcal{M})$ is defined as the space of k -times *continuously differentiable* functions on M , and $C^0(\mathcal{M}) := C(\mathcal{M})$ would be all continuous functions, the Sobolev space $H^k(\mathcal{M})$ is the space of k -times “weakly differentiable” functions, and $H^0(\mathcal{M}) = L^2(\mathcal{M})$. In fact, the set of Sobolev spaces can be extended to having a space $H^s(\mathcal{M}) \subset \mathcal{D}'(\mathcal{M})$ for every $s \in \mathbb{R}$, with $H^s(\mathcal{M}) \subset H^t(\mathcal{M})$ whenever $s \geq t$. We can therefore also define $H^{-\infty}(\mathcal{M}) := \bigcup_{s \in \mathbb{R}} H^s(\mathcal{M})$ and $H^\infty(\mathcal{M}) := \bigcap_{s \in \mathbb{R}} H^s(\mathcal{M})$. For discussion of details on Sobolev spaces, see for example §IX.6 of [RS75], §1.3 of [Sai91], §4 and 5 of [Tay96a] or §9.3 of [FJ98].

According to the *Sobolev Embedding Theorem* (applying it to the case of compact manifolds without boundary; see Prop. 3.3 in §4.3 of [Tay96a]), if \mathcal{M} is an n -dimensional compact manifold (here we’ll say without boundary) then for any $s \in \mathbb{R}$ and $k \in \mathbb{N} \cup \{0\}$,

$$\text{if } s > \frac{n}{2} + k \text{ then } H^s(\mathcal{M}) \subset C^k(\mathcal{M}). \quad (2.13)$$

In our case $n = 2$ and so the condition becomes $s > k + 1$. In particular then, all functions in the domain of the self-adjoint $-\Delta$ operator are continuous.

Now according to the end of §5.1 in [Tay96a], the operator $-\Delta + 1$ (“1” here meaning the identity map) maps $H^{k+1}(\mathcal{M})$ bijectively to $H^{k-1}(\mathcal{M})$ for each $k \in \mathbb{N} \cup \{0\}$, and more generally, $H^{s+2}(\mathcal{M}) \xrightarrow{\text{bij.}} H^s(\mathcal{M})$ for real $s \geq -1$. It follows then that for each $k \in \mathbb{N} \cup \{0\}$ and $u \in H^{k+1}(\mathcal{M})$ we have $-\Delta u \in H^{k-1}(\mathcal{M})$, since $u \in H^{k+1}(\mathcal{M}) \Rightarrow u \in H^{k-1}(\mathcal{M})$, and $(-\Delta + 1)u \in H^{k-1}(\mathcal{M})$, so $-\Delta u = (-\Delta + 1)u - u \in H^{k-1}(\mathcal{M})$. Furthermore, according to Prop. 1.6 in §5.1 of [Tay96a], if $u \in H^1(\mathcal{M})$ and $-\Delta u \in H^{k-1}(\mathcal{M})$ for some $k \in \mathbb{N} \cup \{0\}$ then $u \in H^{k+1}(\mathcal{M})$. Thus, if it is known that $u \in L^2(\mathcal{M})$ and $-\Delta u \in H^{k-1}(\mathcal{M})$ for some $k \in \mathbb{N}$ then $-\Delta u \in H^0(\mathcal{M}) = L^2(\mathcal{M})$, and so $u \in H^2(\mathcal{M}) \subset H^1(\mathcal{M})$, so then by Prop. 1.6 in §5.1 of [Tay96a], $u \in H^{k+1}(\mathcal{M})$. Hence for any $u \in L^2(\mathcal{M})$, given any $k \in \mathbb{N}$ we have $u \in H^{k+1}(\mathcal{M})$ if and only if $-\Delta u \in H^{k-1}(\mathcal{M})$.

So then, suppose $u \in H^{2k}(\mathcal{M})$ for some $k \in \mathbb{N} \cup \{0\}$. Then

$$u \in H^{2k}(\mathcal{M}) \Rightarrow -\Delta u \in H^{2(k-1)}(\mathcal{M}) \Rightarrow \dots \Rightarrow (-\Delta)^k u \in H^0(\mathcal{M}) = L^2(\mathcal{M}), \quad (2.14)$$

and so in particular, $u, -\Delta u, (-\Delta)^2 u, \dots, (-\Delta)^k u \in L^2(\mathcal{M})$. Conversely, suppose $u, -\Delta u, (-\Delta)^2 u, \dots, (-\Delta)^k u \in L^2(\mathcal{M})$. Then

$$(-\Delta)^k u \in L^2(\mathcal{M}) = H^0(\mathcal{M}) \Rightarrow (-\Delta)^{k-1} u \in H^2(\mathcal{M}) \Rightarrow \dots u \in H^{2k}(\mathcal{M}). \quad (2.15)$$

Note in particular that if $u \in C^{2k}(\mathcal{M})$ then $u, -\Delta u, (-\Delta)^2 u, \dots, (-\Delta)^k u \in C(\mathcal{M}) \subset L^\infty(\mathcal{M}) \subset L^2(\mathcal{M})$ since \mathcal{M} is compact. Thus letting $H_{-\Delta}$ denote the self-adjoint $-\Delta$ operator (so as to distinguish from H as in the symbol for Sobolev spaces), for each $k \in \mathbb{N}$ we have

$$C^{2k}(\mathcal{M}) \subset H^{2k}(\mathcal{M}) = \text{Dom}(H_{-\Delta}^k) \subset C^{2(k-1)}(\mathcal{M}). \quad (2.16)$$

It also follows then that

$$H^\infty(\mathcal{M}) = C^\infty(\mathcal{M}) = \bigcap_{k \in \mathbb{N}} \text{Dom}(H_{-\Delta}^k). \quad (2.17)$$

In the case where \mathcal{M} is with boundary, there is a variety of self-adjoint extensions of the operator $-\Delta : C_0^\infty(\mathcal{M}^\circ) \rightarrow C_0^\infty(\mathcal{M}^\circ)$, which are distinguished from one another by *boundary conditions*. Here we shall choose the operator H to satisfy *Dirichlet* boundary conditions. Loosely speaking, this is the condition that functions in $\text{Dom}(H)$ should be zero at the boundary. Now the theory of Sobolev spaces also applies to the case where \mathcal{M} is with boundary, and the precise domain of the self-adjoint Dirichlet $-\Delta$ can be specified with reference to Sobolev spaces (see e.g. Ch. 5 of [Tay96a]). The Sobolev Embedding Theorem likewise applies here, and again yields that $\text{Dom}(H) \subset C(\mathcal{M}^\circ)$, and also that if $u \in L^2(\mathcal{M})$ and $H^j u \in L^2(\mathcal{M}) \forall j \in \mathbb{N}$ then $u \in C^\infty(\mathcal{M}^\circ)$.

2.1.2 Eigenvalues and Eigenfunctions of the Self-Adjoint minus-Laplacian Operator

The operator H has a countable orthonormal basis for $L^2(\mathcal{M})$ consisting of eigenfunctions $\{\Psi_j\}_{j \in \mathbb{N}} \subset \text{Dom}(H) \cap C^\infty(\mathcal{M}^\circ)$, with corresponding non-negative real eigenvalues $\mathcal{E}_1 < \mathcal{E}_2 \leq \mathcal{E}_3 \leq \dots \rightarrow \infty$. Every $f \in L^2(\mathcal{M})$ can then be expanded into this orthonormal basis: $f = \sum_{j=1}^\infty a_j \Psi_j$. This summation converges to f in the L^2 -norm, and the coefficients are uniquely given by $a_j = \langle f, \Psi_j \rangle$. With $\{\Psi_j\}_{j \in \mathbb{N}}$ being a countable orthonormal basis, the Hilbert space $L^2(\mathcal{M})$ behaves with respect to $\{\Psi_j\}_{j \in \mathbb{N}}$ like the Hilbert space l^2 (consisting of column vectors with countably infinitely many entries) behaves with respect to its standard orthonormal basis, in that the following rules are satisfied:

- (i) $\sum_{j=1}^{\infty} a_j \Psi_j \in L^2(\mathcal{M})$ iff $\sum_{j=1}^{\infty} |a_j|^2$ converges,
- (ii) With $f = \sum_{j=1}^{\infty} a_j \Psi_j$ and $g = \sum_{j=1}^{\infty} b_j \Psi_j$, $f + g = \sum_{j=1}^{\infty} (a_j + b_j) \Psi_j$,
- (iii) With $f = \sum_{j=1}^{\infty} a_j \Psi_j$ and $c \in \mathbb{C}$, $cf = \sum_{j=1}^{\infty} (ca_j) \Psi_j$,
- (iv) With $f = \sum_{j=1}^{\infty} a_j \Psi_j$ and $g = \sum_{j=1}^{\infty} b_j \Psi_j$, $\langle f, g \rangle = \sum_{j=1}^{\infty} a_j \bar{b}_j$.

The behaviour of H , when expanding functions into the eigenbasis $\{\Psi_j\}_{j \in \mathbb{N}}$, is straightforwardly given by the following (even though H is not a continuous operator under the L^2 -norm):

Lemma 2.1.1. $\sum_{j=1}^{\infty} a_j \Psi_j \in \text{Dom}(H)$ if and only if $\sum_{j=1}^{\infty} \mathcal{E}_j a_j \Psi_j \in L^2(\mathcal{M})$, in which case,

$$H \left(\sum_{j=1}^{\infty} a_j \Psi_j \right) = \sum_{j=1}^{\infty} \mathcal{E}_j a_j \Psi_j. \quad (2.18)$$

Proof. Firstly, given any $f \in \text{Dom}(H)$, write $f = \sum_{j=1}^{\infty} \langle f, \Psi_j \rangle \Psi_j$. Then

$$\begin{aligned} Hf &= \sum_{j=1}^{\infty} \langle Hf, \Psi_j \rangle \Psi_j = \sum_{j=1}^{\infty} \langle f, H\Psi_j \rangle \Psi_j = \sum_{j=1}^{\infty} \langle f, \mathcal{E}_j \Psi_j \rangle \Psi_j \\ &= \sum_{j=1}^{\infty} \mathcal{E}_j \langle f, \Psi_j \rangle \Psi_j. \end{aligned} \quad (2.19)$$

This proves that if $\sum_{j=1}^{\infty} a_j \Psi_j \in \text{Dom}(H)$ then $\sum_{j=1}^{\infty} \mathcal{E}_j a_j \Psi_j \in L^2(\mathcal{M})$, with (2.18) holding true.

Now write $f = \sum_{j=1}^{\infty} a_j \Psi_j$, $g = \sum_{j=1}^{\infty} \mathcal{E}_j a_j \Psi_j$, and assume $g \in L^2(\mathcal{M})$. Then $\sum_{j=1}^{\infty} \mathcal{E}_j^2 |a_j|^2$ converges, so $\sum_{j=1}^{\infty} |a_j|^2$ converges, and hence $f \in L^2(\mathcal{M})$ also. Next, take any $u = \sum_{j=1}^{\infty} b_j \Psi_j \in \text{Dom}(H)$. Then

$$\langle Hu, f \rangle = \sum_{j=1}^{\infty} (\mathcal{E}_j b_j) \bar{a}_j = \sum_{j=1}^{\infty} b_j (\overline{\mathcal{E}_j a_j}) = \langle u, g \rangle. \quad (2.20)$$

Hence $f \in \text{Dom}(H^*)$ with $H^* f = g$, and thus by self-adjointness of H , $f \in \text{Dom}(H)$ with $Hf = g$. \square

Observe that if we combine Lemma 2.1.1 with (2.17), also applying point (i) above in the description of the l^2 behaviour of $L^2(\mathcal{M})$, we obtain the following:

Corollary 2.1.2. *If \mathcal{M} is without boundary then*

$$C^\infty(\mathcal{M}) = \left\{ \sum_{j=1}^{\infty} a_j \Psi_j : \sum_{j=1}^{\infty} \mathcal{E}_j^n |a_j|^2 < \infty \forall n \in \mathbb{N} \cup \{0\} \right\}. \quad (2.21)$$

2.1.3 Resolvents of the Self-Adjoint minus-Laplacian Operator

Lemma 2.1.3. *For each $z \in \mathbb{C} \setminus \{\mathcal{E}_j\}_{j \in \mathbb{N}}$, the operator $H - z : \text{Dom}(H) \rightarrow L^2(\mathcal{M})$ is bijective and has a bounded inverse.*

Proof.

$$(H - z) \left(\sum_{j=1}^{\infty} a_j \Psi_j \right) = \sum_{j=1}^{\infty} (\mathcal{E}_j - z) a_j \Psi_j. \quad (2.22)$$

Clearly this operator is injective. Now take some $f = \sum_{j=1}^{\infty} a_j \Psi_j \in L^2(\mathcal{M})$, so $\sum_{j=1}^{\infty} |a_j|^2$ converges. It then follows that the following sum converges in \mathbb{R} :

$$\sum_{j=1}^{\infty} \left| \frac{\mathcal{E}_j a_j}{\mathcal{E}_j - z} \right|^2. \quad (2.23)$$

Hence the following sum converges in $L^2(\mathcal{M})$:

$$\sum_{j=1}^{\infty} \frac{\mathcal{E}_j a_j}{\mathcal{E}_j - z} \Psi_j. \quad (2.24)$$

Thus

$$\sum_{j=1}^{\infty} \frac{a_j}{\mathcal{E}_j - z} \Psi_j \in \text{Dom}(H), \quad (2.25)$$

and so

$$\begin{aligned} (H - z) \left(\sum_{j=1}^{\infty} \frac{a_j}{\mathcal{E}_j - z} \Psi_j \right) &= \sum_{j=1}^{\infty} \frac{(\mathcal{E}_j - z) a_j}{\mathcal{E}_j - z} \Psi_j = f \\ \therefore (H - z)^{-1} f &= \sum_{j=1}^{\infty} \frac{a_j}{\mathcal{E}_j - z} \Psi_j. \end{aligned} \quad (2.26)$$

This therefore proves bijectivity. Now the set $\{|1/(\mathcal{E}_j - z)|^2\}_{j \in \mathbb{N}}$ is bounded, and so let $B := \sup_{j \in \mathbb{N}} \{|1/(\mathcal{E}_j - z)|^2\}$. Then

$$\| (H - z)^{-1} f \|^2 = \sum_{j=1}^{\infty} \left| \frac{a_j}{\mathcal{E}_j - z} \right|^2 \leq \sum_{j=1}^{\infty} B |a_j|^2 = B \|f\|^2. \quad (2.27)$$

Hence the operator $(H - z)^{-1}$ is bounded. \square

The operator $(H - z)^{-1}$, for each $z \in \mathbb{C} \setminus \{\mathcal{E}_j\}_{j \in \mathbb{N}}$, is referred to as a *resolvent operator*. $\mathbb{C} \setminus \{\mathcal{E}_j\}_{j \in \mathbb{N}}$ is the *resolvent set* of H , and $\{\mathcal{E}_j\}_{j \in \mathbb{N}}$ is the *spectrum* of H , which shall be denoted $\text{Spec}(H)$.

2.1.4 Further Mathematical Tools

Spectral Projection

Given any set $S \subset \mathbb{R}$, define the *spectral projection operator* $\mathcal{P}_S^{(H)}$ by

$$\mathcal{P}_S^{(H)} f := \sum_{j: \mathcal{E}_j \in S} a_j \Psi_j = \sum_{j: \mathcal{E}_j \in S} \langle f, \Psi_j \rangle \Psi_j \quad \text{for } f = \sum_{j=1}^{\infty} a_j \Psi_j. \quad (2.28)$$

Lemma 2.1.4. *Let $\{\tilde{\Psi}_j\}_{j \in \mathbb{N}}$ be another orthonormal eigenbasis of H . Then letting $\tilde{\mathcal{P}}_S^{(H)}$ be the spectral projection operator defined with reference to the eigenbasis $\{\tilde{\Psi}_j\}_{j \in \mathbb{N}}$ rather than $\{\Psi_j\}_{j \in \mathbb{N}}$, it nevertheless holds that $\tilde{\mathcal{P}}_S^{(H)} = \mathcal{P}_S^{(H)}$.*

Proof. Firstly, we shall prove that for each $\mathcal{E} \in \text{Spec}(H)$, $\tilde{\mathcal{P}}_{\{\mathcal{E}\}}^{(H)} = \mathcal{P}_{\{\mathcal{E}\}}^{(H)}$. Let $\Lambda_{\mathcal{E}}^{(H)}$ be the \mathcal{E} -eigenspace of H , let $\{\psi_1, \dots, \psi_m\}$ be the orthonormal basis of $\Lambda_{\mathcal{E}}^{(H)}$ contained within $\{\Psi_j\}_{j \in \mathbb{N}}$, and let $\{\tilde{\psi}_1, \dots, \tilde{\psi}_m\}$ be the orthonormal basis of $\Lambda_{\mathcal{E}}^{(H)}$ contained within $\{\tilde{\Psi}_j\}_{j \in \mathbb{N}}$. Then for any $f \in L^2(\mathcal{M})$ we have

$$\mathcal{P}_{\{\mathcal{E}\}}^{(H)} f = \sum_{k=1}^m \left\langle \mathcal{P}_{\{\mathcal{E}\}}^{(H)} f, \tilde{\psi}_k \right\rangle \tilde{\psi}_k = \sum_{k=1}^m \left\langle \sum_{j=1}^m \langle f, \psi_j \rangle \psi_j, \tilde{\psi}_k \right\rangle \tilde{\psi}_k \in \Lambda_{\mathcal{E}}^{(H)}. \quad (2.29)$$

But

$$\begin{aligned} \left\langle \sum_{j=1}^m \langle f, \psi_j \rangle \psi_j, \tilde{\psi}_k \right\rangle &= \sum_{j=1}^m \langle f, \psi_j \rangle \langle \psi_j, \tilde{\psi}_k \rangle = \sum_{j=1}^m \langle f, \langle \tilde{\psi}_k, \psi_j \rangle \psi_j \rangle \\ &= \left\langle f, \sum_{j=1}^m \langle \tilde{\psi}_k, \psi_j \rangle \psi_j \right\rangle = \langle f, \tilde{\psi}_k \rangle. \end{aligned} \quad (2.30)$$

Hence

$$\mathcal{P}_{\{\mathcal{E}\}}^{(H)} f = \sum_{k=1}^m \langle f, \tilde{\psi}_k \rangle \tilde{\psi}_k = \tilde{\mathcal{P}}_{\{\mathcal{E}\}}^{(H)} f. \quad (2.31)$$

This proves that $\tilde{\mathcal{P}}_{\{\mathcal{E}\}}^{(H)} = \mathcal{P}_{\{\mathcal{E}\}}^{(H)}$ for each $\mathcal{E} \in \text{Spec}(H)$. But then for any $S \subset \mathbb{R}$, it is easy to see that

$$\mathcal{P}_S^{(H)} f = \sum_{\mathcal{E} \in S \cap \text{Spec}(H)} \mathcal{P}_{\{\mathcal{E}\}}^{(H)} f, \quad \tilde{\mathcal{P}}_S^{(H)} f = \sum_{\mathcal{E} \in S \cap \text{Spec}(H)} \tilde{\mathcal{P}}_{\{\mathcal{E}\}}^{(H)} f. \quad (2.32)$$

[If $S \cap \text{Spec}(H)$ is infinite, equivalently $\{j : \mathcal{E}_j \in S\}$ is infinite, then define these as limits of partial sums of terms arranged in order of increasing index j as in (2.28) for LHS(2.32), and increasing eigenvalue \mathcal{E} for RHS(2.32), in which case the sequence of partial sums for RHS(2.32) is a subsequence of that for LHS(2.32)].

Thus $\tilde{\mathcal{P}}_S^{(H)} f = \mathcal{P}_S^{(H)} f$. □

Order Relations

For two sequences (a_n) and (b_n) , define “ $a_n \ll b_n$ as $n \rightarrow \infty$ ” to hold true if

$$\exists M \in \mathbb{N}, C > 0 \text{ s.t. } |a_n| \leq C|b_n| \forall n \geq M. \quad (2.33)$$

If b_n is nonzero for all sufficiently large n , then this simply means that a_n/b_n is bounded for sufficiently large n .

Furthermore, for sequences (a_n) and (b_n) , define “ $a_n \ll\ll b_n$ as $n \rightarrow \infty$ ” to hold true if

$$\forall \varepsilon > 0 \exists N \in \mathbb{N} \text{ s.t. } |a_n| \leq \varepsilon|b_n| \forall n \geq N. \quad (2.34)$$

If b_n is nonzero for all sufficiently large n , this means that $a_n/b_n \rightarrow 0$.

Given a sequence (b_n) , the notation $O(b_n)$ appearing within an equation shall be used to stand for a sequence which is $\ll b_n$, for example, “ $x_n = y_n + O(b_n)$ as $n \rightarrow \infty$ ” would mean the same as “ $x_n - y_n \ll b_n$ as $n \rightarrow \infty$ ”. Likewise the notation $o(b_n)$ appearing within an equation shall be used to stand for a sequence which is $\ll\ll b_n$.

These notations can apply not only to sequences (i.e. functions on \mathbb{N}), but also for example, to functions of a real variable (say $f(x)$), where we could take $x \rightarrow \infty$, $x \rightarrow -\infty$ or $x \rightarrow a \in \mathbb{R}$ (taking either the two-sided limit or a one-sided limit).

Spectral Counting Function and Weyl’s Law

We introduce the *spectral counting function* $N : \mathbb{R} \rightarrow \mathbb{R}$ as follows:

$$N(E) := \#\{j : \mathcal{E}_j \leq E\}, \quad (2.35)$$

where $\#$ here is the notation we use for the number of elements in a set. For each $x \in \mathcal{M}^\circ$ there is also a corresponding variant of the spectral counting function:

$$N_x(E) := \sum_{j:\mathcal{E}_j \leq E} |\Psi_j(x)|^2. \quad (2.36)$$

For both N and N_x there is the following standard result, known as *Weyl’s law*:

Lemma 2.1.5 (Weyl’s law).

$$N(E) = \frac{\text{area}(\mathcal{M})}{4\pi} E + O(\sqrt{E}) \text{ as } E \rightarrow \infty, \quad (2.37)$$

$$N_x(E) = \frac{E}{4\pi} + O(\sqrt{E}) \text{ as } E \rightarrow \infty \quad \forall x \in \mathcal{M}^\circ. \quad (2.38)$$

(2.38) is sometimes referred to as a *local* Weyl law (later on, in Ch. 5, we introduce another “local Weyl law” for *pseudodifferential operators*).

Corollary 2.1.6. *For each $x \in \mathcal{M}^\circ$,*

$$N_x(E) = \frac{E}{4\pi} + o(E) \text{ as } E \rightarrow \infty, \quad (2.39)$$

equivalently

$$\frac{4\pi N_x(E)}{E} \rightarrow 1 \text{ as } E \rightarrow \infty, \quad (2.40)$$

equivalently

$$\forall \varepsilon > 0 \exists M \geq 0 \text{ s.t. } \forall E \geq M \quad \left(\frac{1}{4\pi} - \varepsilon\right) E \leq N_x(E) \leq \left(\frac{1}{4\pi} + \varepsilon\right) E. \quad (2.41)$$

These also hold for the spectral counting function N , only for each appearance of “ 4π ” in the denominator, “ $\text{area}(\mathcal{M})$ ” would also need to be inserted into the numerator, and likewise for the appearance of “ 4π ” in the numerator, “ $\text{area}(\mathcal{M})$ ” would also need to be inserted into the denominator.

Proof. According to Weyl’s law,

$$\exists L \geq 0, C > 0 \text{ s.t. } \left| N_x(E) - \frac{E}{4\pi} \right| \leq CE^{1/2} \quad \forall E \geq L, \quad (2.42)$$

but for each $\varepsilon > 0$ we have

$$CE^{1/2} \ll \varepsilon E \text{ as } E \rightarrow \infty, \quad (2.43)$$

and thus

$$\exists M_\varepsilon > 0 \text{ s.t. } \left| N_x(E) - \frac{E}{4\pi} \right| \leq \varepsilon E \quad \forall E \geq M_\varepsilon. \quad (2.44)$$

(2.44) here is a statement that $N_x(E) - \frac{E}{4\pi} \ll E$ as $E \rightarrow \infty$, which is a rearrangement of (2.39). (2.44) can also be re-expressed as

$$\left| \frac{4\pi N_x(E)}{E} - 1 \right| \leq 4\pi\varepsilon \quad \forall E \geq M_\varepsilon, \quad (2.45)$$

which in turn is an expression of (2.40). Finally, (2.44) can be re-expressed as

$$-\varepsilon E \leq N_x(E) - \frac{E}{4\pi} \leq \varepsilon E \quad \forall E \geq M_\varepsilon, \quad (2.46)$$

which in turn can be rearranged to give (2.41).

The same arguments work with $N(E)$ as well, starting from (2.37). \square

Corollary 2.1.6 is basically a weaker version of Weyl's law, which can still be useful.

Now we shall also define N^- and N_x^- as follows:

$$N^-(E) := \#\{j : \mathcal{E}_j < E\}, \quad (2.47)$$

$$N_x^-(E) := \sum_{j:\mathcal{E}_j < E} |\Psi_j(x)|^2. \quad (2.48)$$

Thus N^- and N_x^- are left-continuous functions at eigenvalues of H , while N and N_x are right-continuous functions at eigenvalues of H . Lemma 2.1.5 and Corollary 2.1.6 then of course apply to N^- and N_x^- as well as N and N_x .

Sum to Integral Conversion

Lemma 2.1.7. *Let $a, b \in \mathbb{R}$ with $a < b$, let f be a continuously differentiable function on $[a, b]$ and let $x \in \mathcal{M}^\circ$. Then*

$$\sum_{j:a \leq \mathcal{E}_j \leq b} f(\mathcal{E}_j) |\Psi_j(x)|^2 = f(b)N_x(b) - f(a)N_x^-(a) - \int_a^b f'(t)N_x(t)dt. \quad (2.49)$$

Furthermore, let $c \in \mathbb{R}$ and let g be a continuously differentiable function on $[c, \infty)$. In the following equation:

$$\sum_{j:\mathcal{E}_j \geq c} g(\mathcal{E}_j) |\Psi_j(x)|^2 = \lim_{s \rightarrow \infty} g(s)N_x(s) - g(c)N_x^-(c) - \int_c^\infty g'(t)N_x(t)dt, \quad (2.50)$$

if any two of the above three limits to infinity converge, then the third limit also converges and the equation holds true.

These above statements also hold true if the appearances of “ $f(\mathcal{E}_j)|\Psi_j(x)|^2$ ”, “ $g(\mathcal{E}_j)|\Psi_j(x)|^2$ ”, “ N_x ” and “ N_x^- ” are replaced with “ $f(\mathcal{E}_j)$ ”, “ $g(\mathcal{E}_j)$ ”, “ N ” and “ N^- ” respectively.

Remark. In (2.50) we simply take \int_c^∞ to mean $\lim_{s \rightarrow \infty} \int_c^s$, similarly with $\sum_{\mathcal{E}_j \geq c}$.

Proof. Converting the following sum into a Riemann-Stieltjes integral and then applying integration by parts:

$$\begin{aligned} \sum_{j:a < \mathcal{E}_j \leq b} f(\mathcal{E}_j) |\Psi_j(x)|^2 &= \int_a^b f(t) dN_x(t) = f(b)N_x(b) - f(a)N_x(a) - \int_a^b N_x(t) df(t) \\ &= f(b)N_x(b) - f(a)N_x(a) - \int_a^b f'(t)N_x(t)dt. \end{aligned} \quad (2.51)$$

[Note that in the left-hand side of the above equation, the sum is over $a < \mathcal{E}_j \leq b$, not $a \leq \mathcal{E}_j \leq b$]. If a does not coincide with any eigenvalue of H then the left-hand sides

of equations (2.49) and (2.51) are equal, and so are the right-hand sides, thus proving (2.49) in this case. If a does coincide with an eigenvalue \mathcal{E}_k , then

$$\begin{aligned} \sum_{j:a \leq \mathcal{E}_j \leq b} f(\mathcal{E}_j) |\Psi_j(x)|^2 &= f(b)N_x(b) - f(a)N_x(a) + f(a)|\Psi_k(x)|^2 - \int_a^b f'(t)N_x(t)dt \\ &= f(b)N_x(b) - f(a)N_x^-(a) - \int_a^b f'(t)N_x(t)dt. \end{aligned} \quad (2.52)$$

This proves the first part of the lemma. The second part then follows by the algebra of limits.

The last statement in this lemma follows by the same arguments as above, simply replacing the role of “ $|\Psi_j(x)|^2$ ” with the number 1. \square

2.2 The Delta-Perturbed Quantum System

2.2.1 Introduction of the Delta Perturbation

We now perturb the quantum system by adding a *point scatterer / delta potential* at some point $p \in \mathcal{M}^\circ$. The perturbed operator H' is introduced formally as

$$H' = -\Delta + c\delta_p, \quad (2.53)$$

where δ_p is the Dirac delta function with spike at p .

Observe that for a function ϕ on \mathcal{M} which is continuous at p , we can formally write

$$\phi\delta_p = \phi(p)\delta_p = \left(\int_{\mathcal{M}} \phi\delta_p \right) \delta_p = \langle \phi, \delta_p \rangle_{ll} \delta_p, \quad (2.54)$$

and also

$$\phi\delta_p = \phi(p)\delta_p = \left(\int_{\mathcal{M}} \overline{\phi}\delta_p \right) \delta_p = \left(\int_{\mathcal{M}} \phi\overline{\delta_p} \right) \delta_p = \langle \phi, \delta_p \rangle_{lc} \delta_p. \quad (2.55)$$

The subscript ll here means linearity in both arguments as before, and subscript lc means linearity in the first argument and conjugate-linearity in the second argument. Thus we could also formally express the perturbed operator as

$$H' = -\Delta + c\langle \cdot, \delta_p \rangle_{ll} \delta_p = -\Delta + c\langle \cdot, \delta_p \rangle_{lc} \delta_p. \quad (2.56)$$

Observe furthermore that by (2.54)/(2.55), if $\phi(p) = 0$ then $\phi\delta_p = 0$. Thus we can expect that if $\phi \in \text{Dom}(H) \cap \text{Dom}(H')$ and $\phi(p) = 0$ then $H'\phi = H\phi$.

For the rigorous construction of the perturbed operator H' , the requirements we shall specify are

- (i) H' is a self-adjoint operator acting within $L^2(\mathcal{M})$,
- (ii) if $\phi \in \text{Dom}(H)$ and $\phi(p) = 0$ then $\phi \in \text{Dom}(H')$ and $H'\phi = H\phi$.

Although in (2.53) there is the appearance of the parameter c , for the rigorous construction, rather than giving a construction of the operator H' which is dependent on the parameter c , instead we more loosely let the family of all operators satisfying (i) and (ii) above be the rigorously defined family of operators we shall work with, in place of the formally introduced family of operators given by (2.53), “defined” over all $c \in \mathbb{R}$. We do not have any a priori correspondence between the rigorously defined operators and the parameter c , other than $c = 0$ corresponding to the original unperturbed operator H .

Let

$$\mathcal{D}_p := \{\phi \in \text{Dom}(H) : \phi(p) = 0\}, \quad (2.57)$$

and let H_p be the restriction of H to \mathcal{D}_p . We are interested then in the family of self-adjoint extensions of the operator H_p . Trivially H is itself one of these self-adjoint extensions.

As it turns out, \mathcal{D}_p is dense in $L^2(\mathcal{M})$, so H_p has a well-defined adjoint H_p^* , and since H_p is obviously a symmetric operator, it follows that H_p^* is an extension of H . Furthermore, H_p has both *deficiency indices* being 1, where the deficiency indices are defined as the dimensions of the kernels of $H_p^* - i$ and $H_p^* + i$. In other words then, i and $-i$ are both eigenvalues of H_p^* with 1-dimensional corresponding eigenspaces. $\text{Ker}(H_p^* - i)$ and $\text{Ker}(H_p^* + i)$ are referred to as *deficiency subspaces* of H_p .

The von Neumann theory of self-adjoint extensions (see §X.1 of [RS75]) then yields the result that H_p has a family of self-adjoint extensions given by a single angle-like parameter (angle-like in the sense that it is a real-valued parameter except adding 2π has no effect).

Note that for any self-adjoint extension H' of H_p , since $H_p \subset H'$ it follows that $H' = H'^* \subset H_p^*$, where \subset appearing between two operators means that the operator to the left is a restriction of the operator to the right. Thus every self-adjoint extension of H_p is also a self-adjoint restriction of H_p^* . Conversely, if \tilde{H} is a self-adjoint restriction of H_p^* then $H_p^{**} \subset \tilde{H}^* = \tilde{H}$, but H_p^{**} is the closure of H_p (see Thm. VIII.1 in §VIII.1 of [RS80]), and thus \tilde{H} is also a self-adjoint extension of H_p . We also see here that every self-adjoint extension of H_p , equivalently every self-adjoint restriction of H_p^* , is also an extension of the *closure* of H_p .

Now the graph of H is a linear subspace of $L^2(\mathcal{M}) \times L^2(\mathcal{M})$, and the norm given by (2.12) restricted to the graph of H induces a norm on $\text{Dom}(H)$ via the linear isomorphism

$u \in \text{Dom}(H) \mapsto (u, Hu)$, which shall be referred to as the *graph norm* of H . So then, denoting this graph norm $\|\cdot\|_H$,

$$\|u\|_H = \sqrt{\|u\|^2 + \|Hu\|^2} \quad \forall u \in \text{Dom}(H). \quad (2.58)$$

Given that H_p has dense domain in $L^2(\mathcal{M})$, and that H_p has self-adjoint extensions beside H , the following must then hold:

Lemma 2.2.1. *The linear functional $\phi \mapsto \phi(p)$ on $\text{Dom}(H)$ is bounded with respect to the graph norm of H .*

Proof. Firstly, in order for H_p to have any self-adjoint extension beside H , we cannot have the closure of H_p being H , since if it is, then any self-adjoint extension of H_p must also be an extension of H , and at the same time a restriction of $H_p^* = H^* = H$ (see Thm. VIII.1 in §VIII.1 of [RSS0]). Thus the only possible self-adjoint extension of H_p would be H .

Now H , being a self-adjoint extension of H_p , must then be an extension of the closure of H_p , and so in order for H_p to have any self-adjoint extension beside H , the closure of H_p must be a *proper* restriction of H .

Considering now the linear functional $(\phi, H\phi) \mapsto \phi(p)$ on the graph of H , the graph of H_p is then the kernel of this linear functional. Since this linear functional is nonzero, so its kernel is not the whole of its domain, either

- (i) this functional is bounded with respect to the norm given by (2.12) restricted to the graph of H , in which case its kernel is a closed subset of its domain (i.e. the graph of H_p is closed in the graph of H), or
- (ii) this functional is unbounded, in which case its kernel is a dense subset of its domain (i.e. the graph of H_p is dense in the graph of H).

See for example Thm. 1.7.15 and Prop. 1.7.16 in §1.7 of [Meg98] for justification of this.

However, if the graph of H_p is dense in the graph of H , this means that the closure of H_p is H , which has been ruled out if H_p is to have any self-adjoint extension beside H . The only option then is that the linear functional is bounded.

Finally, boundedness of the linear functional $(\phi, H\phi) \mapsto \phi(p)$ on the graph of H with respect to the norm given by (2.12) restricted to the graph of H , is equivalent to boundedness of the linear functional $\phi \mapsto \phi(p)$ on $\text{Dom}(H)$ with respect to the norm given by (2.58). \square

The fact that Lemma 2.2.1 would follow from H_p having dense domain and self-adjoint extensions beside H , is in agreement with statements made in §1.2.1 and 1.2.3 of [AK00]. Ch. 1 of [AK00] which deals with a more general theory of singular rank one perturbations of self-adjoint operators.

Now one property of adjoint operators is that they are always closed operators (see again Thm. VIII.1 in §VIII.1 of [RS80]), meaning that the graph is closed, and so in particular, self-adjoint operators are always closed. So then, the graph of H is closed in $L^2(\mathcal{M}) \times L^2(\mathcal{M})$, but then the proof of Lemma 2.2.1 also reveals that the graph of H_p is closed in the graph of H . Thus the graph of H_p is also closed in $L^2(\mathcal{M}) \times L^2(\mathcal{M})$ (this follows from basic topology / metric space theory), and so H_p is a closed operator. The closure of H_p is therefore just H_p itself.

Corollary 2.2.2. *If $f = \sum_{j=1}^{\infty} a_j \Psi_j \in \text{Dom}(H)$ then $f(p) = \sum_{j=1}^{\infty} a_j \Psi_j(p)$.*

Proof. Let $f_n := \sum_{j=1}^n a_j \Psi_j$ for each $n \in \mathbb{N}$, so $f_n \xrightarrow{n \rightarrow \infty} f$. Then $Hf_n = \sum_{j=1}^n \mathcal{E}_j a_j \Psi_j$, and furthermore, according to Lemma 2.1.1, $Hf = \sum_{j=1}^{\infty} \mathcal{E}_j a_j \Psi_j$. Thus $Hf_n \xrightarrow{n \rightarrow \infty} Hf$. We therefore have $\|f_n - f\| \xrightarrow{n \rightarrow \infty} 0$ and $\|H(f_n - f)\| \xrightarrow{n \rightarrow \infty} 0$, and so

$$\|f_n - f\|_H = \sqrt{\|f_n - f\|^2 + \|H(f_n - f)\|^2} \xrightarrow{n \rightarrow \infty} 0. \quad (2.59)$$

Thus $f_n \xrightarrow{n \rightarrow \infty} f$ under the graph norm of H , and so since the linear functional $\phi \mapsto \phi(p)$ is bounded and therefore continuous on $\text{Dom}(H)$ under this graph norm, it follows that

$$f(p) = \lim_{n \rightarrow \infty} f_n(p) = \sum_{j=1}^{\infty} a_j \Psi_j(p). \quad (2.60)$$

□

Since then, we formally have

$$f(p) = \langle f, \delta_p \rangle_{lc} = \sum_{j=1}^{\infty} a_j \Psi_j(p) \quad \forall f = \sum_{j=1}^{\infty} a_j \Psi_j \in \text{Dom}(H) \quad (2.61)$$

(see (2.55)), we can therefore formally write (given the formula for inner product in terms of orthonormal basis expansion)

$$\delta_p = \sum_{j=1}^{\infty} \overline{\Psi_j(p)} \Psi_j. \quad (2.62)$$

This also makes sense given the formula for the coefficients in an orthonormal basis expansion, since we have $\langle \delta_p, \Psi_j \rangle_{lc} = \overline{\langle \Psi_j, \delta_p \rangle_{lc}} = \overline{\Psi_j(p)}$.

We can likewise then also define, given a set $S \subset \mathbb{R}$,

$$\mathcal{P}_S^{(H)} \delta_p := \sum_{j: \mathcal{E}_j \in S} \overline{\Psi_j(p)} \Psi_j. \quad (2.63)$$

In general, this may or may not converge in $L^2(\mathcal{M})$, depending on the set S . However, this will obviously be in $L^2(\mathcal{M})$, and also in $\text{Dom}(H)$, if S is a bounded set, or more generally if $\#\{j : \mathcal{E}_j \in S\}$ is finite.

Lemma 2.2.3. *Like $\mathcal{P}_S^{(H)} f$ for $f \in L^2(\mathcal{M})$, $\mathcal{P}_S^{(H)} \delta_p$ is also independent of choice of orthonormal eigenbasis of H .*

This can be proved by similar method to the proof of Lemma 2.1.4.

Corollary 2.2.4. *Letting $\{\Psi_j\}_{j \in \mathbb{N}}$ and $\{\tilde{\Psi}_j\}_{j \in \mathbb{N}}$ be two orthonormal eigenbases of H , for each $\mathcal{E} \in \text{Spec}(H)$ we have*

$$\sum_{j: \mathcal{E}_j = \mathcal{E}} |\Psi_j(p)|^2 = \sum_{j: \mathcal{E}_j = \mathcal{E}} |\tilde{\Psi}_j(p)|^2 = \|\mathcal{P}_{\{\mathcal{E}\}}^{(H)} \delta_p\|^2. \quad (2.64)$$

2.2.2 Green's Functions

For each $z \in \mathbb{C} \setminus \{\mathcal{E}_j\}_{j \in \mathbb{N}}$, we have from Lemma 2.1.3 that the operator $(H - z)^{-1} : L^2(\mathcal{M}) \rightarrow \text{Dom}(H)$ is a well-defined bounded operator. We can then consider the linear functional $\sigma_{p,z} : L^2(\mathcal{M}) \rightarrow \mathbb{C}$ given by

$$\sigma_{p,z} f := (H - z)^{-1} f(p) = \sum_{j=1}^{\infty} \frac{a_j}{\mathcal{E}_j - z} \Psi_j(p) \quad \forall f = \sum_{j=1}^{\infty} a_j \Psi_j \in L^2(\mathcal{M}). \quad (2.65)$$

So then, letting $\hat{\delta}_p$ be the linear functional $\phi \in \text{Dom}(H) \mapsto \phi(p)$, we have

$$\sigma_{p,z} = \hat{\delta}_p \circ (H - z)^{-1}. \quad (2.66)$$

Note that while $(H - z)^{-1}$ is a bounded operator, $\hat{\delta}_p$ is an unbounded linear functional, and so we can still consider the question of whether $\sigma_{p,z}$ is a bounded or unbounded linear functional.

Formally writing

$$\sigma_{p,z} f = \left\langle f, \sum_{j=1}^{\infty} \frac{\overline{\Psi_j(p)}}{\mathcal{E}_j - \bar{z}} \Psi_j \right\rangle, \quad (2.67)$$

does the sum in the second part of the above formal inner product converge in $L^2(\mathcal{M})$?

Lemma 2.2.5. For every $z \in \mathbb{C}$, if we take some $c \in \mathbb{R}$ for which $z \notin [c, \infty) \cap \{\mathcal{E}_j\}_{j \in \mathbb{N}}$ then

$$\sum_{j: \mathcal{E}_j \geq c} \frac{|\Psi_j(p)|^2}{|\mathcal{E}_j - z|^2} \quad (2.68)$$

is a convergent sum.

Proof. Let $z = r + is$ with $r, s \in \mathbb{R}$. Then taking some $c' > \max\{c, r\}$, we have

$$\begin{aligned} \sum_{j: \mathcal{E}_j \geq c} \frac{|\Psi_j(p)|^2}{|\mathcal{E}_j - z|^2} &= \sum_{j: \mathcal{E}_j \geq c} \frac{|\Psi_j(p)|^2}{(\mathcal{E}_j - r)^2 + s^2} \\ &\leq \sum_{j: c \leq \mathcal{E}_j < c'} \frac{|\Psi_j(p)|^2}{(\mathcal{E}_j - r)^2 + s^2} + \sum_{j: \mathcal{E}_j \geq c'} \frac{|\Psi_j(p)|^2}{(\mathcal{E}_j - r)^2} \\ &= \sum_{j: c \leq \mathcal{E}_j < c'} \frac{|\Psi_j(p)|^2}{(\mathcal{E}_j - r)^2 + s^2} + \lim_{t \rightarrow \infty} \frac{N_p(t)}{(t - r)^2} - \frac{N_p^-(c')}{(c' - r)^2} \\ &\quad + 2 \int_{c'}^{\infty} \frac{N_p(t)}{(t - r)^3} dt \end{aligned} \quad (2.69)$$

by Lemma 2.1.7. Wishing to show then that the two limits in the last part of the above equation are convergent, taking some $A > \frac{1}{4\pi}$ and applying Corollary 2.1.6, for sufficiently large t we have

$$0 < \frac{N_p(t)}{(t - r)^2} \leq \frac{At}{(t - r)^2} = \frac{A}{t - r} + \frac{Ar}{(t - r)^2} \xrightarrow{t \rightarrow \infty} 0. \quad (2.70)$$

Furthermore, for sufficiently large M ,

$$\int_M^{\infty} \frac{N_p(t)}{(t - r)^3} dt \leq A \int_M^{\infty} \frac{t}{(t - r)^3} dt. \quad (2.71)$$

Now for any $a, b \in \mathbb{R}$ with $a < b$ and $r \notin [a, b]$, we have

$$\begin{aligned} \int_a^b \frac{t}{(t - r)^3} dt &= \int_{a-r}^{b-r} \left(\frac{1}{\tau^2} + \frac{r}{\tau^3} \right) d\tau \\ &= -\frac{1}{b-r} - \frac{r}{2(b-r)^2} + \frac{1}{a-r} + \frac{r}{2(a-r)^2}. \end{aligned} \quad (2.72)$$

Thus

$$\begin{aligned} \int_M^{\infty} \frac{t}{(t - r)^3} dt &= \lim_{T \rightarrow \infty} \left(-\frac{1}{T-r} - \frac{r}{2(T-r)^2} + \frac{1}{M-r} + \frac{r}{2(M-r)^2} \right) \\ &= \frac{1}{M-r} + \frac{r}{2(M-r)^2}. \end{aligned} \quad (2.73)$$

It therefore follows that the two limits in the last part of (2.69) are indeed convergent, and hence the sum in (2.68) is a convergent sum. \square

We can thus conclude that the sum in the second part of the inner product in (2.67) does indeed converge in $L^2(\mathcal{M})$. It also follows then that $\sigma_{p,z}$ is a bounded linear functional. Another approach one might consider for proving $\sigma_{p,z}$ to be bounded is to show that $(H - z)^{-1}$ is a bounded operator from $L^2(\mathcal{M})$ under the usual L^2 -norm to $\text{Dom}(H)$ under the graph norm of H , and then use the boundedness of $\hat{\delta}_p$ on $\text{Dom}(H)$ under the graph norm to deduce that $\sigma_{p,z} = \hat{\delta}_p \circ (H - z)^{-1}$ is a bounded functional. It would then follow from the Riesz representation theorem that $\sigma_{p,z}$ is expressible as an operation taking inner product with some particular function in $L^2(\mathcal{M})$.

Now define $g_z \in L^2(\mathcal{M})$ to be the complex conjugate of the function in the second part of the inner product in (2.67), so

$$\langle f, g_z \rangle_u = \sigma_{p,z} f \quad \forall f \in L^2(\mathcal{M}). \quad (2.74)$$

Then

$$g_z = \sum_{j=1}^{\infty} \langle g_z, \Psi_j \rangle \Psi_j = \sum_{j=1}^{\infty} (\sigma_{p,z} \overline{\Psi_j}) \Psi_j = \sum_{j=1}^{\infty} \frac{\overline{\Psi_j(p)}}{\mathcal{E}_j - z} \Psi_j \quad (2.75)$$

(noting that $(H - z)\overline{\Psi_j} = -\Delta \overline{\Psi_j} - z\overline{\Psi_j} = \overline{-\Delta \Psi_j - z\Psi_j} = \overline{\mathcal{E}_j \Psi_j - z\Psi_j} = (\mathcal{E}_j - z)\overline{\Psi_j}$, so $(H - z)^{-1}\overline{\Psi_j} = (\mathcal{E}_j - z)^{-1}\overline{\Psi_j}$). Hence $\overline{g_z} = g_{\bar{z}}$.

This function g_z is the function $G_z(p, \cdot) = G_z(\cdot, p)$, where $G_z(\cdot, \cdot)$ is the *Green's function* associated with the resolvent operator $(H - z)^{-1}$. Both arguments of $G_z(\cdot, \cdot)$ are positions on \mathcal{M} .

Deriving some further properties of g_z , observe that for every $u \in \text{Dom}(H)$,

$$\begin{aligned} u(p) &= \langle (H - z)u, g_z \rangle_u = \langle Hu, g_z \rangle_u - z \langle u, g_z \rangle_u \\ \Rightarrow \langle Hu, g_z \rangle_u &= \langle u, zg_z \rangle_u + u(p) = \langle u, zg_z + \delta_p \rangle_u. \end{aligned} \quad (2.76)$$

Since H is an extension of the operator $-\Delta$ on $C_0^\infty(\mathcal{M}^\circ)$, it follows that in the distributional sense, we have

$$-\Delta g_z = zg_z + \delta_p. \quad (2.77)$$

Furthermore, taking any $s, z \in \mathbb{C} \setminus \{\mathcal{E}_j\}_{j \in \mathbb{N}}$,

$$\begin{aligned} \langle Hu, g_z - g_s \rangle &= \langle Hu, g_{\bar{z}} \rangle_u - \langle Hu, g_{\bar{s}} \rangle_u = \langle u, \bar{z}g_{\bar{z}} \rangle_u + u(p) - \langle u, \bar{s}g_{\bar{s}} \rangle_u - u(p) \\ &= \langle u, zg_z - sg_s \rangle \quad \forall u \in \text{Dom}(H). \end{aligned} \quad (2.78)$$

Thus by self-adjointness of H , $g_z - g_s \in \text{Dom}(H)$ with

$$H(g_z - g_s) = zg_z - sg_s. \quad (2.79)$$

Now if we take any open $X \subset \mathcal{M}^\circ \setminus \{p\}$, and let $g_z^{(X)}$ be the restriction of g_z to X , then we have

$$\int_X (-\Delta u) g_z^{(X)} = \int_{\mathcal{M}} (Hu) g_z = \int_{\mathcal{M}} u(zg_z) \quad \forall u \in C_0^\infty(X), \quad (2.80)$$

where u is extended to the whole of \mathcal{M} by simply having it be zero everywhere outside X . Thus $-\Delta g_z^{(X)} = zg_z^{(X)}$ in the distributional sense, also meaning then that $(-\Delta)^n g_z^{(X)} = z^n g_z^{(X)} \quad \forall n \in \mathbb{N}$. By the Sobolev embedding theorem it then follows that g_z is C^∞ -smooth on $\mathcal{M}^\circ \setminus \{p\}$ with $-\Delta g_z = zg_z$.

Furthermore, in the case where $\mathcal{M} \subset \mathbb{R}^2$, letting

$$h(x) := -\frac{1}{2\pi} \ln \|x - p\| \quad \forall x \in \mathcal{M}^\circ \setminus \{p\}, \quad (2.81)$$

it is the case that $h \in L^2(\mathcal{M})$, and there is a standard result that

$$-\Delta h = \delta_p. \quad (2.82)$$

Thus $g_z - h \in L^2(\mathcal{M})$ and

$$-\Delta(g_z - h) = zg_z + \delta_p - \delta_p = zg_z \in L^2(\mathcal{M}). \quad (2.83)$$

The Sobolev embedding theorem then yields that $g_z - h \in C(\mathcal{M}^\circ)$, and so

$$g_z(x) = -\frac{1}{2\pi} \ln \|x - p\| + c_{p,z} + o(1) \quad \text{as } x \rightarrow p, \quad (2.84)$$

where $c_{p,z} \in \mathbb{C}$ is a constant (namely the value of $g_z - h$ at p). (2.84) also extends to the case where \mathcal{M} more generally is a 2D Riemannian manifold, only replacing “ $\|x - p\|$ ” with the geodesic distance between x and p .

Finally, another property is that g_z satisfies the boundary conditions (Dirichlet) for functions in $\text{Dom}(H)$ if there is a boundary. In other words, if $\chi \in C_0^\infty(\mathcal{M}^\circ)$ and $\chi = 1$ on a neighbourhood of p then $(1 - \chi)g_z \in \text{Dom}(H)$.

2.2.3 Action of the Delta-Perturbed Operators

Stating the action of the adjoint H_p^* of H_p , and of the self-adjoint extensions $\{H_\Theta : \Theta \in [0, 2\pi)\}$ of H_p (see e.g. [KMW10]),

$$\text{Dom}(H_p^*) = \mathcal{D}_p \oplus \text{span}\{g_i, g_{-i}\}, \quad (2.85)$$

$$H_p^*(\psi + a_+g_i + a_-g_{-i}) = H_p\psi + a_+ig_i - a_-ig_{-i} \quad \forall \psi \in \mathcal{D}_p, \quad a_+, a_- \in \mathbb{C}. \quad (2.86)$$

H_Θ is then the restriction of H_p^* to

$$\text{Dom}(H_\Theta) = \mathcal{D}_p \oplus \text{span}\{g_i - e^{i\Theta}g_{-i}\}. \quad (2.87)$$

Lemma 2.2.6. $H_0 = H$.

Proof. Observe firstly from (2.79) that $g_i - g_{-i} \in \text{Dom}(H)$, with

$$H(g_i - g_{-i}) = ig_i + ig_{-i} = H_p^*(g_i - g_{-i}). \quad (2.88)$$

Thus given any $\psi = \psi_p + a(g_i - g_{-i}) \in \text{Dom}(H_0)$, with $\psi_p \in \mathcal{D}_p$ and $a \in \mathbb{C}$,

$$H_0\psi = H_p\psi_p + ai(g_i + g_{-i}) = H\psi_p + aH(g_i - g_{-i}) = H\psi. \quad (2.89)$$

This so far proves at least that H_0 is a restriction of H .

Now

$$g_i - g_{-i} = \sum_{j=1}^{\infty} \left(\frac{\overline{\Psi_j(p)}}{\mathcal{E}_j - i} - \frac{\overline{\Psi_j(p)}}{\mathcal{E}_j + i} \right) \Psi_j = 2i \sum_{j=1}^{\infty} \frac{\overline{\Psi_j(p)}}{\mathcal{E}_j^2 + 1} \Psi_j, \quad (2.90)$$

and so by Corollary 2.2.2,

$$(g_i - g_{-i})(p) = 2i \sum_{j=1}^{\infty} \frac{|\Psi_j(p)|^2}{\mathcal{E}_j^2 + 1}. \quad (2.91)$$

Since it must hold that $\exists j \in \mathbb{N}$ for which $|\Psi_j(p)|^2 \neq 0$ (otherwise $N_p(E) = 0 \forall E$, which would violate Weyl's law), it follows then that $(g_i - g_{-i})(p) \neq 0$.

Given any $\psi \in \text{Dom}(H)$, letting

$$\psi_p := \psi - \frac{\psi(p)}{(g_i - g_{-i})(p)}(g_i - g_{-i}), \quad (2.92)$$

it follows that $\psi_p \in \text{Dom}(H)$ and $\psi_p(p) = 0$, so $\psi_p \in \mathcal{D}_p$, and thus $\psi \in \text{Dom}(H_0)$. Hence H and H_0 have the same domain, and perform the same operation. \square

Note that the decomposition of any $\psi \in \text{Dom}(H_p^*)$ into the form $\psi = \psi_p + a_+g_i + a_-g_{-i}$, with $\psi_p \in \mathcal{D}_p$, $a_+, a_- \in \mathbb{C}$, is unique. In particular then, for any $\Theta_1, \Theta_2 \in [0, 2\pi)$ with $\Theta_1 \neq \Theta_2$,

$$\text{Dom}(H_{\Theta_1}) \cap \text{Dom}(H_{\Theta_2}) = \mathcal{D}_p. \quad (2.93)$$

Observe that for each $\Theta \in (0, 2\pi)$ (so excluding $\Theta = 0$), every member of $\text{Dom}(H_{\Theta}) \setminus \mathcal{D}_p$ has a logarithmic singularity at p , since by (2.84),

$$(g_i - e^{i\Theta}g_{-i})(x) = \frac{e^{i\Theta} - 1}{2\pi} \ln d_{\mathcal{M}}(x, p) + c_{p,i} - e^{i\Theta}c_{p,-i} + o(1) \quad \text{as } x \rightarrow p, \quad (2.94)$$

where $d_{\mathcal{M}}(\cdot, \cdot)$ denotes geodesic distance between two points on \mathcal{M} . Observe that (2.94) also holds for $\Theta = 0$, yielding

$$c_{p,i} - c_{p,-i} = (g_i - g_{-i})(p) = 2i \sum_{j=1}^{\infty} \frac{|\Psi_j(p)|^2}{\mathcal{E}_j^2 + 1}. \quad (2.95)$$

With H_0 being the unperturbed operator H , the delta perturbed operator H' can be taken to be any H_{Θ} with $\Theta \in (0, 2\pi)$.

2.2.4 Observations on the Strength of the Delta Potential

In a 1-dimensional setting, the operators representing the delta potential can indeed be expressed in the form $-\frac{d^2}{dx^2} + c\delta_p$, with well-defined $c \in \mathbb{R}$ (except one operator effectively corresponding to $c = \pm\infty$). There are effectively boundary conditions at p , consisting of continuity at p but a discontinuity in the derivative at p , whereby the ratio between the value at p and the difference in left-sided and right-sided derivatives at p is determined by the strength c .

Concerning the delta potential in the 2-dimensional setting that we are interested in, observe that we have the following:

Proposition 2.2.7.

$$H_p^* \psi = -\Delta \psi + \left(\lim_{x \rightarrow p} \frac{2\pi \psi(x)}{\ln d_{\mathcal{M}}(x, p)} \right) \delta_p \quad \forall \psi \in \text{Dom}(H_p^*). \quad (2.96)$$

Proof. Given any $\psi \in \text{Dom}(H_p^*)$, writing $\psi = \psi_p + a_+ g_i + a_- g_{-i}$ with $\psi_p \in \mathcal{D}_p$, a_+ , $a_- \in \mathbb{C}$, we have by (2.77),

$$-\Delta \psi = H_p \psi + a_+(ig_i + \delta_p) + a_-(-ig_{-i} + \delta_p), \quad (2.97)$$

so

$$H_p^* \psi = -\Delta \psi - (a_+ + a_-)\delta_p. \quad (2.98)$$

But furthermore by (2.84),

$$\psi(x) = -\frac{a_+ + a_-}{2\pi} \ln d_{\mathcal{M}}(x, p) + a_+ c_{p,i} + a_- c_{p,-i} + o(1) \quad \text{as } x \rightarrow p, \quad (2.99)$$

so dividing through by $\frac{1}{2\pi} \ln d_{\mathcal{M}}(x, p)$ and noting that $\lim_{x \rightarrow p} \frac{1}{\ln d_{\mathcal{M}}(x, p)} = 0$,

$$\lim_{x \rightarrow p} \frac{2\pi \psi(x)}{\ln d_{\mathcal{M}}(x, p)} = -(a_+ + a_-). \quad (2.100)$$

Combining (2.98) and (2.100) then gives (2.96). \square

In light of this, let V_p be a function on \mathcal{M} for which on a neighbourhood of p , $V_p(x) = \frac{2\pi}{\ln d_{\mathcal{M}}(x, p)}$. We can then formally express (2.96) as follows:

$$H_p^* \psi = -\Delta \psi + (\psi V_p) \delta_p. \quad (2.101)$$

Now note that V_p is continuous at p with $V_p(p) = 0$, and that V_p is negative on a punctured neighbourhood of p . This would then mean that formally, $V_p \delta_p = 0$, and so $\psi(V_p \delta_p) = 0$. Nevertheless, $(\psi V_p) \delta_p$ may be nonzero due to a logarithmic singularity at p . Thus we effectively have a violation of the associative law, which is already a recognised phenomenon with multiplication involving distributions (see e.g. [Raj82] or §1.2 in [TK05]).

Consideration of Quadratic Form Representation

One approach that could be attempted for associating the operators H_Θ with values for the strength of the delta potential is to consider the representation of self-adjoint operators by *quadratic forms* (for general theory on this, see e.g. §VIII.6 in [RS80] and Ch. X in [RS75] or Lec. 7 in [Del15]).

Consider the operator \sqrt{H} , which can be defined as follows: \sqrt{H} is the self-adjoint operator with orthonormal eigenbasis $\{\Psi_j\}_{j \in \mathbb{N}}$ and respective corresponding eigenvalues $\{\sqrt{\mathcal{E}_j}\}_{j \in \mathbb{N}}$. By the same arguments as in the proof of Lemma 2.1.1, we have

$$\sum_{j=1}^{\infty} a_j \Psi_j \in \text{Dom}(\sqrt{H}) \quad \text{iff} \quad \sum_{j=1}^{\infty} \sqrt{\mathcal{E}_j} a_j \Psi_j \in L^2(\mathcal{M}), \quad (2.102)$$

$$\sqrt{H} \left(\sum_{j=1}^{\infty} a_j \Psi_j \right) = \sum_{j=1}^{\infty} \sqrt{\mathcal{E}_j} a_j \Psi_j. \quad (2.103)$$

The quadratic form $(\cdot, \cdot)_H$ associated with the operator H is then given by the following:

$$\begin{aligned} (\phi, \psi)_H &= \left\langle \sqrt{H}\phi, \sqrt{H}\psi \right\rangle = \sum_{j=1}^{\infty} \mathcal{E}_j a_j \bar{b}_j \\ \forall \phi &= \sum_{j=1}^{\infty} a_j \Psi_j, \psi = \sum_{j=1}^{\infty} b_j \Psi_j \in \text{Dom}(\sqrt{H}). \end{aligned} \quad (2.104)$$

$\text{Dom}(\sqrt{H})$ here is referred to as the *form domain* of H . Observe that $\text{Dom}(\sqrt{H}) \supset \text{Dom}(H)$ and that $(\cdot, \cdot)_H$ is an extension of

$$\phi, \psi \in \text{Dom}(H) \mapsto \langle H\phi, \psi \rangle. \quad (2.105)$$

For each delta-perturbed operator H_Θ there is likewise an associated quadratic form, which is an extension of

$$\phi, \psi \in \text{Dom}(H_\Theta) \mapsto \langle H_\Theta \phi, \psi \rangle. \quad (2.106)$$

Now quadratic form representation of self-adjoint operators can be a useful tool in the study of perturbations, particularly because a perturbation may leave the quadratic form domain preserved, even when the ordinary domain is not preserved (see e.g. §1.2.3 in [AK00] along with §X.2 in [RS75]). We can then raise the question of whether or not the delta perturbation in our situation preserves the form domain.

Lemma 2.2.8. *For every $z \in \mathbb{C}$, if we take some $c \in \mathbb{R}$ for which $z \notin [c, \infty) \cap \{\mathcal{E}_j\}_{j \in \mathbb{N}}$ then*

$$\sum_{j: \mathcal{E}_j \geq c} \frac{|\Psi_j(p)|^2}{|\mathcal{E}_j - z|} \quad (2.107)$$

is a divergent sum.

Proof. Let $z = r + is$ with $r, s \in \mathbb{R}$. Then taking some $c' > \max\{c, r\}$ and $d > c'$, we have

$$\begin{aligned}
\sum_{j:c \leq \mathcal{E}_j \leq d} \frac{|\Psi_j(p)|^2}{|\mathcal{E}_j - z|} &= \sum_{j:c \leq \mathcal{E}_j \leq d} \frac{|\Psi_j(p)|^2}{\sqrt{(\mathcal{E}_j - r)^2 + s^2}} \\
&\geq \sum_{j:c \leq \mathcal{E}_j < c'} \frac{|\Psi_j(p)|^2}{\sqrt{(\mathcal{E}_j - r)^2 + s^2}} + \sum_{j:c' \leq \mathcal{E}_j \leq d} \frac{|\Psi_j(p)|^2}{\mathcal{E}_j - r + |s|} \\
&= \sum_{j:c \leq \mathcal{E}_j < c'} \frac{|\Psi_j(p)|^2}{\sqrt{(\mathcal{E}_j - r)^2 + s^2}} + \frac{N_p(d)}{d - r + |s|} - \frac{N_p^-(c')}{c' - r + |s|} \\
&\quad + \int_{c'}^d \frac{N_p(t)}{(t - r + |s|)^2} dt. \tag{2.108}
\end{aligned}$$

Now for any $\epsilon \in (0, \frac{1}{4\pi})$, by Corollary 2.1.6 we can take some $M \geq c'$ for which we have $N_p(t) \geq (\frac{1}{4\pi} - \epsilon)t \forall t \geq M$. Interested then in sending d to infinity:

$$\begin{aligned}
\int_M^d \frac{t}{(t - r + |s|)^2} dt &= \int_M^d \left(\frac{1}{t - r + |s|} + \frac{r - |s|}{(t - r + |s|)^2} \right) dt \\
&= \ln(d - r + |s|) + \frac{|s| - r}{d - r + |s|} \\
&\quad - \ln(M - r + |s|) - \frac{|s| - r}{M - r + |s|} \xrightarrow{d \rightarrow \infty} \infty. \tag{2.109}
\end{aligned}$$

It thus follows that LHS(2.108) tends to infinity as $d \rightarrow \infty$. \square

Corollary 2.2.9. For each $z \in \mathbb{C} \setminus \{\mathcal{E}_j\}_{j \in \mathbb{N}}$,

$$\sum_{j=1}^{\infty} \frac{\mathcal{E}_j |\Psi_j(p)|^2}{|\mathcal{E}_j - z|^2} \tag{2.110}$$

is a divergent sum, and thus $g_z \notin \text{Dom}(\sqrt{H})$.

Corollary 2.2.10. For each $\Theta \in (0, 2\pi)$, the form domain of H_Θ is not equal to the form domain of H .

Conclusion of Negative Infinitesimal Strength

The way in which (2.101) could be interpreted intuitively, remembering that the delta-perturbed operators are restrictions of H_p^* , is that the ‘‘delta potential’’ we work with has *negative infinitesimal* strength. This claim is further supported by work done in Ch. 4.

It is perhaps then a partial misnomer that this perturbation is referred to as a ‘‘delta potential’’. Perhaps it would be better referred to as a ‘‘quasi-delta

potential/perturbation”, or to copy terminology from e.g. [LSS05] or [Poh13], it could be referred to as a “regularised delta potential” (by contrast with a “bare delta potential”). In [LSS05], it is even stated that the “regularised” delta potential well in 2D and 3D has infinitesimally small strength (and the use of the word “well” would suggest a negative potential).

2.2.5 Eigenvalues and Eigenfunctions of the Delta-Perturbed Operators

From this point onwards, we work specifically with a choice of orthonormal eigenbasis $\{\Psi_j\}_{j \in \mathbb{N}}$ for which the following requirement is satisfied: *Each distinct eigenvalue has at most one corresponding eigenfunction in the eigenbasis whose value at the point p is nonzero.* It is always possible to select an orthonormal eigenbasis that satisfies this requirement. Now define $\{\Phi_j\}_{j \in \mathbb{N}} \subseteq \{\Psi_k\}_{k \in \mathbb{N}}$ to consist of all those members of the eigenbasis whose values at p are nonzero, and let $\{E_j\}_{j \in \mathbb{N}}$ be the corresponding eigenvalues. Note that we now have, with *strict* inequalities, $E_1 < E_2 < E_3 < \dots \rightarrow \infty$. Deletion of eigenfunctions from the eigenbasis that vanish at p will always still leave infinitely many eigenfunctions left.

Fixing $\Theta \in (0, 2\pi)$, the solutions $\lambda \in \mathbb{R} \setminus \{E_j\}_{j \in \mathbb{N}}$ to the following equation are eigenvalues of H_Θ :

$$\sum_{j=1}^{\infty} \left(\frac{1}{E_j - \lambda} - \frac{E_j}{1 + E_j^2} \right) |\Phi_j(p)|^2 = -\cot\left(\frac{\Theta}{2}\right) \sum_{j=1}^{\infty} \frac{|\Phi_j(p)|^2}{1 + E_j^2}. \quad (2.111)$$

The corresponding eigenfunctions (unnormalised) are then:

$$\phi = \sum_{j=1}^{\infty} \frac{\overline{\Phi_j(p)}}{E_j - \lambda} \Phi_j. \quad (2.112)$$

Now equation (2.111) has one solution within each interval (E_j, E_{j+1}) , and one solution below E_1 . Define λ_j to be the solution lying within the interval (E_j, E_{j+1}) , with λ_0 being the solution below E_1 . If we allow Θ to vary, then as Θ increases from 0 to 2π , λ_j increases from E_j to E_{j+1} , with λ_0 increasing from $-\infty$ to E_1 . [In conjunction with this, see Lemma 4.3.3].

Define ϕ_j to be the eigenfunction given by (2.112), corresponding to eigenvalue λ_j . Define the normalised eigenfunction $\hat{\phi}_j := \phi_j / \|\phi_j\|$.

Observe now that it is also the case that every eigenfunction of H which takes value zero at p is clearly also an eigenfunction of the perturbed operator H_Θ , with the

same corresponding eigenvalue. We have, as a complete orthonormal eigenbasis of the perturbed operator H_Θ :

$$\{\widehat{\phi}_j\}_{j \in \{0\} \cup \mathbb{N}} \cup (\{\Psi_k\}_{k \in \mathbb{N}} \setminus \{\Phi_l\}_{l \in \mathbb{N}}). \quad (2.113)$$

2.3 The Classical System

2.3.1 The Unperturbed Classical System

This is a continuous-time dynamical system for the motion of a particle confined within \mathcal{M} . An *acceptable* trajectory for the particle within \mathcal{M} is one satisfying the following rules:

- The particle's position on \mathcal{M} as a function of time is continuous.
- The particle is at $\partial\mathcal{M}$ for at most finitely many points in time within any finite time period.
- While the particle is on \mathcal{M}° , it moves along a geodesic at constant speed.
- When the particle strikes the boundary, it strikes non-tangentially at a point on the smooth part of the boundary. The out-going velocity vector (a vector on the tangent space) is then the reflection of the incoming velocity vector about the tangent line to $\partial\mathcal{M}$ at the point at which the particle strikes (essentially the same rule as for light reflecting off a mirror).

This system is a dynamical system on position-velocity phase space.

Associated to each point $x \in \mathcal{M}$ is a 2D Euclidean vector space referred to as the *tangent space* at x , denoted $T_x\mathcal{M}$. The velocity of a particle at x is then a vector in this tangent space. The space of linear functionals on this tangent space (the dual space) is referred to as the *cotangent space*, denoted $T_x^*\mathcal{M}$. The tangent space has a scalar product on it, referred to as the *Riemannian metric*. Each tangent vector can therefore be identified isomorphically with a cotangent vector, where this cotangent vector is the linear functional induced by the tangent vector under the scalar product.

We then define the *tangent bundle* $T\mathcal{M} := \{(x, \xi) : x \in \mathcal{M}, \xi \in T_x\mathcal{M}\}$. Likewise define the *cotangent bundle* $T^*\mathcal{M} := \{(x, \xi) : x \in \mathcal{M}, \xi \in T_x^*\mathcal{M}\}$. Either of these could potentially serve as the phase space.

However, since the speed of the particle is always constant over time, and altering the initial speed while keeping the same initial direction will not change the trajectory

(besides from a time rescaling), it is convenient just to take speed = 1, and have the phase space consist of just position and direction of motion. The phase space we shall work with is the *unit cotangent bundle* $S^*\mathcal{M} := \{(x, \xi) : x \in \mathcal{M}, \xi \in T_x^*\mathcal{M}, \|\xi\| = 1\}$, as is done for example in [ZZ96].

The phase space $S^*\mathcal{M}$ then has a natural 3D volume measure on it, which shall be normalised so as to have the total measure of $S^*\mathcal{M}$ being 1. Assume henceforth (if it does not already follow from the conditions stated for \mathcal{M}) that the manifold \mathcal{M} is such that, for almost all (i.e. full measure set of) points $(x, \xi) \in S^*\mathcal{M}$, if the initial state is (x, ξ) , then under the rules stated for an acceptable trajectory, this will give rise to a fully determined trajectory over all time, past and future.

On the set of points in $S^*\mathcal{M}$ that give rise to fully determined trajectories, define the *flow* Φ^t , where $\Phi^t(x, \xi)$ is the state in $S^*\mathcal{M}$ at time $t \in \mathbb{R}$ if the initial state (time $t = 0$) is (x, ξ) , taking speed of motion = 1. This flow is *measure preserving*, meaning that for any measurable set $V \subset S^*\mathcal{M}$ for which all points in V give rise to fully determined trajectories, we have

$$\mu(V) = \mu(\Phi^t(V)) \quad \forall t \in \mathbb{R}, \quad (2.114)$$

where μ is the measure on $S^*\mathcal{M}$.

2.3.2 The Perturbed Classical System

We assume that for as long as the particle confined within \mathcal{M} does not hit the point p , its motion follows the same rules as for the unperturbed classical system. Now only a measure zero set of points in $S^*\mathcal{M}$ would belong to trajectories that ever hit the point p . Since the difference then is only for a measure zero set, the perturbed classical system is considered to be essentially the same dynamical system as the unperturbed classical system.

Chapter 3

Approximation of Some Perturbed Eigenfunctions by a Combination of the Two Surrounding Unperturbed Eigenfunctions

3.1 Overview

In the study of quantum chaos, a common interest is in limiting behaviour of subsequences of an orthonormal eigenbasis of the quantum Hamiltonian, with the functions in the eigenbasis being arranged in order of non-decreasing eigenvalue. In the case where we deal with a delta-perturbed quantum system, it could then be of interest to determine whether knowledge of limiting behaviour of some unperturbed eigenbasis subsequences can be used to infer limiting behaviour of some perturbed eigenbasis subsequences.

As such, one could be interested in a perturbed eigenfunctions subsequence $(\phi_{j_n})_{n \in \mathbb{N}} \subset (\phi_j)_{j \in \mathbb{N}}$ in which for large eigenvalue, the eigenfunctions approximate to a linear combination of only the *two* surrounding unperturbed eigenfunctions Φ_{j_n} and Φ_{j_n+1} . This may enable limiting properties of $(\phi_{j_n})_{n \in \mathbb{N}}$ to be inferred from limiting properties of $(\Phi_{j_n})_{n \in \mathbb{N}}$ and $(\Phi_{j_n+1})_{n \in \mathbb{N}}$. Such approximation of perturbed eigenfunction subsequences to the two surrounding unperturbed eigenfunctions is the subject of this Chapter.

Now of course, as seen in §2.2.5, unperturbed eigenfunctions that vanish at p remain functions of the perturbed operator H_Θ . However, the studies in this Chapter will focus only on the “new” perturbed eigenfunctions $\{\phi_j\}$.

In [KMW10], a class of *quasimodes*, i.e. “approximate eigenfunctions”, for the

delta-perturbed operator is constructed, and analysis is performed on how well these quasimodes can be used to approximate true eigenfunctions of the delta-perturbed operator. Each quasimode is within the domain of the delta-perturbed operator, and associated with each quasimode is a real-valued *quasieigenvalue*. Just as in Chapter 2 here, the setting within [KMW10] is that of a self-adjoint $-\Delta$ on a 2D compact Riemannian manifold, with or without boundary, perturbed by a delta potential.

Particular focus within [KMW10] is placed on a set of quasimodes $\{\psi_{0,I_j}\}_{j \in \mathbb{N}}$ of the perturbed operator H_Θ , where I_j is the interval $[E_j, E_{j+1}]$ and $\psi_{0,I_j} \in \text{span}\{\Phi_j, \Phi_{j+1}\}$. Associated with the quasimode ψ_{0,I_j} is a quasieigenvalue $\mu_j \in (E_j, E_{j+1})$. Again, as defined in §2.2.5, each Φ_j is a member of the eigenbasis of H with $\Phi_j(p) \neq 0$, and E_j is the corresponding eigenvalue. Recall also that the eigenbasis of H has been chosen such that for each distinct eigenvalue, only at most one corresponding member of the eigenbasis may be nonzero at p . Thus with strict inequality, $E_j < E_{j+1}$.

As well as the quasimode ψ_{0,I_j} with quasieigenvalue $\mu_j \in (E_j, E_{j+1})$, there is of course also the true eigenfunction ϕ_j of H_Θ with eigenvalue $\lambda_j \in (E_j, E_{j+1})$. Theorem 4.4 in [KMW10] then gives a pair of conditions under which, for an eigenfunction subsequence $(\phi_{j_n})_{n \in \mathbb{N}} \subset (\phi_j)_{j \in \mathbb{N}}$, it holds that as $n \rightarrow \infty$, $\psi_{0,I_{j_n}}$ and ϕ_{j_n} approach each other under the L^2 norm, when normalised. Thus for large n , the eigenfunction ϕ_{j_n} of H_Θ approximates to a linear combination of only two unperturbed eigenfunctions, namely Φ_{j_n} and Φ_{j_n+1} . This theorem is only stated though for the self-adjoint extension H_π .

In §V of [KMW10], implications of this are then studied in the case of the original *Šeba billiard*, which is a rectangle billiard perturbed with a delta potential. The unperturbed Hamiltonian operator is taken to be the self-adjoint $-\Delta$ with Dirichlet boundary conditions. The position p of the point scatterer is taken to be the centre of the rectangle. It is demonstrated that for the unperturbed rectangle billiard, for large eigenvalues most of the eigenfunctions become localised in momentum space around only four points. These four points in general are different for different eigenfunctions. With $\mathcal{M} \subset \mathbb{R}^2$, the momentum distribution of a wavefunction $\psi \in L^2(\mathcal{M})$ is given by $|\mathcal{F}\{\psi\}|^2$ (normalised), where \mathcal{F} is the Fourier transform.

It is inferred in §V of [KMW10] that there would be a perturbed eigenfunction subsequence $(\phi_{j_n})_{n \in \mathbb{N}} \subset (\phi_j)_{j \in \mathbb{N}}$ in which these eigenfunctions become localised around eight points in momentum space. This is because they approximate to a linear combination of two unperturbed eigenfunctions, each localising around four points in momentum space. Supporting numerical simulations are presented in [BKW03].

Outlining the structure of this Chapter, §3.2 gives a review of Theorem 4.4 in

[KMW10]. This theorem is restated in Prop. 3.2.1. Immediate observations can be made, strengthening the statement of this theorem. This stronger statement of the theorem is given in Cor. 3.2.2.

In §3.3 results are derived which would form a basis for a broadened study of the question of whether a “new” perturbed eigenfunction subsequence approaches linear combinations of only the two surrounding unperturbed eigenfunctions. Distinction here is drawn as to whether or not each approximating linear combination of these two eigenfunctions is demanded to be contained within the domain of the perturbed operator. Cor. 3.3.2 states conditions under which this approximation holds, demanding that the approximating linear combination be contained within the domain of the perturbed operator. Prop. 3.3.3 does the same, but without this demand.

Now Thm. 4.4 in [KMW10] effectively deals with conditions for this approximation, with this demand, since the quasimodes dealt with there are contained in the perturbed domain. However, in this Chapter, the case is considered in which this demand is dropped. In §3.4, the conditions of Prop. 3.3.3 are processed, so as to derive the central result of this Chapter, namely Theorem 3.4.1. From this, Prop. 3.5.1 and Cor. 3.5.2 are then derived. Cor. 3.5.2 permits a transparent comparison with Thm. 4.4 in [KMW10].

Throughout this Chapter, work is carried out within the setting specified in Chapter 2, along with the notation given in Chapter 2.

3.2 Review of Work by Keating, Marklof and Winn

Before defining and discussing quasimodes, first making a basic mathematical observation: given any Hilbert space \mathcal{H} , for any two *normalised* members $\phi, \psi \in \mathcal{H}$,

$$\begin{aligned} \|\phi - e^{i\chi}\psi\|^2 &= \langle \phi - e^{i\chi}\psi, \phi - e^{i\chi}\psi \rangle = 1 - e^{-i\chi} \langle \phi, \psi \rangle - e^{i\chi} \langle \psi, \phi \rangle + 1 \\ &= 2 - 2\operatorname{Re}(e^{i\chi} \langle \psi, \phi \rangle) \quad \forall \chi \in [0, 2\pi). \end{aligned} \quad (3.1)$$

Now let $\chi_0 := -\arg(\langle \psi, \phi \rangle)$, so $\langle \psi, \phi \rangle = |\langle \psi, \phi \rangle| e^{-i\chi_0}$. Then

$$\min_{\chi \in [0, 2\pi)} \|\phi - e^{i\chi}\psi\|^2 = \|\phi - e^{i\chi_0}\psi\|^2 = 2(1 - |\langle \psi, \phi \rangle|). \quad (3.2)$$

3.2.1 Quasimodes

Let T be a self-adjoint operator in a separable Hilbert space \mathcal{H} , having a countable orthonormal eigenbasis $\{u_j\}$, whose spectrum is purely the set of corresponding eigenvalues $\{\Lambda_j\} \subseteq \mathbb{R}$, having $\#\{j : \Lambda_j \in S\} < \infty$ for every bounded set $S \subset \mathbb{R}$. A

member $\psi \in \text{Dom}(T)$ is said to be a *quasimode* of T with *quasieigenvalue* $\mu \in \mathbb{R}$ and *discrepancy* $d \geq 0$ if

$$\|(T - \mu)\psi\| \leq d \|\psi\|. \quad (3.3)$$

Given such a quasimode, as stated in [KMW10], the interval $[\mu - d, \mu + d]$ will contain at least one true eigenvalue of T . Furthermore, it holds that for any $M > 0$,

$$\sum_{j: \Lambda_j \notin [\mu - M, \mu + M]} |\langle \psi, u_j \rangle|^2 = \|\psi\|^2 - \sum_{j: \Lambda_j \in [\mu - M, \mu + M]} |\langle \psi, u_j \rangle|^2 \leq \frac{d^2}{M^2} \|\psi\|^2. \quad (3.4)$$

Rearranging this gives:

$$\sum_{j: \Lambda_j \in [\mu - M, \mu + M]} |\langle \psi, u_j \rangle|^2 \geq \left(1 - \frac{d^2}{M^2}\right) \|\psi\|^2 \quad (3.5)$$

Now suppose that ψ is normalised, and that there is only one eigenvector/eigenfunction u_j non-orthogonal to ψ with corresponding eigenvalue $\Lambda_j \in [\mu - M, \mu + M]$. Let $\chi_0 := -\arg(\langle \psi, u_j \rangle)$. Applying (3.2) followed by (3.4) then gives:

$$\|u_j - e^{i\chi_0}\psi\|^2 = 2(1 - |\langle \psi, u_j \rangle|) \leq 2(1 - |\langle \psi, u_j \rangle|^2) \leq \frac{2d^2}{M^2}. \quad (3.6)$$

Thus

$$\|u_j - e^{i\chi_0}\psi\| \leq \frac{\sqrt{2}d}{M}. \quad (3.7)$$

3.2.2 Approximation of Perturbed Eigenfunctions by Two-Component Quasimodes

Within the family of quasimodes considered in [KMW10], particular attention is paid to quasimodes of the following form: for each interval $I_j := [E_j, E_{j+1}]$ we have an associated quasimode

$$\begin{aligned} \psi_{0, I_j} &= \frac{\overline{\Phi_j(p)}}{E_j - \mu_j} \Phi_j + \frac{\overline{\Phi_{j+1}(p)}}{E_{j+1} - \mu_j} \Phi_{j+1} \\ &= \frac{|\Phi_j(p)|^2 + |\Phi_{j+1}(p)|^2}{E_{j+1} - E_j} \left(\frac{-1}{\Phi_j(p)} \Phi_j + \frac{1}{\Phi_{j+1}(p)} \Phi_{j+1} \right), \end{aligned} \quad (3.8)$$

where

$$\mu_j = \frac{|\Phi_j(p)|^2 E_{j+1} + |\Phi_{j+1}(p)|^2 E_j}{|\Phi_j(p)|^2 + |\Phi_{j+1}(p)|^2} \in (E_j, E_{j+1}). \quad (3.9)$$

ψ_{0, I_j} is shown in [KMW10] to be a quasimode of the delta-perturbed operator H_Θ with quasieigenvalue μ_j and discrepancy $d \leq \frac{1}{2}(E_{j+1} - E_j)$. Let $\widehat{\psi}_{0, I_j} := \psi_{0, I_j} / \|\psi_{0, I_j}\|$.

In Thm. 4.4 of [KMW10], sufficient conditions are derived in the case where $\Theta = \pi$, for which a subsequence $(\widehat{\phi}_{j_n})_{n \in \mathbb{N}}$ of the perturbed eigenfunction sequence $(\widehat{\phi}_j)_{j \in \mathbb{N}}$ approximates to the corresponding sequence of quasimodes $(\widehat{\psi}_{0, I_{j_n}})_{n \in \mathbb{N}}$ in the L^2 norm. More precisely, this theorem states:

Proposition 3.2.1. *Working with the perturbed operator H_π , given a strictly increasing sequence $(j_n)_{n \in \mathbb{N}} \subset \mathbb{N}$, it holds that*

$$\|\widehat{\phi}_{j_n} - e^{i\theta_n} \widehat{\psi}_{0, I_{j_n}}\| \xrightarrow{n \rightarrow \infty} 0 \quad (3.10)$$

for some phases $(e^{i\theta_n})_{n \in \mathbb{N}}$, if the following conditions are satisfied:

- (i) $\exists q \in (0, \frac{1}{2})$, $\rho \in (1, 2(1 - q))$ and sequence $(\varepsilon_n)_{n \in \mathbb{N}} \subset (0, \infty)$ with $\varepsilon_n \xrightarrow{n \rightarrow \infty} 0$ such that

$$E_{j_{n+2}} \ll \varepsilon_n^{-\rho}, \quad (3.11)$$

$$E_{j_{n+1}} - E_{j_n} \ll \varepsilon_n, \quad (3.12)$$

$$E_{j_n} - E_{j_{n-1}} \gg \varepsilon_n^q, \quad (3.13)$$

$$E_{j_{n+2}} - E_{j_{n+1}} \gg \varepsilon_n^q \quad (3.14)$$

as $n \rightarrow \infty$, where \ll is again the order relation $O(\cdot)$, defined in (2.33),

- (ii) $\exists c_0 > 0$ s.t. $|\Phi_{j_n}| \geq c_0$ and $|\Phi_{j_{n+1}}| \geq c_0 \forall n \in \mathbb{N}$.

Remarks. (a) Observe that condition (i) in Prop. 3.2.1 is *stronger* than the following:

$$E_{j_{n+1}} - E_{j_n} \xrightarrow{n \rightarrow \infty} 0, \quad \frac{E_{j_{n+1}} - E_{j_n}}{E_{j_n} - E_{j_{n-1}}} \xrightarrow{n \rightarrow \infty} 0, \quad \frac{E_{j_{n+1}} - E_{j_n}}{E_{j_{n+2}} - E_{j_{n+1}}} \xrightarrow{n \rightarrow \infty} 0. \quad (3.15)$$

- (b) It is remarked in [KMW10] that condition (ii) can in fact be relaxed slightly, by replacing the “ $\geq c_0$ ” requirement with $\gg \varepsilon_n^{r/2}$ for some $r \in (0, 1 - q - \frac{\rho}{2})$.

- (c) Given a strictly increasing sequence $(j_n)_{n \in \mathbb{N}} \subset \mathbb{N}$ and a sequence $(\varepsilon_n)_{n \in \mathbb{N}} \subset (0, \infty)$ with $\varepsilon_n \xrightarrow{n \rightarrow \infty} 0$, suppose (3.11) - (3.14) hold for some $q, \rho \in \mathbb{R}$. Then given any $q', \rho' \in \mathbb{R}$ with $q' \geq q$ and $\rho' \geq \rho$, (3.11) - (3.14) also hold with q' and ρ' in place of q and ρ . This is easy to see since for sufficiently large n , $0 < \varepsilon_n < 1$ and so $\varepsilon_n^{q'} \leq \varepsilon_n^q$ and $\varepsilon_n^{-\rho'} \geq \varepsilon_n^{-\rho}$. This may allow for an automatic weakening of the conditions on q and ρ in Thm. 4.4 of [KMW10].

- (d) Again given a strictly increasing sequence $(j_n)_{n \in \mathbb{N}} \subset \mathbb{N}$ and a sequence $(\varepsilon_n)_{n \in \mathbb{N}} \subset (0, \infty)$ with $\varepsilon_n \xrightarrow{n \rightarrow \infty} 0$, suppose (3.11) - (3.14) hold for some $q, \rho \in \mathbb{R}$. It must then follow that $\rho > 0$ since $E_{j_{n+2}} \xrightarrow{n \rightarrow \infty} \infty$, and that $q \geq -\rho$ since $E_{j_n} - E_{j_{n-1}} < E_{j_{n+2}}$ and $E_{j_{n+2}} - E_{j_{n+1}} < E_{j_{n+2}}$.

(e) The appearance of phases $e^{i\theta_n}$ in (3.10) can be eliminated. This is because

$$\begin{aligned} \langle \widehat{\psi}_{0,I_{j_n}}, \widehat{\phi}_{j_n} \rangle &= \frac{1}{\|\widehat{\psi}_{0,I_{j_n}}\| \|\widehat{\phi}_{j_n}\|} \left(\frac{|\Phi_{j_n}(p)|^2}{(E_{j_n} - \mu_{j_n})(E_{j_n} - \lambda_{j_n})} \right. \\ &\quad \left. + \frac{|\Phi_{j_n+1}(p)|^2}{(E_{j_n+1} - \mu_{j_n})(E_{j_n+1} - \lambda_{j_n})} \right) > 0, \end{aligned} \quad (3.16)$$

so $\arg \left(\langle \widehat{\psi}_{0,I_{j_n}}, \widehat{\phi}_{j_n} \rangle \right) = 0$, and thus from (3.2) it follows that

$$\|\widehat{\phi}_{j_n} - \widehat{\psi}_{0,I_{j_n}}\| \leq \|\widehat{\phi}_{j_n} - e^{i\theta_n} \widehat{\psi}_{0,I_{j_n}}\|. \quad (3.17)$$

Hence

$$\exists (\theta_n)_{n \in \mathbb{N}} \subset \mathbb{R} \quad \text{s.t.} \quad \|\widehat{\phi}_{j_n} - e^{i\theta_n} \widehat{\psi}_{0,I_{j_n}}\| \xrightarrow{n \rightarrow \infty} 0 \quad (3.18)$$

if and only if

$$\|\widehat{\phi}_{j_n} - \widehat{\psi}_{0,I_{j_n}}\| \xrightarrow{n \rightarrow \infty} 0. \quad (3.19)$$

In light of remarks (c), (d) and (e), the following corollary may thus be derived:

Corollary 3.2.2. *Working with the perturbed operator H_π , given a strictly increasing sequence $(j_n)_{n \in \mathbb{N}} \subset \mathbb{N}$, it holds that*

$$\|\widehat{\phi}_{j_n} - \widehat{\psi}_{0,I_{j_n}}\| \xrightarrow{n \rightarrow \infty} 0 \quad (3.20)$$

if conditions (i) and (ii) from Prop. 3.2.1 hold, only now weakening the specification for q and ρ in condition (i) to the following:

$$-2 < q < \frac{1}{2}, \quad \begin{cases} 0 < \rho < 2(1-q) & \text{if } 0 \leq q < \frac{1}{2} \\ -q \leq \rho < 2 & \text{if } -2 < q < 0. \end{cases} \quad (3.21)$$

In what follows, we shall rename ψ_{0,I_j} as ψ_j° . We also shall *not* restrict to the case of $\Theta = \pi$ henceforth. It would be useful to make the following observation:

Lemma 3.2.3. *For given $j \in \mathbb{N}$, for any $u \in \text{span}\{\Phi_j, \Phi_{j+1}\}$, it holds that $u \in \text{Dom}(H_\Theta)$ iff $u \in \mathcal{D}_p$ iff $u = s\psi_j^\circ$ for some scalar $s \in \mathbb{C}$.*

Proof. Clearly $u \in \text{Dom}(H)$. Since $\text{Dom}(H) \cap \text{Dom}(H_\Theta) = \mathcal{D}_p$, it follows that $u \in \text{Dom}(H_\Theta)$ iff $u \in \mathcal{D}_p$. Writing $u = b\Phi_j + c\Phi_{j+1}$, $u(p) = 0$ iff $c = -b\Phi_j(p)/\Phi_{j+1}(p)$. Comparing with the right-hand side of (3.8), this clearly holds iff u is a scalar multiple of ψ_j° . \square

Again, in [KMW10], interest is expressed in a perturbed eigenfunction subsequence $(\widehat{\phi}_{j_n})_{n \in \mathbb{N}}$ for which, as $n \rightarrow \infty$, $\widehat{\phi}_{j_n}$ approximates to a linear combination of Φ_{j_n} and Φ_{j_n+1} . However, only the case where this linear combination is contained within the domain of the perturbed operator is considered. It would seem reasonable to broaden the investigation by also considering the case where this restriction is dropped.

3.3 Further Work: Initial Observations on Conditions for Approximation

Proposition 3.3.1. *Given a sequence $\{j_n\} \subseteq \mathbb{N}$ with $j_n \rightarrow \infty$ as $n \rightarrow \infty$, and sequence $\{u_{j_n}\} \subseteq L^2(\mathcal{M})$ with $u_{j_n} = b_{j_n}\Phi_{j_n} + c_{j_n}\Phi_{j_n+1} \neq 0$, consider the following statement: $\exists \{s_{j_n}\}, \{z_{j_n}\} \subseteq \mathbb{C}$ such that*

- (i) $\|s_{j_n}\phi_{j_n} - z_{j_n}u_{j_n}\| \rightarrow 0$ as $n \rightarrow \infty$,
- (ii) \nexists subsequence $\{k_n\} \subseteq \{j_n\}$ such that both $\|s_{k_n}\phi_{k_n}\|, \|z_{k_n}u_{k_n}\| \rightarrow 0$.

The above statement holds true iff

$$\left\| \widehat{\phi}_{j_n} - e^{i\chi_{j_n}} \widehat{u}_{j_n} \right\| \rightarrow 0, \quad (3.22)$$

equivalently

$$\left| \left\langle \widehat{u}_{j_n}, \widehat{\phi}_{j_n} \right\rangle \right| \rightarrow 1, \quad (3.23)$$

where $\widehat{u}_{j_n} := u_{j_n}/\|u_{j_n}\|$ and $\chi_{j_n} := -\arg\left(\left\langle \widehat{u}_{j_n}, \widehat{\phi}_{j_n} \right\rangle\right)$. Here

$$\left\| \widehat{\phi}_{j_n} - e^{i\chi_{j_n}} \widehat{u}_{j_n} \right\|^2 = 2 \left(1 - \left| \left\langle \widehat{u}_{j_n}, \widehat{\phi}_{j_n} \right\rangle \right| \right), \quad (3.24)$$

$$\left| \left\langle \widehat{u}_{j_n}, \widehat{\phi}_{j_n} \right\rangle \right| = \frac{\left| \frac{b_{j_n}\Phi_{j_n}(p)}{E_{j_n}-\lambda_{j_n}} + \frac{c_{j_n}\Phi_{j_n+1}(p)}{E_{j_n+1}-\lambda_{j_n}} \right|}{\sqrt{|b_{j_n}|^2 + |c_{j_n}|^2} \sqrt{\sum_{k=1}^{\infty} \frac{|\Phi_k(p)|^2}{(E_k-\lambda_{j_n})^2}}}. \quad (3.25)$$

Proof. Trivially, if (3.22) holds true then the statement in question holds true, as (3.22) would serve as an example.

Now suppose the statement in question holds true. We wish then to prove (3.22).

For each j_n , let w_{j_n} be the larger out of $s_{j_n}\phi_{j_n}$ and $z_{j_n}u_{j_n}$, and let v_{j_n} be the smaller, where “larger” (“smaller”) means having larger (smaller) norm. From (ii), it follows that

$$\exists M > 0, N_1 \in \mathbb{N} \text{ s.t. } \|w_{j_n}\| \geq M \quad \forall n \geq N_1. \quad (3.26)$$

Now take some $L \in (0, M)$, $\varepsilon \in (0, M - L)$ and (by (i)) $N_2 \geq N_1$ such that $\|s_{j_n}\phi_{j_n} - z_{j_n}u_{j_n}\| = \|w_{j_n} - v_{j_n}\| < \varepsilon \quad \forall n \geq N_2$. Then for each $n \geq N_2$:

$$M \leq \|w_{j_n}\| \leq \|w_{j_n} - v_{j_n}\| + \|v_{j_n}\| < \varepsilon + \|v_{j_n}\| \quad (3.27)$$

$$\therefore \|v_{j_n}\| > M - \varepsilon > L. \quad (3.28)$$

Hence it follows that

$$\|s_{j_n}\phi_{j_n}\|, \|z_{j_n}u_{j_n}\| > L \quad \forall n \geq N_2. \quad (3.29)$$

From now on, assume $n \geq N_2$. Define

$$\tilde{u}_{j_n} := \frac{z_{j_n}u_{j_n}}{s_{j_n}\|\phi_{j_n}\|}. \quad (3.30)$$

Then

$$\left\| \widehat{\phi}_{j_n} - \tilde{u}_{j_n} \right\| = \left\| \frac{s_{j_n}\phi_{j_n} - z_{j_n}u_{j_n}}{s_{j_n}\|\phi_{j_n}\|} \right\| \leq \frac{\|s_{j_n}\phi_{j_n} - z_{j_n}u_{j_n}\|}{L}. \quad (3.31)$$

Hence by (i),

$$\left\| \widehat{\phi}_{j_n} - \tilde{u}_{j_n} \right\| \rightarrow 0 \text{ as } n \rightarrow \infty. \quad (3.32)$$

Now define $\acute{u}_{j_n} := \tilde{u}_{j_n}/\|\tilde{u}_{j_n}\|$, so \acute{u}_{j_n} is normalised. Then

$$\begin{aligned} \left\| \widehat{\phi}_{j_n} - \acute{u}_{j_n} \right\| &\leq \left\| \widehat{\phi}_{j_n} - \tilde{u}_{j_n} \right\| + \|\tilde{u}_{j_n} - \acute{u}_{j_n}\| = \left\| \widehat{\phi}_{j_n} - \tilde{u}_{j_n} \right\| + \left\| \tilde{u}_{j_n} \left(1 - \frac{1}{\|\tilde{u}_{j_n}\|} \right) \right\| \\ &= \left\| \widehat{\phi}_{j_n} - \tilde{u}_{j_n} \right\| + |(\|\tilde{u}_{j_n}\| - 1)| \\ &= \left\| \widehat{\phi}_{j_n} - \tilde{u}_{j_n} \right\| + \left| \left(\|\tilde{u}_{j_n}\| - \left\| \widehat{\phi}_{j_n} \right\| \right) \right| \leq 2 \left\| \widehat{\phi}_{j_n} - \tilde{u}_{j_n} \right\|. \end{aligned} \quad (3.33)$$

Hence

$$\left\| \widehat{\phi}_{j_n} - \acute{u}_{j_n} \right\| \rightarrow 0 \text{ as } n \rightarrow \infty. \quad (3.34)$$

Finally by (3.2),

$$\left\| \widehat{\phi}_{j_n} - e^{ix_{j_n}}\widehat{u}_{j_n} \right\| \leq \left\| \widehat{\phi}_{j_n} - \acute{u}_{j_n} \right\|. \quad (3.35)$$

Thus (3.22) holds true.

The rest then follows from (3.2), (2.112) and basic Hilbert space formulae. \square

Corollary 3.3.2. *Given a sequence $\{j_n\} \subseteq \mathbb{N}$ with $j_n \rightarrow \infty$ as $n \rightarrow \infty$, consider the following statement: $\exists \{s_{j_n}\} \subseteq \mathbb{C}, \{v_{j_n}\} \subseteq L^2(\mathcal{M})$ with $v_{j_n} = x_{j_n}\Phi_{j_n} + y_{j_n}\Phi_{j_n+1} \in \text{Dom}(H_\Theta)$, such that*

$$(i) \quad \|s_{j_n}\phi_{j_n} - v_{j_n}\| \rightarrow 0 \text{ as } n \rightarrow \infty,$$

$$(ii) \quad \nexists \text{ subsequence } \{k_n\} \subseteq \{j_n\} \text{ such that both } \|s_{k_n}\phi_{k_n}\|, \|v_{k_n}\| \rightarrow 0.$$

The above statement holds true iff

$$\left\| \widehat{\phi}_{j_n} - \widehat{\psi}_{j_n}^\circ \right\| \rightarrow 0, \quad (3.36)$$

equivalently

$$\left\langle \widehat{\psi}_{j_n}^\circ, \widehat{\phi}_{j_n} \right\rangle \rightarrow 1. \quad (3.37)$$

Here

$$\left\| \widehat{\phi}_{j_n} - \widehat{\psi}_{j_n}^\circ \right\|^2 = 2 \left(1 - \left\langle \widehat{\psi}_{j_n}^\circ, \widehat{\phi}_{j_n} \right\rangle \right), \quad (3.38)$$

$$\left\langle \widehat{\psi}_{j_n}^\circ, \widehat{\phi}_{j_n} \right\rangle = \frac{(E_{j_n+1} - E_{j_n}) |\Phi_{j_n}(p) \Phi_{j_n+1}(p)|}{(E_{j_n+1} - \lambda_{j_n})(\lambda_{j_n} - E_{j_n}) \sqrt{|\Phi_{j_n}(p)|^2 + |\Phi_{j_n+1}(p)|^2} \sqrt{\sum_{k=1}^{\infty} \frac{|\Phi_k(p)|^2}{(E_k - \lambda_{j_n})^2}}}. \quad (3.39)$$

Proof. Given Lemma 3.2.3, the statement in question here is equivalent to the statement in question in Proposition 3.3.1, with $u_{j_n} = \psi_{j_n}^\circ$. Thus the Corollary follows from Proposition 3.3.1, using the formula (3.8) for ψ_j° . Observe from (3.39) (or from (3.16)) that $\left\langle \widehat{\psi}_{j_n}^\circ, \widehat{\phi}_{j_n} \right\rangle > 0$, and so $\left| \left\langle \widehat{\psi}_{j_n}^\circ, \widehat{\phi}_{j_n} \right\rangle \right| = \left\langle \widehat{\psi}_{j_n}^\circ, \widehat{\phi}_{j_n} \right\rangle$, $\arg \left(\left\langle \widehat{\psi}_{j_n}^\circ, \widehat{\phi}_{j_n} \right\rangle \right) = 0$. \square

Now for given $j \in \mathbb{N}$, define

$$\psi_j^+ := \mathcal{P}_{[E_j, E_{j+1}]} \phi_j = \frac{\overline{\Phi_j(p)}}{E_j - \lambda_j} \Phi_j + \frac{\overline{\Phi_{j+1}(p)}}{E_{j+1} - \lambda_j} \Phi_{j+1}. \quad (3.40)$$

Define $\widehat{\psi}_j^+ := \psi_j^+ / \|\psi_j^+\|$.

Proposition 3.3.3. *Given a sequence $\{j_n\} \subseteq \mathbb{N}$ with $j_n \rightarrow \infty$ as $n \rightarrow \infty$, consider the following statement: $\exists \{s_{j_n}\} \subseteq \mathbb{C}, \{v_{j_n}\} \subseteq L^2(\mathcal{M})$ with $v_{j_n} = x_{j_n} \Phi_{j_n} + y_{j_n} \Phi_{j_n+1}$, such that*

- (i) $\|s_{j_n} \phi_{j_n} - v_{j_n}\| \rightarrow 0$ as $n \rightarrow \infty$,
- (ii) \nexists subsequence $\{k_n\} \subseteq \{j_n\}$ such that both $\|s_{k_n} \phi_{k_n}\|, \|v_{k_n}\| \rightarrow 0$.

The above statement holds true iff

$$\left\| \widehat{\phi}_{j_n} - \widehat{\psi}_{j_n}^+ \right\| \rightarrow 0, \quad (3.41)$$

equivalently

$$\left\langle \widehat{\psi}_{j_n}^+, \widehat{\phi}_{j_n} \right\rangle \rightarrow 1. \quad (3.42)$$

Here

$$\left\| \widehat{\phi}_{j_n} - \widehat{\psi}_{j_n}^+ \right\|^2 = 2 \left(1 - \left\langle \widehat{\psi}_{j_n}^+, \widehat{\phi}_{j_n} \right\rangle \right), \quad (3.43)$$

$$\left\langle \widehat{\psi}_{j_n}^+, \widehat{\phi}_{j_n} \right\rangle = \sqrt{\frac{\frac{|\Phi_{j_n}(p)|^2}{(E_{j_n} - \lambda_{j_n})^2} + \frac{|\Phi_{j_n+1}(p)|^2}{(E_{j_n+1} - \lambda_{j_n})^2}}{\sum_{k=1}^{\infty} \frac{|\Phi_k(p)|^2}{(E_k - \lambda_{j_n})^2}}}. \quad (3.44)$$

Given (3.44), this condition can equivalently be written down as:

$$\sum_{k=1}^{j_n-1} \frac{|\Phi_k(p)|^2}{(E_k - \lambda_{j_n})^2} + \sum_{k=j_n+2}^{\infty} \frac{|\Phi_k(p)|^2}{(E_k - \lambda_{j_n})^2} \ll \frac{|\Phi_{j_n}(p)|^2}{(E_{j_n} - \lambda_{j_n})^2} + \frac{|\Phi_{j_n+1}(p)|^2}{(E_{j_n+1} - \lambda_{j_n})^2} \text{ as } n \rightarrow \infty. \quad (3.45)$$

Remark. The key difference between the statement at the start of Prop. 3.3.3 and that of Cor. 3.3.2 is that in Cor. 3.3.2, it is demanded that $v_{j_n} \in \text{Dom}(H_\Theta)$. This is not demanded in Prop. 3.3.3.

Proof. (3.43), (3.44) and the equivalence of (3.41) and (3.42) follow easily from (3.2), (2.112), (3.40) and basic Hilbert space formulae. The equivalence of (3.42) and (3.45) follows easily by placing (3.44) into (3.42) and rearranging. Trivially, if (3.41) holds true then the statement in question holds true, as (3.41) would serve as an example. It remains to show that (3.41) follows from the statement in question.

Assume the statement in question holds true. Note that (i) and (ii) together rule out the possibility of a subsequence $\{k_n\} \subseteq \{j_n\}$ for which $v_{k_n} = 0$, and thus v_{j_n} is nonzero for all sufficiently large n . Applying Proposition 3.3.1 then gives:

$$\left\| \widehat{\phi}_{j_n} - e^{i\chi_{j_n}} \widehat{v}_{j_n} \right\| \rightarrow 0. \quad (3.46)$$

Write

$$\widehat{\phi}_{j_n} = \sum_{k=1}^{\infty} a_{j_n}^{(k)} \Phi_k, \quad (3.47)$$

$$e^{i\chi_{j_n}} \widehat{v}_{j_n} = b_{j_n} \Phi_{j_n} + c_{j_n} \Phi_{j_n+1}. \quad (3.48)$$

Observe that by (3.43), (3.44) and (2.112):

$$\left\| \widehat{\phi}_{j_n} - \widehat{\psi}_{j_n}^+ \right\|^2 = 2 \left(1 - \sqrt{|a_{j_n}^{(j_n)}|^2 + |a_{j_n}^{(j_n+1)}|^2} \right). \quad (3.49)$$

Also

$$\left\| \widehat{\phi}_{j_n} \right\|^2 = \sum_{k=1}^{\infty} |a_{j_n}^{(k)}|^2 = 1, \quad (3.50)$$

$$\left\| \widehat{\phi}_{j_n} - e^{i\chi_{j_n}} \widehat{v}_{j_n} \right\|^2 = \sum_{k=1}^{j_n-1} |a_{j_n}^{(k)}|^2 + |a_{j_n}^{(j_n)} - b_{j_n}|^2 + |a_{j_n}^{(j_n+1)} - c_{j_n}|^2 + \sum_{k=j_n+2}^{\infty} |a_{j_n}^{(k)}|^2. \quad (3.51)$$

Thus

$$\begin{aligned} \left\| \widehat{\phi}_{j_n} - \widehat{\psi}_{j_n}^+ \right\|^2 &= 2 \left(1 - \sqrt{|a_{j_n}^{(j_n)}|^2 + |a_{j_n}^{(j_n+1)}|^2} \right) \leq 2 \left(1 - |a_{j_n}^{(j_n)}|^2 - |a_{j_n}^{(j_n+1)}|^2 \right) \\ &= 2 \left(\sum_{k=1}^{j_n-1} |a_{j_n}^{(k)}|^2 + \sum_{k=j_n+2}^{\infty} |a_{j_n}^{(k)}|^2 \right) \leq 2 \left\| \widehat{\phi}_{j_n} - e^{i\chi_{j_n}} \widehat{v}_{j_n} \right\|^2. \end{aligned} \quad (3.52)$$

Hence (3.41) holds true. \square

3.4 Derived Results

Theorem 3.4.1. *Given a sequence $\{j_n\} \subseteq \mathbb{N}$ with $j_n \rightarrow \infty$ as $n \rightarrow \infty$, sufficient for $\left\| \widehat{\phi}_{j_n} - \widehat{\psi}_{j_n}^+ \right\| \rightarrow 0$ is the following:*

$$\frac{E_{j_{n+1}} - E_{j_n}}{E_{j_n} - E_{j_{n-1}}} \ll \sqrt{\frac{|\Phi_{j_n}(p)|^2 + |\Phi_{j_{n+1}}(p)|^2}{E_{j_{n-1}}}}, \quad (3.53)$$

$$\frac{E_{j_{n+1}} - E_{j_n}}{E_{j_{n+2}} - E_{j_{n+1}}} \ll \sqrt{\frac{|\Phi_{j_n}(p)|^2 + |\Phi_{j_{n+1}}(p)|^2}{E_{j_{n+2}}}} \quad (3.54)$$

as $n \rightarrow \infty$, where \ll is again the order relation $o(\cdot)$, defined in (2.34).

Proof. Firstly, (3.45) is a necessary and sufficient condition for $\left\| \widehat{\phi}_{j_n} - \widehat{\psi}_{j_n}^+ \right\| \rightarrow 0$. Now observe that sufficient for (3.45) is the following:

$$\sum_{k=1}^{j_n-1} \frac{|\Phi_k(p)|^2}{(E_k - E_{j_n})^2} + \sum_{k=j_{n+2}}^{\infty} \frac{|\Phi_k(p)|^2}{(E_k - E_{j_{n+1}})^2} \ll \frac{|\Phi_{j_n}(p)|^2 + |\Phi_{j_{n+1}}(p)|^2}{(E_{j_{n+1}} - E_{j_n})^2}, \quad (3.55)$$

since $\text{LHS}(3.55) > \text{LHS}(3.45)$ and $\text{RHS}(3.55) < \text{RHS}(3.45)$. Here we have removed the explicit appearance of λ_{j_n} . Note that the second term in $\text{LHS}(3.55)$ is convergent by Lemma 2.2.5.

Now if we fix some $M \in \mathbb{R} \setminus \{E_j\}_{j \in \mathbb{N}}$ independent of n , then for each sufficiently large n we have, by Lemma 2.1.7,

$$\begin{aligned} \sum_{k=1}^{j_n-1} \frac{|\Phi_k(p)|^2}{(E_k - E_{j_n})^2} &= \sum_{k:E_k < M} \frac{|\Phi_k(p)|^2}{(E_k - E_{j_n})^2} + \frac{N_p(E_{j_{n-1}})}{(E_{j_{n-1}} - E_{j_n})^2} - \frac{N_p(M)}{(M - E_{j_n})^2} \\ &\quad + 2 \int_M^{E_{j_{n-1}}} \frac{N_p(t)}{(t - E_{j_n})^3} dt. \end{aligned} \quad (3.56)$$

Likewise

$$\sum_{k=j_{n+2}}^{\infty} \frac{|\Phi_k(p)|^2}{(E_k - E_{j_{n+1}})^2} = -\frac{N_p(E_{j_{n+1}})}{(E_{j_{n+2}} - E_{j_{n+1}})^2} + 2 \int_{E_{j_{n+2}}}^{\infty} \frac{N_p(t)}{(t - E_{j_{n+1}})^3} dt, \quad (3.57)$$

noting that if we fix any $A > \frac{1}{4\pi}$, then for sufficiently large t we have by Corollary 2.1.6 (weaker form of Weyl's law),

$$0 < \frac{N_p(t)}{(t - E_{j_{n+1}})^2} \leq \frac{At}{(t - E_{j_{n+1}})^2} = \frac{A}{t - E_{j_{n+1}}} + \frac{AE_{j_{n+1}}}{(t - E_{j_{n+1}})^2} \xrightarrow{t \rightarrow \infty} 0, \quad (3.58)$$

and also noting obviously that $N_p^-(E_{j_{n+2}}) = N_p(E_{j_{n+1}})$.

We can now use Weyl's law to derive upper bounds on the expressions given in (3.56) and (3.57). With the stronger form of Weyl's law (Lemma 2.1.5), provided M is set to be sufficiently large, $\exists C > 0$ for which we have

$$\frac{E}{4\pi} - C\sqrt{E} \leq N_p(E) \leq \frac{E}{4\pi} + C\sqrt{E} \quad \forall E \geq M. \quad (3.59)$$

Thus

$$\begin{aligned} \sum_{k=1}^{j_n-1} \frac{|\Phi_k(p)|^2}{(E_k - E_{j_n})^2} &\leq \sum_{k:E_k < M} \frac{|\Phi_k(p)|^2}{(E_k - E_{j_n})^2} + \frac{\frac{E_{j_n-1}}{4\pi} + C\sqrt{E_{j_n-1}}}{(E_{j_n-1} - E_{j_n})^2} - \frac{\frac{M}{4\pi} - C\sqrt{M}}{(M - E_{j_n})^2} \\ &\quad + 2 \int_M^{E_{j_n-1}} \frac{\frac{t}{4\pi} - C\sqrt{t}}{(t - E_{j_n})^3} dt \\ &= \sum_{k:E_k \leq M} \frac{|\Phi_k(p)|^2}{(E_k - E_{j_n})^2} \\ &\quad + \frac{1}{4\pi} \left(\frac{E_{j_n-1}}{(E_{j_n-1} - E_{j_n})^2} - \frac{M}{(M - E_{j_n})^2} + 2 \int_M^{E_{j_n-1}} \frac{t}{(t - E_{j_n})^3} dt \right) \\ &\quad + C \left(\frac{\sqrt{E_{j_n-1}}}{(E_{j_n-1} - E_{j_n})^2} + \frac{\sqrt{M}}{(M - E_{j_n})^2} - 2 \int_M^{E_{j_n-1}} \frac{\sqrt{t}}{(t - E_{j_n})^3} dt \right). \end{aligned} \quad (3.60)$$

Likewise

$$\begin{aligned} \sum_{k=j_n+2}^{\infty} \frac{|\Phi_k(p)|^2}{(E_k - E_{j_n+1})^2} &\leq -\frac{\frac{E_{j_n+2}}{4\pi} - C\sqrt{E_{j_n+2}}}{(E_{j_n+2} - E_{j_n+1})^2} + 2 \int_{E_{j_n+2}}^{\infty} \frac{\frac{t}{4\pi} + C\sqrt{t}}{(t - E_{j_n+1})^3} dt \\ &= \frac{1}{4\pi} \left(-\frac{E_{j_n+2}}{(E_{j_n+2} - E_{j_n+1})^2} + 2 \int_{E_{j_n+2}}^{\infty} \frac{t}{(t - E_{j_n+1})^3} dt \right) \\ &\quad + C \left(\frac{\sqrt{E_{j_n+2}}}{(E_{j_n+2} - E_{j_n+1})^2} + 2 \int_{E_{j_n+2}}^{\infty} \frac{\sqrt{t}}{(t - E_{j_n+1})^3} dt \right). \end{aligned} \quad (3.61)$$

Note that for any E_j we have $N_p(E_j) = N_p(E) \quad \forall E \in [E_j, E_{j+1})$, and so provided E_j is sufficiently large,

$$\frac{E}{4\pi} - C\sqrt{E} \leq N_p(E_j) \leq \frac{E}{4\pi} + C\sqrt{E} \quad \forall E \in [E_j, E_{j+1}] \quad (3.62)$$

(obviously E_{j+1} can be included in the interval by continuity). Wherever in (3.60) and (3.61) estimates for some $N_p(E_j)$ have been involved, the choice of $E \in [E_j, E_{j+1}]$ has been made so as to optimise the tightness of these upper bounds for the two parts of LHS(3.55). This would probably in general only make a fairly minor difference though, if any.

Now $\int \sqrt{t}/(t - E_j)^3 dt$ may be rather difficult to compute and then analyse. Considering then upper bounds obtained via the weaker form of Weyl's law (Corollary 2.1.6), given any $\varepsilon > 0$ and sufficiently large $M \geq 0$ (where ‘‘sufficiently large’’ M would depend on the choice of ε) we have

$$\begin{aligned} \sum_{k=1}^{j_n-1} \frac{|\Phi_k(p)|^2}{(E_k - E_{j_n})^2} &\leq \sum_{k:E_k < M} \frac{|\Phi_k(p)|^2}{(E_k - E_{j_n})^2} \\ &+ \frac{1}{4\pi} \left(\frac{E_{j_n-1}}{(E_{j_n-1} - E_{j_n})^2} - \frac{M}{(M - E_{j_n})^2} + 2 \int_M^{E_{j_n-1}} \frac{t}{(t - E_{j_n})^3} dt \right) \\ &+ \varepsilon \left(\frac{E_{j_n-1}}{(E_{j_n-1} - E_{j_n})^2} + \frac{M}{(M - E_{j_n})^2} - 2 \int_M^{E_{j_n-1}} \frac{t}{(t - E_{j_n})^3} dt \right), \end{aligned} \quad (3.63)$$

$$\begin{aligned} \sum_{k=j_n+2}^{\infty} \frac{|\Phi_k(p)|^2}{(E_k - E_{j_n+1})^2} &\leq \frac{1}{4\pi} \left(-\frac{E_{j_n+2}}{(E_{j_n+2} - E_{j_n+1})^2} + 2 \int_{E_{j_n+2}}^{\infty} \frac{t}{(t - E_{j_n+1})^3} dt \right) \\ &+ \varepsilon \left(\frac{E_{j_n+2}}{(E_{j_n+2} - E_{j_n+1})^2} + 2 \int_{E_{j_n+2}}^{\infty} \frac{t}{(t - E_{j_n+1})^3} dt \right). \end{aligned} \quad (3.64)$$

Abbreviate (3.60), (3.61), (3.63) and (3.64) respectively as follows:

$$\sum_{k=1}^{j_n-1} \frac{|\Phi_k(p)|^2}{(E_k - E_{j_n})^2} \leq \mathcal{A}_n + \frac{1}{4\pi} \mathcal{B}_n + C\mathcal{C}_n, \quad (3.65)$$

$$\sum_{k=j_n+2}^{\infty} \frac{|\Phi_k(p)|^2}{(E_k - E_{j_n+1})^2} \leq \frac{1}{4\pi} \mathcal{F}_n + C\mathcal{G}_n, \quad (3.66)$$

$$\sum_{k=1}^{j_n-1} \frac{|\Phi_k(p)|^2}{(E_k - E_{j_n})^2} \leq \mathcal{A}_n + \frac{1}{4\pi} \mathcal{B}_n + \varepsilon \mathcal{C}'_n, \quad (3.67)$$

$$\sum_{k=j_n+2}^{\infty} \frac{|\Phi_k(p)|^2}{(E_k - E_{j_n+1})^2} \leq \frac{1}{4\pi} \mathcal{F}_n + \varepsilon \mathcal{G}'_n \quad (3.68)$$

(noting that for fixed C and ε , we can choose a common value of M for both the strong Weyl and weak Weyl estimates). It is easy to see already that $\mathcal{A}_n, \mathcal{C}_n, \mathcal{G}_n, \mathcal{C}'_n, \mathcal{G}'_n > 0$.

Now

$$\begin{aligned} \int_M^{E_{j_n-1}} \frac{t}{(t - E_{j_n})^3} dt &= -\frac{1}{E_{j_n-1} - E_{j_n}} - \frac{E_{j_n}}{2(E_{j_n-1} - E_{j_n})^2} \\ &+ \frac{1}{M - E_{j_n}} + \frac{E_{j_n}}{2(M - E_{j_n})^2}, \end{aligned} \quad (3.69)$$

(see (2.72)), and so

$$\mathcal{B}_n = \frac{1}{E_{j_n} - E_{j_{n-1}}} - \frac{1}{E_{j_n} - M} = \frac{E_{j_{n-1}} - M}{(E_{j_n} - E_{j_{n-1}})(E_{j_n} - M)} > 0. \quad (3.70)$$

Note also that

$$\mathcal{C}'_n = -\mathcal{B}_n + \frac{2E_{j_{n-1}}}{(E_{j_{n-1}} - E_{j_n})^2}. \quad (3.71)$$

Likewise

$$\int_{E_{j_{n+2}}}^{\infty} \frac{t}{(t - E_{j_{n+1}})^3} dt = \frac{1}{E_{j_{n+2}} - E_{j_{n+1}}} + \frac{E_{j_{n+1}}}{2(E_{j_{n+2}} - E_{j_{n+1}})^2} \quad (3.72)$$

(see (2.73)), and so

$$\mathcal{F}_n = \frac{1}{E_{j_{n+2}} - E_{j_{n+1}}} > 0, \quad (3.73)$$

$$\mathcal{G}'_n = \mathcal{F}_n + \frac{2E_{j_{n+2}}}{(E_{j_{n+2}} - E_{j_{n+1}})^2}. \quad (3.74)$$

It can now be stated that $\text{RHS}(3.65) \ll \text{RHS}(3.55)$ as $n \rightarrow \infty$ if and only if $\mathcal{A}_n, \mathcal{B}_n, \mathcal{C}_n \ll \text{RHS}(3.55)$, and likewise with $\text{RHS}(3.66)$, $\text{RHS}(3.67)$ and $\text{RHS}(3.68)$ (for each of these equations, taking whichever members of $\{\mathcal{A}_n, \mathcal{B}_n, \mathcal{C}_n, \mathcal{F}_n, \mathcal{G}_n, \mathcal{C}'_n, \mathcal{G}'_n\}$ appear in the equation).

Settling with the weaker Weyl estimates, observe firstly that a particular *necessary* condition for $\text{RHS}(3.67) \ll \text{RHS}(3.55)$ is

$$\frac{\mathcal{B}_n + \mathcal{C}'_n}{2} = \frac{E_{j_{n-1}}}{(E_{j_n} - E_{j_{n-1}})^2} \ll \frac{|\Phi_{j_n}(p)|^2 + |\Phi_{j_{n+1}}(p)|^2}{(E_{j_{n+1}} - E_{j_n})^2}. \quad (3.75)$$

This can be rearranged to obtain the following:

$$\frac{E_{j_{n+1}} - E_{j_n}}{E_{j_n} - E_{j_{n-1}}} \ll \sqrt{\frac{|\Phi_{j_n}(p)|^2 + |\Phi_{j_{n+1}}(p)|^2}{E_{j_{n-1}}}}. \quad (3.76)$$

Now let

$$\tilde{\mathcal{B}}_n := \frac{E_{j_{n-1}}}{E_{j_n}(E_{j_n} - E_{j_{n-1}})}, \quad (3.77)$$

so

$$\frac{\tilde{\mathcal{B}}_n}{\mathcal{B}_n} = \frac{E_{j_{n-1}}}{E_{j_{n-1}} - M} \cdot \frac{E_{j_n} - M}{E_{j_n}} \rightarrow 1, \quad (3.78)$$

and so $\mathcal{B}_n \ll \text{RHS}(3.55)$ if and only if $\tilde{\mathcal{B}}_n \ll \text{RHS}(3.55)$, i.e.

$$\frac{E_{j_{n-1}}}{E_{j_n}(E_{j_n} - E_{j_{n-1}})} \ll \frac{|\Phi_{j_n}(p)|^2 + |\Phi_{j_{n+1}}(p)|^2}{(E_{j_{n+1}} - E_{j_n})^2}. \quad (3.79)$$

Dividing both sides by $E_{j_n} - E_{j_{n-1}}$, rearranging and then taking square roots, we obtain

$$\frac{E_{j_{n+1}} - E_{j_n}}{E_{j_n} - E_{j_{n-1}}} \ll \sqrt{\frac{|\Phi_{j_n}(p)|^2 + |\Phi_{j_{n+1}}(p)|^2}{E_{j_{n-1}}}} \cdot \sqrt{\frac{E_{j_n}}{E_{j_n} - E_{j_{n-1}}}}. \quad (3.80)$$

Clearly if (3.76) is satisfied then (3.80) is automatically satisfied. Thus (3.76) is a sufficient condition for both $\mathcal{B}_n \ll \text{RHS}(3.55)$ and $\mathcal{C}'_n \ll \text{RHS}(3.55)$.

Now if $\{k : E_k < M\} \neq \emptyset$ then $\mathcal{A}_n \ll \text{RHS}(3.55)$ if and only if for each k with $E_k < M$,

$$\frac{|\Phi_k(p)|^2}{(E_k - E_{j_n})^2} \ll \frac{|\Phi_{j_n}(p)|^2 + |\Phi_{j_{n+1}}(p)|^2}{(E_{j_{n+1}} - E_{j_n})^2}, \quad (3.81)$$

which simplifies to

$$\frac{1}{E_{j_n}^2} \ll \frac{|\Phi_{j_n}(p)|^2 + |\Phi_{j_{n+1}}(p)|^2}{(E_{j_{n+1}} - E_{j_n})^2}, \quad (3.82)$$

which then rearranges to

$$E_{j_{n+1}} - E_{j_n} \ll E_{j_n} \sqrt{|\Phi_{j_n}(p)|^2 + |\Phi_{j_{n+1}}(p)|^2}. \quad (3.83)$$

Observe that (3.80) can be re-written as

$$E_{j_{n+1}} - E_{j_n} \ll \sqrt{E_{j_n}(|\Phi_{j_n}(p)|^2 + |\Phi_{j_{n+1}}(p)|^2)} \cdot \sqrt{\frac{E_{j_n} - E_{j_{n-1}}}{E_{j_{n-1}}}}. \quad (3.84)$$

Since $\sqrt{\frac{E_{j_n} - E_{j_{n-1}}}{E_{j_{n-1}}}} < \sqrt{E_{j_n}}$ for sufficiently large n , it follows that if (3.80)/(3.84) is satisfied then (3.83) is automatically satisfied.

We can now conclude that (3.76) is both a *necessary* and *sufficient* condition for $\text{RHS}(3.67) \ll \text{RHS}(3.55)$.

Moving on now to conditions for $\text{RHS}(3.68) \ll \text{RHS}(3.55)$, we have the following *necessary* condition:

$$\frac{\mathcal{G}'_n - \mathcal{F}_n}{2} = \frac{E_{j_{n+2}}}{(E_{j_{n+2}} - E_{j_{n+1}})^2} \ll \frac{|\Phi_{j_n}(p)|^2 + |\Phi_{j_{n+1}}(p)|^2}{(E_{j_{n+1}} - E_{j_n})^2}. \quad (3.85)$$

This rearranges to

$$\frac{E_{j_{n+1}} - E_{j_n}}{E_{j_{n+2}} - E_{j_{n+1}}} \ll \sqrt{\frac{|\Phi_{j_n}(p)|^2 + |\Phi_{j_{n+1}}(p)|^2}{E_{j_{n+2}}}}. \quad (3.86)$$

This is also a *sufficient* condition for $\text{RHS}(3.68) \ll \text{RHS}(3.55)$, because

$$\begin{aligned} \frac{\mathcal{G}'_n - \mathcal{F}_n}{2} &= \frac{E_{j_{n+2}}}{(E_{j_{n+2}} - E_{j_{n+1}})^2} = \frac{1}{E_{j_{n+2}} - E_{j_{n+1}}} \cdot \frac{E_{j_{n+2}}}{E_{j_{n+2}} - E_{j_{n+1}}} \\ &> \frac{1}{E_{j_{n+2}} - E_{j_{n+1}}} = \mathcal{F}_n, \end{aligned} \quad (3.87)$$

and so if (3.85)/(3.86) is satisfied, then it follows automatically that $\mathcal{F}_n \ll \text{RHS}(3.55)$. It then follows from (3.85)/(3.86) combined with $\mathcal{F}_n \ll \text{RHS}(3.55)$ that $\mathcal{G}'_n \ll \text{RHS}(3.55)$. \square

Observe that if for this $\{j_n\}$ sequence, $|\Phi_{j_n}(p)|^2 + |\Phi_{j_{n+1}}(p)|^2$ has a strictly positive lower bound (equivalently $\max\{|\Phi_{j_n}(p)|, |\Phi_{j_{n+1}}(p)|\}$ has a strictly positive lower bound), then *sufficient* for (3.53), (3.54) is:

$$\frac{E_{j_{n+1}} - E_{j_n}}{E_{j_n} - E_{j_{n-1}}} \ll \frac{1}{\sqrt{E_{j_{n-1}}}}, \quad (3.88)$$

$$\frac{E_{j_{n+1}} - E_{j_n}}{E_{j_{n+2}} - E_{j_{n+1}}} \ll \frac{1}{\sqrt{E_{j_{n+2}}}}. \quad (3.89)$$

If $|\Phi_{j_n}(p)|^2 + |\Phi_{j_{n+1}}(p)|^2$ is bounded above (equivalently $\max\{|\Phi_{j_n}(p)|, |\Phi_{j_{n+1}}(p)|\}$ is bounded above), then (3.88), (3.89) are *necessary* for (3.53), (3.54). Note that $\max\{|\Phi_{j_n}(p)|, |\Phi_{j_{n+1}}(p)|\}$ here simply means the larger of the two values for each n , rather than the maximum over the whole sequence.

3.5 Analysis of Results: Comparison with Result by Keating, Marklof and Winn

On the basis of having derived Thm. 3.4.1, subsequent results may be derived which are analogous to Thm. 4.4 in [KMW10], which again is stated here as Prop. 3.2.1. This will allow for clearer comparison with Thm. 4.4 in [KMW10].

Proposition 3.5.1. *Given a sequence $\{j_n\} \subseteq \mathbb{N}$ with $j_n \rightarrow \infty$ as $n \rightarrow \infty$, sufficient for $\left\| \widehat{\phi}_{j_n} - \widehat{\psi}_{j_n}^+ \right\| \rightarrow 0$ is the following:*

(i) $\exists q, \rho \in \mathbb{R}$ and sequence $(\varepsilon_n)_{n \in \mathbb{N}} \subset (0, \infty)$ such that

$$E_{j_{n+2}} \ll \varepsilon_n^{-\rho}, \quad (3.90)$$

$$E_{j_{n+1}} - E_{j_n} \ll \varepsilon_n, \quad (3.91)$$

$$E_{j_n} - E_{j_{n-1}} \gg \varepsilon_n^q, \quad (3.92)$$

$$E_{j_{n+2}} - E_{j_{n+1}} \gg \varepsilon_n^q, \quad (3.93)$$

$$\varepsilon_n^{1-q-\rho/2} \rightarrow 0 \quad (3.94)$$

as $n \rightarrow \infty$,

(ii) $\exists c_0 > 0$ s.t. $\max\{|\Phi_{j_n}(p)|, |\Phi_{j_{n+1}}(p)|\} \geq c_0 \forall n \in \mathbb{N}$.

Proof. Assume (3.90) - (3.93) hold true for some $q, \rho \in \mathbb{R}$ and sequence $(\varepsilon_n)_{n \in \mathbb{N}} \subset (0, \infty)$, and also assume condition (ii) holds. So then, for sufficiently large n , \exists constants $A, C, B_1, B_2 > 0$ such that

$$E_{j_n+2} \leq A\varepsilon_n^{-\rho}, \quad (3.95)$$

$$E_{j_n+1} - E_{j_n} \leq C\varepsilon_n, \quad (3.96)$$

$$E_{j_n} - E_{j_n-1} \geq B_1\varepsilon_n^q, \quad (3.97)$$

$$E_{j_n+2} - E_{j_n+1} \geq B_2\varepsilon_n^q. \quad (3.98)$$

It then follows that

$$\frac{(E_{j_n+1} - E_{j_n})\sqrt{E_{j_n-1}}}{E_{j_n} - E_{j_n-1}} \leq \frac{\sqrt{AC}}{B_1} \varepsilon_n^{1-q-\rho/2}, \quad (3.99)$$

$$\frac{(E_{j_n+1} - E_{j_n})\sqrt{E_{j_n+2}}}{E_{j_n+2} - E_{j_n+1}} \leq \frac{\sqrt{AC}}{B_2} \varepsilon_n^{1-q-\rho/2}. \quad (3.100)$$

Hence if $\varepsilon_n^{1-q-\rho/2} \xrightarrow{n \rightarrow \infty} 0$ then (3.88) and (3.89) are satisfied, and thus with condition (ii) also holding true, it follows that (3.53) and (3.54) are satisfied. \square

Observe that in condition (i), if it furthermore holds that $\varepsilon_n \rightarrow 0$ then from (3.90) - (3.93) it must follow that $\rho > 0$ and $q \geq -\rho$, since $E_{j_n+2} \rightarrow \infty$, $E_{j_n} - E_{j_n-1} < E_{j_n+2}$ and $E_{j_n+2} - E_{j_n+1} < E_{j_n+2}$. Then from (3.94) it would follow that $1 - q - \frac{\rho}{2} > 0$. Conversely, if in place of condition (i) we specify that $(\varepsilon_n)_{n \in \mathbb{N}} \subset (0, \infty)$ satisfies $\varepsilon_n \rightarrow 0$, $q, \rho \in \mathbb{R}$ satisfy

$$\rho > 0, \quad q \geq -\rho, \quad 1 - q - \frac{\rho}{2} > 0, \quad (3.101)$$

and (3.90) - (3.93) are satisfied, then it will follow that (3.94) is also satisfied. Thus together with condition (ii), it will follow that $\left| \widehat{\phi}_{j_n} - \widehat{\psi}_{j_n}^+ \right| \rightarrow 0$. [In fact, for (3.101) it would be sufficient simply to state $1 - q - \frac{\rho}{2} > 0$, since $\rho > 0$ and $q \geq -\rho$ would again follow automatically from (3.90) - (3.93)].

Finally, reworking (3.101) into a form more easily comparable with the inequalities on q and ρ stated in [KMW10], (3.101) can firstly be rewritten as follows:

$$\rho > 0, \quad -q \leq \rho < 2(1 - q). \quad (3.102)$$

This obviously requires $-q < 2(1 - q)$, equivalently $q < 2$. This also requires $2(1 - q) > 0$, equivalently $q < 1$. (3.102) can then be rewritten as follows:

$$q < 1, \quad \begin{cases} 0 < \rho < 2(1 - q) & \text{if } 0 \leq q < 1 \\ -q \leq \rho < 2(1 - q) & \text{if } q < 0. \end{cases} \quad (3.103)$$

Hence:

Corollary 3.5.2. *Given a sequence $\{j_n\} \subseteq \mathbb{N}$ with $j_n \rightarrow \infty$ as $n \rightarrow \infty$, sufficient for $\left\| \widehat{\phi}_{j_n} - \widehat{\psi}_{j_n}^+ \right\| \rightarrow 0$ is the following:*

(i) $\exists q, \rho \in \mathbb{R}$ satisfying

$$q < 1, \quad \begin{cases} 0 < \rho < 2(1 - q) & \text{if } 0 \leq q < 1 \\ -q \leq \rho < 2(1 - q) & \text{if } q < 0, \end{cases} \quad (3.104)$$

and sequence $(\varepsilon_n)_{n \in \mathbb{N}} \subset (0, \infty)$ with $\varepsilon_n \xrightarrow{n \rightarrow \infty} 0$, such that

$$E_{j_{n+2}} \ll \varepsilon_n^{-\rho}, \quad (3.105)$$

$$E_{j_{n+1}} - E_{j_n} \ll \varepsilon_n, \quad (3.106)$$

$$E_{j_n} - E_{j_{n-1}} \gg \varepsilon_n^q, \quad (3.107)$$

$$E_{j_{n+2}} - E_{j_{n+1}} \gg \varepsilon_n^q \quad (3.108)$$

as $n \rightarrow \infty$,

(ii) $\exists c_0 > 0$ s.t. $\max\{|\Phi_{j_n}(p)|, |\Phi_{j_{n+1}}(p)|\} \geq c_0 \forall n \in \mathbb{N}$.

Comparing then Cor. 3.5.2 here with Thm. 4.4 of [KMW10] (here Prop. 3.2.1) and Cor. 3.2.2, the inequalities on q and ρ stated in [KMW10] are:

$$0 < q < \frac{1}{2}, \quad 1 < \rho < 2(1 - q), \quad (3.109)$$

and those stated in Cor. 3.2.2 are:

$$-2 < q < \frac{1}{2}, \quad \begin{cases} 0 < \rho < 2(1 - q) & \text{if } 0 \leq q < \frac{1}{2} \\ -q \leq \rho < 2 & \text{if } -2 < q < 0. \end{cases} \quad (3.110)$$

(3.104) is weaker than both (3.109) and (3.110).

Hence condition (i) in Cor. 3.5.2 is weaker than condition (i) in Thm. 4.4 of [KMW10]. Likewise, condition (ii) in Cor. 3.5.2 is clearly weaker than condition (ii) in Thm. 4.4 of [KMW10]. Observe also, from the above derivations of Prop. 3.5.1 and Cor. 3.5.2, that conditions (i) and (ii) together from Cor. 3.5.2 imply (3.53) and (3.54) from Thm. 3.4.1. Hence (3.53) and (3.54) together from Thm. 3.4.1 are weaker than conditions (i) and (ii) together from Thm. 4.4 of [KMW10].

Obviously, *weakening* the *conditions* of a proposition will *strengthen* the proposition, as will *strengthening* the *conclusion* of the proposition. Now from Thm. 4.4 of [KMW10] to Thm. 3.4.1, Prop. 3.5.1 or Cor. 3.5.2, there is a weakening of conditions, as has been

demonstrated. However, it follows from Prop. 3.3.3 that the $\left\| \widehat{\phi}_{j_n} - \widehat{\psi}_{j_n}^+ \right\| \rightarrow 0$ conclusion in Thm. 3.4.1, Prop. 3.5.1 and Cor. 3.5.2 is also weaker than the $\left\| \widehat{\phi}_{j_n} - e^{i\theta_n} \widehat{\psi}_{j_n}^\circ \right\| \rightarrow 0$ conclusion in Thm. 4.4 of [KMW10].

Finally, remember again that in Thm. 4.4 of [KMW10], a statement is made only for the case where $\Theta = \pi$. However, all of the results in §3.3, 3.4 and 3.5 here apply for any perturbed operator H_Θ with $\Theta \in (0, 2\pi)$.

Chapter 4

Approximation of the Delta Potential by Non-Singular Rank-One Perturbations

4.1 Overview

The delta potential is not a smooth potential, but rather a *singular* potential, being concentrated at the point $p \in \mathcal{M}^\circ$. However, one can address the task of constructing a sequence of self-adjoint operators, constituting *non-singular* perturbations of the self-adjoint $-\Delta$ operator H , which nevertheless approach the delta-perturbed operator H_Θ . This shall be the subject of this Chapter.

By analogy with (2.53), one could consider perturbing H by a multiplication operator which approaches the delta potential. In other words, letting $(H^N)_{N \in \mathbb{N}}$ be the sequence of self-adjoint operators involving non-singular perturbations of H ,

$$H^N \psi = H\psi + \nu_N V_N \psi, \quad (4.1)$$

with $\nu_N \in \mathbb{R}$, $V_N \in C^\infty(\mathcal{M}^\circ, \mathbb{R}) \cap L^\infty(\mathcal{M})$ and $V_N \rightarrow \delta_p$. Alternatively, by analogy with (2.56), one could consider perturbing H by a rank-one operator which approaches the delta potential. In other words,

$$H^N \psi = H\psi + \nu_N \langle \psi, Y_N \rangle Y_N, \quad (4.2)$$

with $\nu_N \in \mathbb{R}$, $Y_N \in C^\infty(\mathcal{M}^\circ) \cap L^2(\mathcal{M})$ and $Y_N \rightarrow \delta_p$.

The latter approach, involving rank-one perturbations, shall be taken within the investigations in this Chapter.

Studies which have already been carried out in the problem of approximating delta potentials by non-singular potentials can be found for example in [BF61], [Zor80], [AGHHE88], [AK00] and [GN12]. These however, work mainly within the setting of a whole Euclidean space \mathbb{R}^n , rather than a compact manifold. Approach of a sequence of self-adjoint operators towards the delta potential has been studied within these works, particularly by considering *strong resolvent convergence*, *norm resolvent convergence*, and behaviour of spectrum and corresponding “generalised eigenfunctions”.

For the investigations in this Chapter, convergence of eigenvalues and eigenfunctions of H^N towards those of H_Θ shall be examined. This shall be via means of direct analysis of the constructions of these eigenvalues and eigenfunctions, paying attention to the formulae involved.

Within the study of semiclassical analysis involving high-energy limits, there are a variety of results which can be applied quite generally to self-adjoint quantum Hamiltonian operators of appropriate form. See for example [Sch01]. It could happen then that such results may apply for non-singular perturbations of H approaching H_Θ . One could then be interested in deriving results in the high-energy limit for the delta-perturbed operator H_Θ , on the basis of these non-singular approximations of the delta potential.

To such an end, it may be of interest to examine how the eigenvalues and eigenfunctions of the approximating operators approach those of the delta-perturbed operator. In particular, it may be of interest to examine their *rate of convergence*, especially because there are two limits involved here, namely the high-energy limit, and the approach towards the delta potential. It would be of interest to be able to swap the order of these two limits, and for this, rate of convergence is relevant. See for example, Lemmas 4.4.8 and 4.4.9, and Cor. 4.4.10, later on in this Chapter.

The results stated in this Chapter give statements about convergence of eigenvalues and eigenfunctions, but not statements about their rate of convergence. Nevertheless, due to this method involving direct analysis of the constructions and formulae, analysing the means of development of these results may be a helpful starting point if one does wish to analyse rate of convergence.

Outlining the structure of this Chapter, in §4.2 is a review of work already done, particularly [Zor80], followed by discussion of suggestions for adaptation from the whole Euclidean space \mathbb{R}^2 to the two-dimensional compact manifold \mathcal{M} . Basic features of rank-one perturbations are also stated and proved within §4.2. In §4.3, a construction is derived for an orthonormal eigenbasis of a rank-one perturbation of H , together with

the corresponding eigenvalues. The construction of the eigenbasis and eigenvalues of H_Θ is also restated in such a way as to demonstrate clear resemblance. Based on this resemblance, in §4.4, results are derived regarding convergence of eigenvalues and eigenfunctions of rank-one-perturbed operators to those of the delta-perturbed operator.

The central result of this Chapter is Theorem 4.4.19 in §4.4.4. This theorem specifies conditions for a sequence of rank-one-perturbed operators $(H^N)_{N \in \mathbb{N}}$ and an interval $[E_K, E_L]$ under which all eigenvalues of H^N in $[E_K, E_L]$ and corresponding eigenbasis members converge to those of the delta-perturbed operator H_Θ .

Leading up to this, §4.4.1 deals with convergence of “old” eigenfunctions for each “old” eigenvalue, §4.4.2 deals with convergence of “new” eigenvalues and §4.4.3 deals with convergence of “new” eigenfunctions. In §4.4.1 only a basic condition is assumed on the limiting behaviour of the coefficients in the H -eigenbasis expansion of Y_N . The mathematical analysis involved in §4.4.1 largely corresponds simply to analysis on a finite-dimensional Hilbert space. In §4.4.2 and 4.4.3 it is found that further conditions on (Y_N) and (ν_N) are needed. Some significant results within §4.4.2 and 4.4.3 are Propositions 4.4.6, 4.4.12, 4.4.16 and 4.4.18. Lemmas 4.4.8 and 4.4.9, and Cor. 4.4.10, dealing with the question of when the order of two nested limits can be swapped, prove to be particularly useful mathematical tools in §4.4.2 and 4.4.3.

Regarding attainability of the conditions in Theorem 4.4.19, relevant results are Lemma 4.4.14, Prop. 4.4.20 and Cor. 4.4.22.

4.2 Introducing Rank-One Perturbations and their Use as Approximations

4.2.1 Review of Work by Zorbas on Whole Euclidean Space

In [Zor80], methods of constructing operators formally expressed in the form

$$-\Delta + V(x) + \sum_{j=1}^N \nu_j \delta(x - a_j), \quad (4.3)$$

on Euclidean spaces \mathbb{R}^1 and \mathbb{R}^3 , are discussed. The failure of these methods in dimension ≥ 4 is also discussed. Some of this paper focusses specifically on the case of a single delta spike at the origin:

$$-\Delta + V(x) + \nu \delta(x). \quad (4.4)$$

Here we shall review the relevant work in [Zor80], focussing only on the rigorous formulations of (4.4) with $V = 0$, since the addition of any potential beside that of a

single delta-scatterer will not be of particular relevance for our consideration.

Such delta-perturbed operators are constructed first of all by means of self-adjoint extension theory, and the construction is very much akin to that described in §2.2.3. Let H_\circ be the unperturbed self-adjoint $-\Delta$ acting within $L^2(\mathbb{R}^n)$, where $n = 1$ or 3 , and let $\mathcal{D} := \{\phi \in \text{Dom}(H_\circ) : \phi(0) = 0\}$. For each $\theta \in [0, 2\pi)$ there is then a perturbed self-adjoint operator K_θ whose domain consists of all functions ψ of the form

$$\psi = \phi + c \left(G(\cdot, 0; i) + e^{i\theta} G(\cdot, 0; -i) \right), \quad (4.5)$$

with $\phi \in \mathcal{D}$ and $c \in \mathbb{C}$. Here $G(\cdot, 0; i)$ is the equivalent of g_i in \mathbb{R}^n and $G(\cdot, 0; -i)$ is the equivalent of g_{-i} in \mathbb{R}^n . The operation of K_θ on ψ is then

$$K_\theta \psi = H_\circ \phi + c \left(iG(\cdot, 0; i) - ie^{i\theta} G(\cdot, 0; -i) \right). \quad (4.6)$$

By comparison with Lemma 2.2.6, it is evident that K_π coincides with the unperturbed operator H_\circ .

Now in §VIII of [Zor80], a sequence of operators is constructed which converges to the operator K_θ in the *strong resolvent sense*. This strong resolvent convergence forms another method of rigorous construction of self-adjoint operators associated with the formal expression (4.4).

Definition. Given a sequence of self-adjoint operators $(T_N)_{N \in \mathbb{N}}$ acting within a Hilbert space \mathcal{H} , and another self-adjoint operator T acting within \mathcal{H} , it is said that $T_N \xrightarrow{N \rightarrow \infty} T$ in the *strong resolvent sense* if

$$(\lambda - T_N)^{-1} v \xrightarrow{N \rightarrow \infty} (\lambda - T)^{-1} v \quad \forall v \in \mathcal{H}, \lambda \in \mathbb{C} \setminus \mathbb{R}. \quad (4.7)$$

The operators $(\lambda - T_N)^{-1}$ and $(\lambda - T)^{-1}$ here will always be well-defined bounded linear operators on \mathcal{H} when $\lambda \in \mathbb{C} \setminus \mathbb{R}$. For discussion on strong resolvent (and also *norm resolvent*) convergence, see §VIII.7 of [RS80].

From Thm. 8.1 in §VIII of [Zor80], we have the following:

Proposition 4.2.1. *For each $N \in \mathbb{N}$ define an operator H^N acting within $L^2(\mathbb{R}^n)$ by the following:*

$$\mathcal{F}\{H^N \psi\}(\xi) = \mathcal{F}\{H_\circ \psi\}(\xi) + \frac{1}{(2\pi)^n} \nu_N \chi_N(\xi) \int_{\mathbb{R}^n} \chi_N(\omega) \widehat{\psi}(\omega) d\omega, \quad (4.8)$$

where $\mathcal{F}\{f\}(\xi)$ or $\widehat{f}(\xi)$ is the Fourier transform of f evaluated at ξ , $(\nu_N)_{N \in \mathbb{N}} \subset \mathbb{R}$ and $(\chi_N)_{N \in \mathbb{N}} \subset C_0^\infty(\mathbb{R}^n, [0, 1])$, with

$$\chi_N(\xi) := \begin{cases} 1 & \text{if } \|\xi\| \leq N \\ 0 & \text{if } \|\xi\| \geq N + 1. \end{cases} \quad (4.9)$$

If $n = 1$, then given any $\theta \in [0, 2\pi) \setminus \{\frac{3\pi}{2}\}$, H^N converges to K_θ in the strong resolvent sense if

$$\nu_N = -\frac{2 \cos\left(\frac{\theta}{2}\right)}{\cos\left(\frac{\theta}{2} - \frac{\pi}{4}\right)} \quad \forall N \in \mathbb{N}. \quad (4.10)$$

If $n = 3$, then given any $\theta \in [0, 2\pi) \setminus \{\pi\}$, H^N converges to K_θ in the strong resolvent sense if

$$\nu_N = -\frac{8\pi^3}{4\pi N - 2\pi^2\beta + \gamma_N} \quad (4.11)$$

\forall suff. large $N \in \mathbb{N}$, where

$$\beta = -\frac{\sin\left(\frac{\theta}{2} - \frac{\pi}{4}\right)}{\cos\left(\frac{\theta}{2}\right)}, \quad (4.12)$$

$$\gamma_N = \frac{1}{1 + e^{i\theta}} \left\{ \int_{N \leq \|q\| \leq N+1} \frac{(\chi_N(q))^2}{\|q\|^2 - i} dq + e^{i\theta} \int_{N \leq \|q\| \leq N+1} \frac{(\chi_N(q))^2}{\|q\|^2 + i} dq \right\}. \quad (4.13)$$

This is proved in [Zor80] via means of proving that K_θ is the *strong graph limit* of H^N (see again §VIII.7 of [RS80]). This in turn is proved by showing that for every $\psi \in \text{Dom}(K_\theta)$ there exists $\psi_N \in \text{Dom}(H^N)$ such that $\psi_N \rightarrow \psi$ and $H^N \psi_N \rightarrow K_\theta \psi$. A formula for ψ_N is given in [Zor80] based on the decomposition of ψ given by (4.5).

Remarks. (a) It is not explicitly stated in [Zor80] that the image of χ_N (within $N < \|\xi\| < N + 1$) is to be restricted to $[0, 1]$. However, in light of the analysis in the following subsection, it is reasonable to assume χ_N to be real-valued in order to ensure self-adjointness. It is also reasonable to assume $(\chi_N)_{N \in \mathbb{N}}$ to be uniformly bounded in order to ensure the δ -like limiting behaviour of $\mathcal{F}^{-1}\{\chi_N\}$ which shall be demonstrated. Such conditions on χ_N may therefore have been assumed in [Zor80], despite not being stated plainly. As such, having the image of χ_N be restricted to $[0, 1]$ seems to be a reasonable “safety assumption”.

(b) With $n = 1$ we see a well-defined strength ν of delta potential associated with each operator K_θ , except for $K_{3\pi/2}$, which evidently corresponds to $\nu = \pm\infty$. Observe also that associated with K_π is $\nu = 0$. However, with $n = 3$, as shall be shown in the following subsection, for every K_θ other than K_π , the strength ν_N is negative real-valued for sufficiently large N and tends to zero.

(c) The original statement of this theorem in [Zor80] allows for the addition of a potential V beside the delta potential, provided V belongs to an appropriate class of functions, as specified in [Zor80]. However, for our purposes here, it will suffice to have $V = 0$.

4.2.2 Further Analysis of Result by Zorbas

There is more than one convention for the precise definition of the Fourier transform, but in general it would take the form:

$$\mathcal{F}\{f\}(\xi) := A \int_{\mathbb{R}^n} f(x) e^{-iB\xi \cdot x} dx \quad (4.14)$$

for $f \in L^1(\mathbb{R}^n)$, where A and B are real constants (usually both positive). There is also a standard extension of the Fourier transform to the space of *tempered distributions* $\mathcal{S}'(\mathbb{R}^n)$.

Tempered distributions are distributions for which the space of test functions (that is, the domain of these distributions as linear functionals) is not $C_0^\infty(\mathbb{R}^n)$ but a larger space known as *Schwartz space* $\mathcal{S}(\mathbb{R}^n)$ (also known as the space of *rapidly decreasing functions*). Schwartz space is the space of functions $u \in C^\infty(\mathbb{R}^n)$ for which $x_1^{\alpha_1} \dots x_n^{\alpha_n} \partial_{x_1}^{\beta_1} \dots \partial_{x_n}^{\beta_n} u$ is a bounded function for every choice of $\alpha_1, \dots, \alpha_n, \beta_1, \dots, \beta_n \in \{0\} \cup \mathbb{N}$. For each $p \in [1, \infty) \cup \{\infty\}$,

$$C_0^\infty(\mathbb{R}^n) \subset \mathcal{S}(\mathbb{R}^n) \subset L^p(\mathbb{R}^n) \subset \mathcal{S}'(\mathbb{R}^n) \subset \mathcal{D}'(\mathbb{R}^n). \quad (4.15)$$

The Fourier transform maps $\mathcal{S}(\mathbb{R}^n) \rightarrow \mathcal{S}(\mathbb{R}^n)$, $\mathcal{S}'(\mathbb{R}^n) \rightarrow \mathcal{S}'(\mathbb{R}^n)$ and $L^2(\mathbb{R}^n) \rightarrow L^2(\mathbb{R}^n)$ bijectively. It also maps $L^1(\mathbb{R}^n) \rightarrow C(\mathbb{R}^n) \cap L^\infty(\mathbb{R}^n)$ injectively but not surjectively. Furthermore, the Fourier transform of every compactly supported distribution is C^∞ -smooth and even analytic (see §10.2, 11.1 of [FJ98]).

With $A = B = 1$, the inverse Fourier transform is given by:

$$\mathcal{F}^{-1}\{\hat{f}\}(x) := f(x) = \frac{1}{(2\pi)^n} \int_{\mathbb{R}^n} \hat{f}(\xi) e^{i\xi \cdot x} d\xi, \quad (4.16)$$

where $\hat{}$ represents the Fourier transform, so then for general $A, B > 0$:

$$\mathcal{F}^{-1}\{\hat{f}\}(x) := f(x) = \frac{1}{(2\pi)^n} \int_{\mathbb{R}^n} \frac{1}{A} \hat{f}\left(\frac{1}{B}\xi\right) e^{i\xi \cdot x} d\xi = \frac{1}{A} \left(\frac{B}{2\pi}\right)^n \int_{\mathbb{R}^n} \hat{f}(k) e^{iBk \cdot x} dk. \quad (4.17)$$

Furthermore, with $A = 1$ and $B = 2\pi$, the Fourier transform as a bijective operator from $L^2(\mathbb{R}^n)$ to $L^2(\mathbb{R}^n)$ is unitary, meaning that the L^2 inner product is preserved under the Fourier transform:

$$\int_{\mathbb{R}^n} \hat{f}(\xi) \overline{\hat{g}(\xi)} d\xi = \int_{\mathbb{R}^n} f(x) \overline{g(x)} dx. \quad (4.18)$$

Thus for general $A, B > 0$:

$$\begin{aligned} \int_{\mathbb{R}^n} \hat{f}(\xi) \overline{\hat{g}(\xi)} d\xi &= \left(\frac{2\pi}{B}\right)^n \int_{\mathbb{R}^n} \hat{f}\left(\frac{2\pi}{B}k\right) \overline{\hat{g}\left(\frac{2\pi}{B}k\right)} dk \\ &= A^2 \left(\frac{2\pi}{B}\right)^n \int_{\mathbb{R}^n} \frac{1}{A} \hat{f}\left(\frac{2\pi}{B}k\right) \overline{\frac{1}{A} \hat{g}\left(\frac{2\pi}{B}k\right)} dk = A^2 \left(\frac{2\pi}{B}\right)^n \int_{\mathbb{R}^n} f(x) \overline{g(x)} dx. \end{aligned} \quad (4.19)$$

Equation (4.19) also has a distributional extension whereby, if the g function is in \mathcal{S} , then the f function can be any member of \mathcal{S}' (see e.g. §1.1, 1.2 of [Sai91] or §3.3, 3.4 of [Tay96a]). In particular, if $g \in \mathcal{S}$ then the equation works for any $f \in L^p \cap \mathcal{F}^{-1}(L^q)$, $p, q \in [1, \infty]$.

It is not explicitly stated precisely what convention for the Fourier transform is used in [Zor80], but assuming it takes the form given in (4.14) with $A, B > 0$, and letting Z_N be the inverse Fourier transform of χ_N , it follows from (4.19) that

$$\int_{\mathbb{R}^n} \widehat{\psi}(\omega) \chi_N(\omega) d\omega = A^2 \left(\frac{2\pi}{B} \right)^n \int_{\mathbb{R}^n} \psi(y) \overline{Z_N(y)} dy. \quad (4.20)$$

Thus taking the inverse Fourier transform of both sides of (4.8), we have:

$$\begin{aligned} H^N \psi(x) &= H_\circ \psi(x) + \frac{A^2}{B^n} \nu_N Z_N(x) \int_{\mathbb{R}^n} \psi(y) \overline{Z_N(y)} dy \\ &= H_\circ \psi(x) + \frac{A^2}{B^n} \nu_N \langle \psi, Z_N \rangle Z_N(x). \end{aligned} \quad (4.21)$$

Establishing then the self-adjointness of H^N , we have the following two lemmas:

Lemma 4.2.2. *On a Hilbert space \mathcal{H} , a linear operator $T : \mathcal{H} \rightarrow \mathcal{H}$ is bounded, self-adjoint and rank-one if and only if $\exists v \in \mathcal{H} \setminus \{0\}$, $\alpha \in \mathbb{R} \setminus \{0\}$ such that*

$$Tu = \alpha \langle u, v \rangle v \quad \forall u \in \mathcal{H}. \quad (4.22)$$

Proof. Clearly T is a bounded rank-one operator if and only if $\exists v \in \mathcal{H} \setminus \{0\}$ and a nonzero bounded linear functional $\sigma : \mathcal{H} \rightarrow \mathbb{R}$ such that $T = \sigma v$. Then by the Riesz representation theorem, $\exists w \in \mathcal{H} \setminus \{0\}$ such that $\sigma = \langle \cdot, w \rangle$. Likewise every operator of the form $\langle \cdot, w \rangle$ with $w \neq 0$ is a nonzero bounded linear functional.

So then, T is a bounded rank-one operator if and only if it can be expressed in the form $T = \langle \cdot, w \rangle v$, with $v, w \neq 0$. Suppose then we do have $T = \langle \cdot, w \rangle v$ with $v, w \neq 0$. Let $S := \langle \cdot, v \rangle w$. Then

$$\langle T\phi, \psi \rangle = \langle \langle \phi, w \rangle v, \psi \rangle = \langle \phi, w \rangle \langle v, \psi \rangle = \langle \phi, \langle \psi, v \rangle w \rangle = \langle \phi, S\psi \rangle \quad \forall \phi, \psi \in \mathcal{H}, \quad (4.23)$$

so $T^* = S$. If then T is self-adjoint, i.e. $S = T$, then

$$Sv = \langle v, v \rangle w = Tv = \langle v, w \rangle v \xrightarrow{\langle v, v \rangle \neq 0} w = \frac{\langle v, w \rangle}{\langle v, v \rangle} v =: \alpha v, \quad \alpha \neq 0. \quad (4.24)$$

Note also that

$$\langle w, v \rangle = \langle \alpha v, v \rangle = \alpha \langle v, v \rangle = \frac{\langle v, w \rangle}{\langle v, v \rangle} \langle v, v \rangle = \langle v, w \rangle \Rightarrow \langle v, w \rangle \in \mathbb{R} \xrightarrow{\langle v, v \rangle \in \mathbb{R}} \alpha \in \mathbb{R}. \quad (4.25)$$

Thus

$$Tu = \langle u, w \rangle v = \langle u, \alpha v \rangle v = \alpha \langle u, v \rangle v. \quad (4.26)$$

Conversely, suppose we are given an operator T of the form $T = \alpha \langle \cdot, v \rangle v$ with $v \in \mathcal{H} \setminus \{0\}$, $\alpha \in \mathbb{R} \setminus \{0\}$. Then $T = \langle \cdot, v \rangle (\alpha v)$ so

$$T^* = \langle \cdot, \alpha v \rangle v = \bar{\alpha} \langle \cdot, v \rangle v = \alpha \langle \cdot, v \rangle v = T, \quad (4.27)$$

so T is self-adjoint. \square

Lemma 4.2.3. *On a Hilbert space \mathcal{H} , if $T : \text{Dom}(T) \subset \mathcal{H} \rightarrow \mathcal{H}$, with $\text{Dom}(T)$ being dense in \mathcal{H} , is a self-adjoint operator, and $B : \mathcal{H} \rightarrow \mathcal{H}$ is a bounded self-adjoint operator, then $T + B : \text{Dom}(T) \rightarrow \mathcal{H}$ is a self-adjoint operator.*

Proof. Firstly given any $v \in \text{Dom}(T)$, we have

$$\begin{aligned} \langle (T + B)u, v \rangle &= \langle Tu, v \rangle + \langle Bu, v \rangle = \langle u, Tv \rangle + \langle u, Bv \rangle \\ &= \langle u, (T + B)v \rangle \quad \forall u \in \text{Dom}(T), \end{aligned} \quad (4.28)$$

so $\text{Dom}((T + B)^*) \supset \text{Dom}(T)$ with $(T + B)^*v = (T + B)v \quad \forall v \in \text{Dom}(T)$.

Next, given any $v \in \text{Dom}((T + B)^*)$, we have

$$\begin{aligned} \langle u, (T + B)^*v \rangle &= \langle (T + B)u, v \rangle = \langle Tu, v \rangle + \langle Bu, v \rangle = \langle Tu, v \rangle + \langle u, Bv \rangle \\ \Rightarrow \langle Tu, v \rangle &= \langle u, (T + B)^*v \rangle - \langle u, Bv \rangle = \langle u, ((T + B)^* - B)v \rangle \quad \forall u \in \text{Dom}(T), \end{aligned} \quad (4.29)$$

so $v \in \text{Dom}(T^*) = \text{Dom}(T)$ (with $Tv = T^*v = ((T + B)^* - B)v \Rightarrow (T + B)^*v = (T + B)v$). Thus $\text{Dom}((T + B)^*) \subset \text{Dom}(T)$, and hence $\text{Dom}((T + B)^*) = \text{Dom}(T)$. \square

Hence H^N is indeed self-adjoint.

Approach Towards the Delta Function

Observe that χ_N loosely speaking approaches the constant function 1 as $N \rightarrow \infty$, and that $\mathcal{F} \left\{ \frac{1}{A} \delta \right\} = 1$, suggesting therefore that Z_N loosely speaking approaches $\frac{1}{A} \delta$. This then suggests that we have the following:

$$\begin{aligned} \frac{A^2}{B^n} Z_N(x) \int_{\mathbb{R}^n} \psi(y) \overline{Z_N(y)} dy &\xrightarrow{N \rightarrow \infty} \frac{1}{B^n} \delta(x) \int_{\mathbb{R}^n} \psi(y) \overline{\delta(y)} dy \\ &= \frac{1}{B^n} \delta(x) \int_{\mathbb{R}^n} \overline{\psi(y) \delta(y)} dy = \frac{1}{B^n} \psi(0) \delta(x) = \frac{1}{B^n} \delta(x) \psi(x). \end{aligned} \quad (4.30)$$

So then, for large N we have:

$$H^N \approx H_\circ + \frac{1}{B^n} \nu_N \langle \cdot, \delta \rangle \delta = H_\circ + \frac{1}{B^n} \nu_N \delta. \quad (4.31)$$

It seems likely then that in [Zor80] a convention for the Fourier transform is assumed in which $B = 1$.

More rigorously, observe firstly that $Z_N \in \mathcal{S}(\mathbb{R}^n)$ and

$$\int_{\mathbb{R}^n} Z_N(x) dx = \frac{1}{A} \mathcal{F}\{Z_N\}(0) = \frac{1}{A} \chi_N(0) = \frac{1}{A}. \quad (4.32)$$

Secondly, recall that $\chi_N(\xi) \in [0, 1] \forall \xi \in \mathbb{R}^n \forall N \in \mathbb{N}$, so in particular then, $|1 - \chi_N(\xi)| \leq 1 \forall \xi \in \mathbb{R}^n \forall N \in \mathbb{N}$. Let $\mathcal{B}_N^{(n)} := \{\xi \in \mathbb{R}^n : \|\xi\| < N\}$, so $1 - \chi_N(\xi) = 0 \forall \xi \in \mathcal{B}_N^{(n)}$. Take some $\psi \in \mathcal{F}(L^1(\mathbb{R}^n))$, noting that

$$\mathcal{S}(\mathbb{R}^n) \subset \mathcal{F}(L^1(\mathbb{R}^n)) = \mathcal{F}^{-1}(L^1(\mathbb{R}^n)) \subset C(\mathbb{R}^n) \cap L^\infty(\mathbb{R}^n) \subset \mathcal{S}'(\mathbb{R}^n). \quad (4.33)$$

Then

$$\begin{aligned} & \left| \frac{1}{A} \psi(0) - \int_{\mathbb{R}^n} \psi Z_N \right| = \left| \frac{1}{A} \mathcal{F}^{-1}\{\widehat{\psi}\}(0) - \int_{\mathbb{R}^n} \psi Z_N \right| \\ &= \left| \frac{1}{A^2} \left(\frac{B}{2\pi}\right)^n \int_{\mathbb{R}^n} \widehat{\psi} - \frac{1}{A^2} \left(\frac{B}{2\pi}\right)^n \int_{\mathbb{R}^n} \widehat{\psi} \overline{\mathcal{F}\{Z_N\}} \right| \\ &= \frac{1}{A^2} \left(\frac{B}{2\pi}\right)^n \left| \int_{\mathbb{R}^n} \widehat{\psi}(\xi) (1 - \chi_N(-\xi)) d\xi \right| \\ &\leq \frac{1}{A^2} \left(\frac{B}{2\pi}\right)^n \int_{\mathbb{R}^n \setminus \mathcal{B}_N^{(n)}} |\widehat{\psi}(\xi) (1 - \chi_N(-\xi))| d\xi \\ &\leq \frac{1}{A^2} \left(\frac{B}{2\pi}\right)^n \int_{\mathbb{R}^n \setminus \mathcal{B}_N^{(n)}} |\widehat{\psi}| \xrightarrow{N \rightarrow \infty} 0, \end{aligned} \quad (4.34)$$

so

$$\int_{\mathbb{R}^n} \psi(x) Z_N(x) dx \xrightarrow{N \rightarrow \infty} \frac{1}{A} \psi(0). \quad (4.35)$$

It then follows that as members of $\mathcal{S}'(\mathbb{R}^n)$:

$$Z_N \xrightarrow[\text{weak}^*]{N \rightarrow \infty} \frac{1}{A} \delta, \quad (4.36)$$

meaning that if we consider the representation of Z_N and $\frac{1}{A} \delta$ as linear functionals on $\mathcal{S}(\mathbb{R}^n)$, we have

$$\langle u, Z_N \rangle_u \xrightarrow{N \rightarrow \infty} \left\langle u, \frac{1}{A} \delta \right\rangle_u \quad \forall u \in \mathcal{S}(\mathbb{R}^n) \quad (4.37)$$

(see §3.4 of [Tay96a]). Again the subscript ll means linearity in both arguments, rather than conjugate-linearity in one of the arguments. Note also that if in (4.34), the appearance of Z_N is replaced with $\overline{Z_N}$, then the only effect this will have is to change the appearance of $\chi_N(-\xi)$ to $\chi_N(\xi)$, and thus

$$\int_{\mathbb{R}^n} \psi(x) \overline{Z_N(x)} dx \xrightarrow{N \rightarrow \infty} \frac{1}{A} \psi(0) \quad \forall \psi \in \mathcal{F}(L^1(\mathbb{R}^n)). \quad (4.38)$$

Strength of the Rank-One Perturbation

Now regarding the behaviour of ν_N , in dimension 1 it is clear from (4.10) that ν_N is an N -independent real value for each $\theta \in [0, 2\pi) \setminus \{\frac{3\pi}{2}\}$. For dimension 3, we shall verify that ν_N , as given by (4.11), (4.12) and (4.13), is indeed real-valued for each $\theta \in [0, 2\pi) \setminus \{\pi\}$ and sufficiently large N . We shall also determine its basic limiting behaviour as $N \rightarrow \infty$.

To this end, note firstly that

$$\frac{1}{1 + e^{i\theta}} = \frac{1 + e^{-i\theta}}{2(1 + \cos \theta)}, \quad \frac{e^{i\theta}}{1 + e^{i\theta}} = \frac{1 + e^{i\theta}}{2(1 + \cos \theta)}. \quad (4.39)$$

Thus from (4.13),

$$\begin{aligned} \gamma_N &= \int_{N \leq \|q\| \leq N+1} (\chi_N(q))^2 \left\{ \frac{1}{(1 + e^{i\theta})(\|q\|^2 - i)} + \frac{e^{i\theta}}{(1 + e^{i\theta})(\|q\|^2 + i)} \right\} dq \\ &= \int_{N \leq \|q\| \leq N+1} (\chi_N(q))^2 \left\{ \frac{1 + e^{-i\theta}}{2(1 + \cos \theta)(\|q\|^2 - i)} + \frac{1 + e^{i\theta}}{2(1 + \cos \theta)(\|q\|^2 + i)} \right\} dq. \end{aligned} \quad (4.40)$$

The two terms within the curly brackets here are complex conjugates of each other, and so their sum is real-valued. χ_N again is also real-valued. Hence γ_N is real-valued. It then follows that ν_N is indeed real-valued, provided the denominator in (4.11) does not come to zero.

Now to compute a bound on γ_N ,

$$\begin{aligned} |\gamma_N| &\leq \int_{N \leq \|q\| \leq N+1} |\chi_N(q)|^2 \left\{ \left| \frac{1}{(1 + e^{i\theta})(\|q\|^2 - i)} \right| + \left| \frac{e^{i\theta}}{(1 + e^{i\theta})(\|q\|^2 + i)} \right| \right\} dq \\ &= \int_{N \leq \|q\| \leq N+1} |\chi_N(q)|^2 \left\{ \frac{2}{\sqrt{2(1 + \cos \theta)(\|q\|^4 + 1)}} \right\} dq \\ &\leq \sqrt{\frac{2}{1 + \cos \theta}} \int_{N \leq \|q\| \leq N+1} \frac{1}{\|q\|^2} dq \\ &= \sqrt{\frac{2}{1 + \cos \theta}} 4\pi \int_{N \leq r \leq N+1} \frac{1}{r^2} r^2 dr = \sqrt{\frac{32\pi^2}{1 + \cos \theta}}. \end{aligned} \quad (4.41)$$

Hence for fixed $\theta \in [0, 2\pi) \setminus \{\pi\}$, (γ_N) is a bounded sequence in N . It then follows from (4.11) that ν_N is negative for all sufficiently large N , and that $\nu_N \rightarrow 0$ as $N \rightarrow \infty$.

Removal of the Appearance of Constants A and B

It is very common, when defining the Fourier transform, to follow the convention in which A and B , as appearing in (4.14), are both 1. If in [Zor80], the Fourier

transform is to be understood with this convention, then obviously the appearances of multiplication/division by (powers of) A and B in the above analysis can be removed. However, without assuming this to be so, but only assuming $A, B > 0$, let

$$\tilde{Z}_N := AZ_N, \quad \tilde{\nu}_N := \frac{\nu_N}{B^n}. \quad (4.42)$$

In this case, (4.21) becomes

$$\begin{aligned} H^N \psi(x) &= H_\circ \psi(x) + \tilde{\nu}_N \tilde{Z}_N(x) \int_{\mathbb{R}^n} \psi(y) \overline{\tilde{Z}_N(y)} dy \\ &= H_\circ \psi(x) + \tilde{\nu}_N \langle \psi, \tilde{Z}_N \rangle \tilde{Z}_N(x). \end{aligned} \quad (4.43)$$

Likewise (4.35) and (4.38) become

$$\int_{\mathbb{R}^n} \psi(x) \tilde{Z}_N(x) dx \xrightarrow{N \rightarrow \infty} \psi(0), \quad (4.44)$$

$$\int_{\mathbb{R}^n} \psi(x) \overline{\tilde{Z}_N(x)} dx \xrightarrow{N \rightarrow \infty} \psi(0) \quad \forall \psi \in \mathcal{F}(L^1(\mathbb{R}^n)). \quad (4.45)$$

4.2.3 Overview of Other Work on Operators Approaching the Delta Potential in Whole Euclidean Space

Norm Resolvent Convergence

Within the book [AGHHE88] is included the construction of self-adjoint operators approaching the self-adjoint delta-perturbed $-\Delta$ in the *norm resolvent sense*. This is discussed in the settings of \mathbb{R}^1 , \mathbb{R}^2 and \mathbb{R}^3 .

Definition. Given a sequence of self-adjoint operators $(T_N)_{N \in \mathbb{N}}$ acting within a Hilbert space \mathcal{H} , and another self-adjoint operator T acting within \mathcal{H} , it is said that $T_N \xrightarrow{N \rightarrow \infty} T$ in the *norm resolvent sense* if

$$(\lambda - T_N)^{-1} \xrightarrow{N \rightarrow \infty} (\lambda - T)^{-1} \quad \forall \lambda \in \mathbb{C} \setminus \mathbb{R}. \quad (4.46)$$

This convergence is with respect to the standard operator norm on the space of bounded linear operators from \mathcal{H} to \mathcal{H} .

Note that norm resolvent convergence is *stronger* than strong resolvent convergence. Again, see §VIII.7 of [RS80] for further discussion on strong and norm resolvent convergence.

[AGHHE88] is divided into three Parts. Part I deals with the addition of a delta potential concentrated on a single point in \mathbb{R}^n (and also a δ' potential in \mathbb{R}^1). Part II

deals with the addition of finitely many such point-perturbations. Part III deals with the addition of infinitely many such perturbations. In Parts I and II, the Hilbert space is $L^2(\mathbb{R}^n)$. However, included within Part III is discussion on the case of a periodic potential throughout \mathbb{R}^n , so the point-perturbations would be positioned according to some periodic pattern. In this case, letting Λ be the periodic lattice, this system is studied using the Hilbert space $L^2(\mathbb{R}^n/\Lambda)$. This could then be seen as a study on a flat compact manifold rather than the whole Euclidean space.

§1.5.1 of the book [AK00] also gives a construction of self-adjoint operators approaching the delta-perturbed $-\Delta$, in the setting of \mathbb{R}^3 . It refers to the convergence here as “strong resolvent” convergence, yet the definition of strong resolvent convergence in [AK00] is equivalent to the definition of norm resolvent convergence in [RS80].

These approximating operators are rank-one perturbations of the self-adjoint $-\Delta$, following essentially the same construction as described above in §4.2.1 and 4.2.2, which again review Thm. 8.1 in [Zor80]. However:

- (i) The cutoff functions χ_N (see (4.9)) are now sharp cutoff functions rather than smooth ones:

$$\chi_N(\xi) := \begin{cases} \frac{1}{(2\pi)^{3/2}} & \text{if } \|\xi\| < N \\ 0 & \text{if } \|\xi\| > N. \end{cases} \quad (4.47)$$

Observe that in this case, $\mathcal{F}^{-1}\{\chi_N\} \notin \mathcal{S}(\mathbb{R}^3)$, but rather $\mathcal{F}^{-1}\{\chi_N\} \in C^\infty(\mathbb{R}^3) \cap L^2(\mathbb{R}^3) \setminus L^1(\mathbb{R}^3)$.

- (ii) A valid example formula for the sequence of perturbation strengths (ν_N) stated in [AK00] is

$$\nu_N = \frac{\alpha}{1 - \frac{\alpha N}{2\pi^2}}. \quad (4.48)$$

[AK00] does not give a specification for ν_N which explicitly references the self-adjoint extension index parameter θ , as [Zor80] does. It is evident though that there would be a correlation between θ and $\alpha \in \mathbb{R}$. Observe that for $\alpha \neq 0$, (4.48) yields the result that again, $\nu_N < 0$ for all sufficiently large N and $\nu_N \xrightarrow{N \rightarrow \infty} 0$.

In [AK00], the value representing the strength of a rank-one perturbation (here ν_N) is referred to as the *coupling constant*. This variation of ν_N with N here, so as to achieve approximation to the delta potential, is referred to as *renormalisation* of the coupling constant.

Having sharp rather than smooth cutoff functions χ_N , letting $Z_N := \mathcal{F}^{-1}\{\chi_N\}$, (4.35) and (4.38) still hold for all $\psi \in \mathcal{F}(L^1(\mathbb{R}^3)) \cap L^2(\mathbb{R}^3)$ (give-or-take multiplication by an appropriate constant, dependent on the convention for defining the Fourier transform).

Spectrum and Generalised Eigenfunctions

In the setting of a whole Euclidean space \mathbb{R}^n , the self-adjoint $-\Delta$ operator does not have a discrete spectrum and corresponding countable orthonormal eigenbasis. In particular, given any $\psi \in L^2(\mathbb{R}^n)$, let $\widehat{\psi}$ be the Fourier transform of ψ (with $A = B = 1$ in (4.14)), so $\widehat{\psi} \in L^2(\mathbb{R}^n)$ also. Then

$$\mathcal{F}\{-\Delta\psi\}(\xi) = \|\xi\|^2 \widehat{\psi}(\xi). \quad (4.49)$$

Now it is of course impossible for any nonzero L^p function on \mathbb{R}^n , under the Lebesgue measure, to have its support confined within a zero measure set such as an $(n-1)$ -sphere of any radius. Hence if $\psi \neq 0$ then $\nexists E \in \mathbb{R}$ such that $\|\xi\|^2 \widehat{\psi}(\xi) = E\widehat{\psi}(\xi)$, and thus $\nexists E \in \mathbb{R}$ such that $-\Delta\psi = E\psi$. The self-adjoint $-\Delta$ acting within $L^2(\mathbb{R}^n)$ therefore has no eigenvalues.

Nevertheless, the spectrum of the self-adjoint $-\Delta$ is $[0, \infty)$. Furthermore, although the self-adjoint $-\Delta$ has no eigenfunctions in $L^2(\mathbb{R}^n)$, one can still consider “generalised eigenfunctions” outside $L^2(\mathbb{R}^n)$ corresponding to the points in its spectrum. In particular, for any $k \in \mathbb{R}^n$,

$$-\Delta e^{ik \cdot x} = \|k\|^2 e^{ik \cdot x}. \quad (4.50)$$

$e^{ik \cdot x}$ may then serve as a generalised eigenfunction of the self-adjoint $-\Delta$, with generalised eigenvalue $\|k\|^2$. One can also consider expansion of a function into these generalised eigenfunctions $\{e^{ik \cdot x}\}_{k \in \mathbb{R}^n}$, which would be given by the Fourier transform of the function.

The study of self-adjoint operators approaching the delta-perturbed $-\Delta$ in whole Euclidean space has also been carried out by examination of spectrum and (generalised) eigenfunctions. Such study can be found in [BF61], [AGHHE88] and [GN12]. [BF61] deals specifically in three dimensions and [GN12] deals specifically in two dimensions.

Briefly describing the work in [GN12], associated with the N^{th} operator in the sequence of self-adjoint operators approaching the delta-perturbed operator, is a set of *classical scattering eigenfunctions* $\{\psi_N^+(k, \cdot) : k \in \mathbb{R}^2 \setminus \{0\}\}$ and a set of *Faddeev eigenfunctions* $\{\psi_N(k, \cdot) : k \in \mathbb{C}^2 \setminus \mathbb{R}^2\}$. For each of these eigenfunctions the corresponding energy (i.e. generalised eigenvalue) is $E = \|k\|^2$. These eigenfunctions are then shown to approach certain limiting functions as $N \rightarrow \infty$, which would correspond to the delta-perturbed operator. Explicit formulae are given for these eigenfunctions of the approximating operators and of the delta-perturbed operator.

These approximating operators are again rank-one perturbations of the self-adjoint $-\Delta$ operator following essentially the same construction as in [Zor80] and [AK00]. Again,

the cutoff functions involved are sharp:

$$\chi_N(\xi) := \begin{cases} 1 & \text{if } \|\xi\| \leq N \\ 0 & \text{if } \|\xi\| > N. \end{cases} \quad (4.51)$$

It follows again that letting $Z_N := \mathcal{F}^{-1}\{\chi_N\}$, (4.35) and (4.38) still hold for all $\psi \in \mathcal{F}(L^1(\mathbb{R}^2)) \cap L^2(\mathbb{R}^2)$. The formula for the sequence of perturbation strengths (ν_N) given in [GN12] is

$$\nu_N = \frac{\alpha}{1 - \frac{\alpha}{2\pi} \ln N}. \quad (4.52)$$

Again, if $\alpha \neq 0$ then $\nu_N < 0$ for all sufficiently large N and $\nu_N \xrightarrow{N \rightarrow \infty} 0$.

4.2.4 Rank-One Perturbations on the Compact Manifold

In \mathbb{R}^2 , consider a sequence of self-adjoint operators

$$H^N = -\Delta + \nu_N \langle \cdot, Z_N \rangle Z_N, \quad (4.53)$$

where $(\nu_N) \subset \mathbb{R}$, $(Z_N) \subset C^\infty(\mathbb{R}^2) \cap L^2(\mathbb{R}^2)$ and

$$\int_{\mathbb{R}^2} \psi(x) Z_N(x) dx \xrightarrow{N \rightarrow \infty} \psi(0), \quad (4.54)$$

$$\int_{\mathbb{R}^2} \psi(x) \overline{Z_N(x)} dx \xrightarrow{N \rightarrow \infty} \psi(0) \quad \forall \psi \in C_0^\infty(\mathbb{R}^n). \quad (4.55)$$

Suppose this sequence of operators has been shown to approach the self-adjoint delta-perturbed $-\Delta$ in \mathbb{R}^2 , in some appropriate sense. One may then be interested in adapting this from the whole Euclidean space \mathbb{R}^2 to the case of the δ_p -perturbation of H on the two-dimensional compact manifold \mathcal{M} , introduced in Chapter 2.

In attempting this, here is a reasonable trial construction for the sequence of approximating self-adjoint operators:

For each operator H^N acting in $L^2(\mathbb{R}^2)$ given by (4.53), consider a corresponding operator $H_{(\mathcal{M},p)}^N$ acting in $L^2(\mathcal{M})$ of the form

$$H_{(\mathcal{M},p)}^N \psi = H\psi + \nu_N \langle \psi, Y_N \rangle Y_N \quad \forall \psi \in \text{Dom}(H), \quad (4.56)$$

where each $Y_N \in C_0^\infty(\mathcal{M}^\circ) \subset L^2(\mathcal{M})$ is constructed as follows:

- (i) Take a *normal coordinate chart* about the point p on some open ball $\mathcal{B}_R(p) \subset \mathcal{M}^\circ$ (that is, an open ball of radius R about p , defined in terms of geodesic distance), with the metric tensor g_{ij} at p being δ_{ij} . So then, this chart has the following properties:

- (a) $\mathcal{B}_R(p)$ is mapped homeomorphically onto $\mathcal{B}_R(0) \subset \mathbb{R}^2$, with p being mapped to 0.
- (b) On the tangent space at p , the coordinate basis $\{(1, 0), (0, 1)\}$ under this chart is orthonormal under the metric.
- (c) Letting σ denote the map from $\mathcal{B}_R(p) \subset \mathcal{M}^\circ$ to $\mathcal{B}_R(0) \subset \mathbb{R}^2$ which defines this chart, for every line segment Γ lying within $\mathcal{B}_R(0)$ which passes through 0, $\sigma^{-1}(\Gamma)$ is a geodesic segment within $\mathcal{B}_R(p)$ passing through p .
- (d) For any point $x \in \mathcal{B}_R(p)$, the geodesic distance between p and x is equal to the Euclidean distance between 0 and $\sigma(x)$, i.e. $\|\sigma(x)\|$.
- (ii) Take some $Q \in C_0^\infty(\mathcal{B}_R(p))$ with $Q = 1$ on a neighbourhood of p .

(iii) Define

$$Y_N(x) := \begin{cases} Q(x)Z_N(\sigma(x)) & \text{if } x \in \mathcal{B}_R(p) \\ 0 & \text{if } x \in \mathcal{M} \setminus \mathcal{B}_R(p). \end{cases} \quad (4.57)$$

Now given any $\phi : \mathcal{M} \rightarrow \mathbb{C}$ which is C^∞ -smooth on a neighbourhood of $\text{supp } Q$, define $\psi \in C_0^\infty(\mathbb{R}^2)$ as follows:

$$\psi(x) := \begin{cases} \phi(\sigma^{-1}(x))Q(\sigma^{-1}(x))\mathbf{g}_\sigma(\sigma^{-1}(x)) & \text{if } x \in \mathcal{B}_R(0) \\ 0 & \text{if } x \in \mathbb{R}^2 \setminus \mathcal{B}_R(0), \end{cases} \quad (4.58)$$

where \mathbf{g} is a chart-dependent, C^∞ -smooth positive real-valued function called the *Riemannian density*. The Riemannian density is defined in such a way that for an open region $\Omega \subset \mathcal{M}$ and a chart $\omega : \Omega \rightarrow \omega(\Omega) \subset \mathbb{R}^2$, letting \mathbf{g}_ω be the Riemannian density on Ω under ω , we have:

$$\int_\Omega f(x)dx = \int_{\omega(\Omega)} f(\omega^{-1}(y))\mathbf{g}_\omega(\omega^{-1}(y))dy. \quad (4.59)$$

The formula for the Riemannian density is

$$\mathbf{g}(x) = \sqrt{\det(g_{ij})_{i,j=1}^2}. \quad (4.60)$$

Note then that

$$\phi(p) = \psi(0), \quad (4.61)$$

$$\begin{aligned} \int_{\mathcal{M}} \phi(x)Y_N(x)dx &= \int_{\mathcal{B}_R(p)} \phi(x)Q(x)Z_N(\sigma(x))dx \\ &= \int_{\mathcal{B}_R(0)} \phi(\sigma^{-1}(y))Q(\sigma^{-1}(y))Z_N(y)\mathbf{g}_\sigma(\sigma^{-1}(y))dy = \int_{\mathbb{R}^2} \psi(y)Z_N(y)dy. \end{aligned} \quad (4.62)$$

Thus given (4.54), it follows that

$$\int_{\mathcal{M}} \phi(x) Y_N(x) dx \xrightarrow{N \rightarrow \infty} \phi(p). \quad (4.63)$$

Furthermore, in case Q may take non-real values at some points on \mathcal{M} , define $\tilde{\psi} \in C_0^\infty(\mathbb{R}^2)$ similarly to ψ in (4.58), only replacing Q with \bar{Q} . Then in (4.61) and (4.62), by replacing ψ , Y_N , Q and Z_N with $\tilde{\psi}$, \bar{Y}_N , \bar{Q} and \bar{Z}_N respectively, it follows from (4.55) that

$$\int_{\mathcal{M}} \phi(x) \bar{Y}_N(x) dx \xrightarrow{N \rightarrow \infty} \phi(p). \quad (4.64)$$

In particular then, writing

$$Y_N = \sum_{j=1}^{\infty} y_j^N \Psi_j, \quad (4.65)$$

so

$$y_j^N = \langle Y_N, \Psi_j \rangle, \quad (4.66)$$

and since for each $j \in \mathbb{N}$, $\Psi_j \in C^\infty(\mathcal{M}^\circ)$, it follows that

$$y_j^N = \overline{\int_{\mathcal{M}} \Psi_j(x) \bar{Y}_N(x) dx} \xrightarrow{N \rightarrow \infty} \bar{\Psi}_j(p). \quad (4.67)$$

4.2.5 Consideration of Eigenvalues and Eigenfunctions

When interested in a sequence of rank-one perturbations of H approaching the delta-perturbed operator H_Θ , it may be of particular interest to consider this in relation to eigenvalues and eigenfunctions of the rank-one perturbations approaching those of the delta-perturbed operator.

Definition. Consider a Hilbert space \mathcal{H} and a closed linear operator $T : \text{Dom}(T) \rightarrow \mathcal{H}$ with $\text{Dom}(T) \subset \mathcal{H}$ being dense in \mathcal{H} . If $\lambda - T : \text{Dom}(T) \rightarrow \mathcal{H}$ is bijective for some $\lambda \in \mathbb{C}$, and $(\lambda - T)^{-1}$ is a bounded operator on \mathcal{H} , then $(\lambda - T)^{-1}$ is referred to as a *resolvent* of T , and λ is said to be in the *resolvent set* of T . The complement of the resolvent set of T within \mathbb{C} is referred to as the *spectrum* of T , which shall be denoted $\text{Spec}(T)$.

Again, T being *closed* means that the graph of T is a closed subset of $\mathcal{H} \times \mathcal{H}$. In particular, if T is self-adjoint then it is indeed closed and has dense domain. Furthermore, the spectrum of a self-adjoint operator is always contained within \mathbb{R} .

Observe that every eigenvalue of T is contained within its spectrum, because $\lambda \in \mathbb{C}$ is an eigenvalue of T if and only if $\lambda - T : \text{Dom}(T) \rightarrow \mathcal{H}$ fails to be injective. The set of eigenvalues of T is referred to as the *point spectrum* of T .

A variety of different classifications for points in the spectrum of an operator have been developed, such as the aforementioned *point spectrum*. Other examples are continuous spectrum, residual spectrum, discrete spectrum and essential spectrum. Sometimes there is even more than one different convention for defining such terms. Below we shall define *discrete* and *essential* spectrum in the case of a self-adjoint operator, in accordance with the convention found in e.g. §VII.3 and VIII.3 of [RS80] and §4.1 of [Dav95].

Definition. Consider a self-adjoint operator T acting within a Hilbert space \mathcal{H} . Given any $\lambda \in \text{Spec}(T)$, λ is said to belong to the *discrete spectrum* of T if λ is an eigenvalue of T whose corresponding eigenspace is finite-dimensional, and $(\lambda - \epsilon, \lambda + \epsilon) \cap \text{Spec}(T) = \{\lambda\}$ for some $\epsilon > 0$. Otherwise, λ is said to belong to the *essential spectrum* of T .

A more general definition of discrete and essential spectrum, beyond the case of T being self-adjoint, nevertheless coinciding with the above when T is self-adjoint, can be found in [RS78].

Definition. In a Hilbert space \mathcal{H} , a linear operator $B : \mathcal{H} \rightarrow \mathcal{H}$ is said to be *compact* if the image of every bounded set in \mathcal{H} under B is precompact. Equivalently, B is compact iff for every bounded sequence $(v_n)_{n=1}^\infty \subset \mathcal{H}$, $(Bv_n)_{n=1}^\infty$ has a convergent subsequence in \mathcal{H} .

Note that a compact linear operator is always bounded. Furthermore, a bounded linear operator of finite rank (i.e. finite dimensional image) is always compact.

The above definition of a compact operator also applies more generally to a linear operator from a Banach space to another Banach space.

Proposition 4.2.4. *Given some $Y \in L^2(\mathcal{M})$ and $\nu \in \mathbb{R}$, define the operator*

$$H' := H + \nu \langle \cdot, Y \rangle Y, \quad (4.68)$$

with $\text{Dom}(H') = \text{Dom}(H)$. Then there exists an orthonormal basis $(\psi_j)_{j=1}^\infty$ of $L^2(\mathcal{M})$ consisting of eigenfunctions of H' , with respective corresponding eigenvalues $\mu_1 \leq \mu_2 \leq \mu_3 \leq \dots \rightarrow \infty$, and $\text{Spec}(H') = \{\mu_j\}_{j=1}^\infty$.

Proof. Firstly, the spectrum of H is purely the set of eigenvalues $\{\mathcal{E}_j\}_{j=1}^\infty$, since as shown in Lemma 2.1.3, $H - z : \text{Dom}(H) \rightarrow L^2(\mathcal{M})$ is a bijective operator with bounded inverse for every $z \in \mathbb{C} \setminus \{\mathcal{E}_j\}_{j=1}^\infty$. Furthermore, every eigenvalue of H clearly belongs to the discrete spectrum, and so the essential spectrum of H is empty.

Now according to Example 3 in §XIII.4 of [RS78], perturbing a self-adjoint operator by adding a compact operator leaves the essential spectrum unchanged. Thus since $\nu \langle \cdot, Y \rangle Y$

has rank being at most 1, and so is a compact operator, it follows that H' also has empty essential spectrum. Furthermore, by Lemmas 4.2.2, 4.2.3 and the self-adjointness of H , H' is also self-adjoint. With the Hilbert space $L^2(\mathcal{M})$ being infinite-dimensional but separable, it then follows that according to Thm. 4.1.5 in §4.1 of [Dav95], H' has an orthonormal eigenbasis $(\psi_j)_{j=1}^\infty$ and corresponding eigenvalues $(\mu_j)_{j=1}^\infty$ with $|\mu_j| \rightarrow \infty$ as $j \rightarrow \infty$.

Next, it shall be shown that the set of eigenvalues of H' must have a finite lower bound. Given any $\phi = \sum_{j=1}^\infty a_j \Psi_j \in \text{Dom}(H)$, it follows from Lemma 2.1.1 and the formula for the inner product in terms of orthonormal basis expansion that

$$\langle H\phi, \phi \rangle = \sum_{j=1}^\infty \mathcal{E}_j |a_j|^2 \geq \sum_{j=1}^\infty \mathcal{E}_1 |a_j|^2 = \mathcal{E}_1 \|\phi\|^2. \quad (4.69)$$

Furthermore, letting $B := \nu \langle \cdot, Y \rangle Y$,

$$\begin{aligned} \langle B\phi, \phi \rangle &= \langle \nu \langle \phi, Y \rangle Y, \phi \rangle = \nu \langle \phi, Y \rangle \langle Y, \phi \rangle = \nu |\langle \phi, Y \rangle|^2 \\ &\geq \min\{0, \nu \|Y\|^2\} \|\phi\|^2 =: C \|\phi\|^2. \end{aligned} \quad (4.70)$$

Hence

$$\langle H'\phi, \phi \rangle = \langle H\phi, \phi \rangle + \langle B\phi, \phi \rangle \geq (\mathcal{E}_1 + C) \|\phi\|^2. \quad (4.71)$$

Now letting $\mu \in \mathbb{R}$ be an eigenvalue of H' and $\psi \in \text{Dom}(H) \setminus \{0\}$ be a corresponding eigenfunction,

$$\langle H'\psi, \psi \rangle = \mu \|\psi\|^2 \geq (\mathcal{E}_1 + C) \|\psi\|^2, \quad (4.72)$$

and so $\mu \geq \mathcal{E}_1 + C$. Thus $\mathcal{E}_1 + C$ is a lower bound for the set of all eigenvalues of H' .

It may now be concluded that the orthonormal eigenbasis of H' can be arranged in a sequence $(\psi_j)_{j=1}^\infty$ with which the corresponding eigenvalues $(\mu_j)_{j=1}^\infty$ satisfy $\mu_1 \leq \mu_2 \leq \mu_3 \leq \dots \rightarrow \infty$. H' may have no other eigenvalues beside $\{\mu_j\}_{j=1}^\infty$, since if it did, the corresponding eigenfunctions would be orthogonal to all members of $\{\psi_j\}_{j=1}^\infty$, and thus could not be expanded into $\{\psi_j\}_{j=1}^\infty$ as all coefficients would be zero. Furthermore, the spectrum of H' may have no other points beside $\{\mu_j\}_{j=1}^\infty$, since as already stated, the essential spectrum is empty. Thus the spectrum is purely discrete, and all points in the discrete spectrum are eigenvalues. \square

Suppose one has obtained a sequence of rank-one-perturbed operators (H^N) approaching the delta-perturbed operator H_Θ in either the strong or norm resolvent sense. This may then enable analysis of the limiting behaviour of eigenvalues and eigenfunctions of H^N in relation to the eigenvalues and eigenfunctions of H . Theorems VIII.23 and VIII.24 in [RS80] would then be of use in this pursuit.

However, in the approach that shall be taken in the following sections of Chapter, the limiting behaviour of the eigenvalues and eigenfunctions of H^N , in relation to those of H_Θ , shall be studied via direct analysis of their formulae. This approach shall begin by assuming only that (4.67) holds. Further conditions would then be added as the investigation progresses.

4.3 Eigenvalues and Eigenfunctions of the Rank-One Perturbed Operators

4.3.1 Construction of Eigenvalues and Eigenfunctions

In §3 of [RU12], there is a discussion on the eigenvalues and eigenfunctions of a rank-one perturbation of a self-adjoint operator on a finite-dimensional Hilbert space, observing that the delta potential can be formally represented in a form akin to that of a rank-one perturbation. Now we wish to derive the complete set of eigenvalues and eigenfunctions for rank-one perturbations of the operator H on the Hilbert space $L^2(\mathcal{M})$. Then we seek to approximate the eigenvalues and eigenfunctions of the rigorously constructed delta potential by those of rank-one perturbations of H .

So then, given some $Y \in L^2(\mathcal{M}) \setminus \{0\}$ and $\nu \in \mathbb{R} \setminus \{0\}$, we wish to obtain an orthonormal eigenbasis and corresponding eigenvalues of the self-adjoint operator

$$H' := H + \nu \langle \cdot, Y \rangle Y. \quad (4.73)$$

To this end, take some $\psi \in \text{Dom}(H)$ (noting that $\text{Dom}(H') = \text{Dom}(H)$) and $E \in \mathbb{R}$, for which we wish to determine whether or not $H'\psi = E\psi$. Expanding ψ and Y into the orthonormal eigenbasis of H :

$$\psi = \sum_{j=1}^{\infty} a_j \Psi_j, \quad Y = \sum_{j=1}^{\infty} y_j \Psi_j, \quad (4.74)$$

it follows that

$$\begin{aligned} H'\psi = E\psi \quad \text{iff} \quad H\psi + \nu \langle \psi, Y \rangle Y = E\psi \quad \text{iff} \quad (E - H)\psi = \nu \langle \psi, Y \rangle Y \\ \text{iff} \quad (E - \mathcal{E}_j)a_j = \nu \langle \psi, Y \rangle y_j \quad \forall j \in \mathbb{N}. \end{aligned} \quad (4.75)$$

Now split the situation into three possible cases, namely:

- (i) $\langle \psi, Y \rangle = 0$;

(ii) $\langle \psi, Y \rangle \neq 0$ and $E \notin \text{Spec}(H)$;

(iii) $\langle \psi, Y \rangle \neq 0$ and $E \in \text{Spec}(H)$.

Again, ‘‘Spec’’ means spectrum, so $\text{Spec}(H) = \{\mathcal{E}_j\}_{j \in \mathbb{N}}$.

In case (i), $H'\psi = H\psi$, and thus $H'\psi = E\psi$ if and only if $H\psi = E\psi$.

So then, for each eigenspace of H , calling the eigenvalue \mathcal{E} , if $\mathcal{P}_{\{\mathcal{E}\}}^{(H)}Y := \sum_{j:\mathcal{E}_j=\mathcal{E}} y_j \Psi_j = 0$ then \mathcal{E} is an eigenvalue of H' also, with the \mathcal{E} -eigenspace $\Lambda_{\mathcal{E}}^{(H)}$ of H being a subspace of the \mathcal{E} -eigenspace $\Lambda_{\mathcal{E}}^{(H')}$ of H' . If $\mathcal{P}_{\{\mathcal{E}\}}^{(H)}Y \neq 0$ and the dimension of $\Lambda_{\mathcal{E}}^{(H)}$ is ≥ 2 then \mathcal{E} is an eigenvalue of H' also, with the orthogonal complement of $\text{span}\{\mathcal{P}_{\{\mathcal{E}\}}^{(H)}Y\}$ in $\Lambda_{\mathcal{E}}^{(H)}$ being a subspace of $\Lambda_{\mathcal{E}}^{(H')}$. This covers all eigenfunctions of H' that are orthogonal to Y .

In case (ii), noting that the operator $E - H : \text{Dom}(H) \rightarrow L^2(\mathcal{M})$ is then bijective, it follows from (4.75) that

$$H'\psi = E\psi \quad \text{iff} \quad \psi = \nu \langle \psi, Y \rangle (E - H)^{-1}Y. \quad (4.76)$$

Let

$$\psi_E := (E - H)^{-1}Y = \sum_{j=1}^{\infty} \frac{y_j}{E - \mathcal{E}_j} \Psi_j \in \text{Dom}(H) \setminus \{0\}. \quad (4.77)$$

So then, if $H'\psi = E\psi$ then $\psi \in \text{span}\{\psi_E\} \setminus \{0\}$, and writing $\psi = \alpha\psi_E$, we have

$$\begin{aligned} \psi = \nu \langle \psi, Y \rangle \psi_E &= \nu \langle \alpha\psi_E, Y \rangle \psi_E = \alpha\psi_E \Rightarrow \nu \langle \alpha\psi_E, Y \rangle = \alpha \\ &\Rightarrow \langle \psi_E, Y \rangle = \sum_{j=1}^{\infty} \frac{|y_j|^2}{E - \mathcal{E}_j} = \frac{1}{\nu}. \end{aligned} \quad (4.78)$$

Conversely (now without even assuming beforehand that $\langle \psi, Y \rangle \neq 0$, but still assuming $E \notin \text{Spec}(H)$), suppose $\psi \in \text{span}\{\psi_E\} \setminus \{0\}$ and $\sum_{j=1}^{\infty} \frac{|y_j|^2}{E - \mathcal{E}_j} = \frac{1}{\nu}$. Then writing $\psi = \alpha\psi_E$, we have

$$\begin{aligned} \langle \psi, Y \rangle &= \alpha \langle \psi_E, Y \rangle = \alpha \sum_{j=1}^{\infty} \frac{|y_j|^2}{E - \mathcal{E}_j} = \frac{\alpha}{\nu} \neq 0 \\ &\Rightarrow \alpha = \nu \langle \psi, Y \rangle \Rightarrow \psi = \alpha\psi_E = \nu \langle \psi, Y \rangle \psi_E \stackrel{(4.76)}{\implies} H'\psi = E\psi. \end{aligned} \quad (4.79)$$

In case (iii), defining

$$\psi_E := \sum_{j:\mathcal{E}_j \neq E} \frac{y_j}{E - \mathcal{E}_j} \Psi_j \in \text{Dom}(H), \quad (4.80)$$

it then follows from (4.75) that

$$\begin{aligned}
H'\psi = E\psi & \quad \text{iff} \quad \begin{cases} y_j = 0 & \text{for } \mathcal{E}_j = E \\ a_j = \nu \langle \psi, Y \rangle \frac{y_j}{E - \mathcal{E}_j} & \text{for } \mathcal{E}_j \neq E \end{cases} \\
\text{iff} \quad \begin{cases} \mathcal{P}_{\{E\}}^{(H)} Y = 0 \\ \mathcal{P}_{\mathbb{R} \setminus \{E\}}^{(H)} \psi = \nu \langle \psi, Y \rangle \psi_E \end{cases} & \quad \text{iff} \quad \begin{cases} \mathcal{P}_{\{E\}}^{(H)} Y = 0 \\ \mathcal{P}_{\mathbb{R} \setminus \{E\}}^{(H)} \psi = \nu \langle \mathcal{P}_{\mathbb{R} \setminus \{E\}}^{(H)} \psi, Y \rangle \psi_E. \end{cases} \quad (4.81)
\end{aligned}$$

So then, if $H'\psi = E\psi$ then $\mathcal{P}_{\{E\}}^{(H)} Y = 0$, so $\mathcal{P}_{\mathbb{R} \setminus \{E\}}^{(H)} Y \neq 0$, and so $\psi_E \neq 0$. Furthermore, $\langle \mathcal{P}_{\mathbb{R} \setminus \{E\}}^{(H)} \psi, Y \rangle = \langle \psi, Y \rangle \neq 0$, so $\mathcal{P}_{\mathbb{R} \setminus \{E\}}^{(H)} \psi \in \text{span}\{\psi_E\} \setminus \{0\}$, equivalently $\psi \in (\text{span}\{\psi_E\} \setminus \{0\}) + \Lambda_E^{(H)}$. Then following the same argument as in (4.78), only replacing ψ with $\mathcal{P}_{\mathbb{R} \setminus \{E\}}^{(H)} \psi$, we have

$$\langle \psi_E, Y \rangle = \sum_{j: \mathcal{E}_j \neq E} \frac{|y_j|^2}{E - \mathcal{E}_j} = \sum_{j: y_j \neq 0} \frac{|y_j|^2}{E - \mathcal{E}_j} = \frac{1}{\nu}. \quad (4.82)$$

Conversely (again without assuming beforehand that $\langle \psi, Y \rangle \neq 0$, but still assuming $E \in \text{Spec}(H)$), suppose $\mathcal{P}_{\{E\}}^{(H)} Y = 0$ (so $\mathcal{P}_{\mathbb{R} \setminus \{E\}}^{(H)} Y \neq 0 \Rightarrow \psi_E \neq 0$), $\psi \in (\text{span}\{\psi_E\} \setminus \{0\}) + \Lambda_E^{(H)}$ (so $\mathcal{P}_{\mathbb{R} \setminus \{E\}}^{(H)} \psi \in \text{span}\{\psi_E\} \setminus \{0\}$) and $\sum_{j: y_j \neq 0} \frac{|y_j|^2}{E - \mathcal{E}_j} = \frac{1}{\nu}$ (so $\sum_{j: \mathcal{E}_j \neq E} \frac{|y_j|^2}{E - \mathcal{E}_j} = \frac{1}{\nu}$). Note then that again, $\langle \psi, Y \rangle = \langle \mathcal{P}_{\mathbb{R} \setminus \{E\}}^{(H)} \psi, Y \rangle$. Now following the same argument as in (4.79), only replacing ψ with $\mathcal{P}_{\mathbb{R} \setminus \{E\}}^{(H)} \psi$ and applying (4.81) instead of (4.76), it follows that $\langle \psi, Y \rangle = \langle \mathcal{P}_{\mathbb{R} \setminus \{E\}}^{(H)} \psi, Y \rangle \neq 0$ and $H'\psi = E\psi$. Observe finally that ψ_E is clearly orthogonal to all members of $\Lambda_E^{(H)}$.

Given all of this, we can now construct all eigenvalues of H' , and an orthonormal basis of each corresponding eigenspace. Note, either from the above analysis or from Prop. 4.2.4, that every eigenspace is finite-dimensional. By Prop. 4.2.4, H' has a complete countable orthonormal eigenbasis. It then follows in particular that if we take any orthonormal basis of each eigenspace, and then take the union over all eigenspaces, this will give such a complete orthonormal eigenbasis.

Now stating the construction of an orthonormal eigenbasis of H' :

- (i) Start off with an orthonormal eigenbasis of H , whereby for each eigenspace $\Lambda_E^{(H)}$ with $\mathcal{P}_{\{E\}}^{(H)} Y \neq 0$, the basis for this eigenspace is chosen in such a way that one of the members is in $\text{span}\{\mathcal{P}_{\{E\}}^{(H)} Y\}$. Note that $\mathcal{P}_{\{E\}}^{(H)} Y = 0$ if and only if $y_j = 0 \forall j$ with $\mathcal{E}_j = E$.
- (ii) Then for each eigenvalue E of H with $\mathcal{P}_{\{E\}}^{(H)} Y \neq 0$, delete the member of $\text{span}\{\mathcal{P}_{\{E\}}^{(H)} Y\}$.

(iii) Find all $E \in \mathbb{R} \setminus \{\mathcal{E} \in \text{Spec}(H) : \mathcal{P}_{\{\mathcal{E}\}}^{(H)} Y \neq 0\}$ that solve the equation

$$\sum_{j:y_j \neq 0} \frac{|y_j|^2}{E - \mathcal{E}_j} = \frac{1}{\nu}, \quad (4.83)$$

noting that this sum here does indeed converge for each $E \in \mathbb{R} \setminus \{\mathcal{E} \in \text{Spec}(H) : \mathcal{P}_{\{\mathcal{E}\}}^{(H)} Y \neq 0\}$, since $\sum_{j=1}^{\infty} |y_j|^2$ converges to $\|Y\|^2 < \infty$.

(iv) For each E that solves (4.83), insert the function

$$\widehat{\psi}_E := \frac{\psi_E}{\|\psi_E\|}, \quad (4.84)$$

where

$$\psi_E := \sum_{j:y_j \neq 0} \frac{y_j}{E - \mathcal{E}_j} \Psi_j \in \text{Dom}(H). \quad (4.85)$$

For each eigenfunction that we have after step (ii), the corresponding eigenvalue is the same as the corresponding eigenvalue of H . For each eigenfunction $\widehat{\psi}_E$ introduced in step (iv), the corresponding eigenvalue is E .

Note that in LHS(4.83) and LHS(4.85), the reason for having $\sum_{j:y_j \neq 0}$ rather than $\sum_{j=1}^{\infty}$ is so as to allow for the possibility of E coinciding with an eigenvalue \mathcal{E} of H with $\mathcal{P}_{\{\mathcal{E}\}}^{(H)} Y = 0$ (i.e. $y_j = 0 \forall j$ with $\mathcal{E}_j = \mathcal{E}$), without having terms in the sum where the denominator is zero. With $E \in \mathbb{R} \setminus \{\mathcal{E} \in \text{Spec}(H) : \mathcal{P}_{\{\mathcal{E}\}}^{(H)} Y \neq 0\}$, LHS(4.83) and LHS(4.85) can equivalently be written with $\sum_{j:\mathcal{E}_j \neq E}$, and if $E \notin \text{Spec}(H)$ then obviously this is just equivalent to $\sum_{j=1}^{\infty}$.

Let $R(E)$ denote the LHS of (4.83). We wish to describe qualitatively the behaviour of this function $R : \mathbb{R} \setminus \{\mathcal{E} \in \text{Spec}(H) : \mathcal{P}_{\{\mathcal{E}\}}^{(H)} Y \neq 0\} \rightarrow \mathbb{R}$. Observe first of all that each term in the sum in the LHS of (4.83) is a strictly decreasing function of E on $(-\infty, \mathcal{E}_j)$ and on (\mathcal{E}_j, ∞) , with a singularity at \mathcal{E}_j , tending to $-\infty$ from the left and $+\infty$ from the right.

Given any $M \in \mathbb{N}$, define

$$R^{(M)}(E) := \sum_{j \in \{1, \dots, M\} : y_j \neq 0} \frac{|y_j|^2}{E - \mathcal{E}_j}. \quad (4.86)$$

Then (provided M is large enough that $\{j \in \{1, \dots, M\} : y_j \neq 0\} \neq \emptyset$) $R^{(M)}$ has a singularity at each \mathcal{E}_j with $j \in \{1, \dots, M\}$ and $y_j \neq 0$, tending to $-\infty$ from the left and $+\infty$ from the right, and is continuous and strictly decreasing on every interval which does not intersect one of the singularities.

We now verify that these basic behaviours of the finite sum $R^{(M)}$ also extend to the potentially infinite sum R .

Lemma 4.3.1. $R : \mathbb{R} \setminus \{\mathcal{E} \in \text{Spec}(H) : \mathcal{P}_{\{\mathcal{E}\}}^{(H)} Y \neq 0\} \rightarrow \mathbb{R}$ has the following properties:

- (i) It is strictly decreasing on every interval whose intersection with $\{\mathcal{E} \in \text{Spec}(H) : \mathcal{P}_{\{\mathcal{E}\}}^{(H)} Y \neq 0\}$ is empty.
- (ii) For each $\mathcal{E} \in \text{Spec}(H)$ with $\mathcal{P}_{\{\mathcal{E}\}}^{(H)} Y \neq 0$, $\lim_{E \rightarrow \mathcal{E}^-} R(E) = -\infty$ and $\lim_{E \rightarrow \mathcal{E}^+} R(E) = +\infty$.
- (iii) It is Lipschitz continuous on every compact interval whose intersection with $\{\mathcal{E} \in \text{Spec}(H) : \mathcal{P}_{\{\mathcal{E}\}}^{(H)} Y \neq 0\}$ is empty.

Proof. (i) Take some $a, b \in \mathbb{R}$ with $a < b$ and $[a, b] \cap \{\mathcal{E} \in \text{Spec}(H) : \mathcal{P}_{\{\mathcal{E}\}}^{(H)} Y \neq 0\} = \emptyset$. Then given any $M \in \mathbb{N}$ with $\{j \in \{1, \dots, M\} : y_j \neq 0\} \neq \emptyset$,

$$\begin{aligned} R^{(M+1)}(a) - R^{(M+1)}(b) &= R^{(M)}(a) - R^{(M)}(b) + \left(\frac{|y_{M+1}|^2}{a - \mathcal{E}_{M+1}} - \frac{|y_{M+1}|^2}{b - \mathcal{E}_{M+1}} \right) \\ &\geq R^{(M)}(a) - R^{(M)}(b) > 0. \end{aligned} \quad (4.87)$$

Then by induction, if $M_1, M_2 \in \mathbb{N} \cap [M, \infty)$ and $M_1 < M_2$ then $R^{(M_1)}(a) - R^{(M_1)}(b) \leq R^{(M_2)}(a) - R^{(M_2)}(b)$. Hence

$$R(a) - R(b) = \lim_{K \rightarrow \infty} (R^{(K)}(a) - R^{(K)}(b)) \geq R^{(M)}(a) - R^{(M)}(b) > 0. \quad (4.88)$$

- (ii) Given any $k \in \mathbb{N}$ with $y_k \neq 0$, take some $M \in \mathbb{N} \cap [k, \infty)$ and some $a < \mathcal{E}_k$ with $[a, \mathcal{E}_k] \cap \{\mathcal{E} \in \text{Spec}(H) : \mathcal{P}_{\{\mathcal{E}\}}^{(H)} Y \neq 0\} = \emptyset$. Then with variable $E \in (a, \mathcal{E}_k)$, we have, by applying (4.88) together with $\lim_{E \rightarrow \mathcal{E}_k^-} R^{(M)}(E) = -\infty$,

$$R(a) - R(E) \geq R^{(M)}(a) - R^{(M)}(E) \xrightarrow{E \rightarrow \mathcal{E}_k^-} \infty \Rightarrow R(E) \xrightarrow{E \rightarrow \mathcal{E}_k^-} -\infty. \quad (4.89)$$

Next, still keeping the same k and M , take some $b > \mathcal{E}_k$ with $(\mathcal{E}_k, b] \cap \{\mathcal{E} \in \text{Spec}(H) : \mathcal{P}_{\{\mathcal{E}\}}^{(H)} Y \neq 0\} = \emptyset$, and take variable $E \in (\mathcal{E}_k, b)$. Then

$$R(E) - R(b) \geq R^{(M)}(E) - R^{(M)}(b) \xrightarrow{E \rightarrow \mathcal{E}_k^+} \infty \Rightarrow R(E) \xrightarrow{E \rightarrow \mathcal{E}_k^+} \infty. \quad (4.90)$$

- (iii) Define

$$T_Y(E) := \sum_{j: y_j \neq 0} \frac{|y_j|^2}{(E - \mathcal{E}_j)^2}, \quad T_Y^{(M)}(E) := \sum_{j \in \{1, \dots, M\}: y_j \neq 0} \frac{|y_j|^2}{(E - \mathcal{E}_j)^2}. \quad (4.91)$$

Observe that $T_Y(E)$ is a convergent sum for each $E \in \mathbb{R} \setminus \{\mathcal{E} \in \text{Spec}(H) : \mathcal{P}_{\{\mathcal{E}\}}^{(H)} Y \neq 0\}$, converging to $\|\psi_E\|^2$, with ψ_E defined in (4.85). Observe also that

$$\frac{d}{dE} R^{(M)}(E) = -T_Y^{(M)}(E). \quad (4.92)$$

Fix a compact interval $[a, b]$ of positive length (i.e. $b > a$) with $[a, b] \cap \{\mathcal{E} \in \text{Spec}(H) : \mathcal{P}_{\{\mathcal{E}\}}^{(H)} Y \neq 0\} = \emptyset$. Then taking any $x, z \in [a, b]$ with $x < z$, and applying the mean value theorem,

$$0 < R(x) - R(z) = \lim_{K \rightarrow \infty} (R^{(K)}(x) - R^{(K)}(z)) = \lim_{K \rightarrow \infty} T_Y^{(K)}(\sigma_K)(z - x) \quad (4.93)$$

for some $(\sigma_K)_{K \in \mathbb{N}} \subset (x, z)$. For each $E \in (x, z)$ and $j \in \mathbb{N}$ with $y_j \neq 0$, if $\mathcal{E}_j > b$ then $\frac{|y_j|^2}{(E - \mathcal{E}_j)^2} < \frac{|y_j|^2}{(b - \mathcal{E}_j)^2}$, and if $\mathcal{E}_j < a$ then $\frac{|y_j|^2}{(E - \mathcal{E}_j)^2} < \frac{|y_j|^2}{(a - \mathcal{E}_j)^2}$. In either case, $\frac{|y_j|^2}{(E - \mathcal{E}_j)^2} < \frac{|y_j|^2}{(a - \mathcal{E}_j)^2} + \frac{|y_j|^2}{(b - \mathcal{E}_j)^2}$. Hence

$$\begin{aligned} T_Y^{(K)}(\sigma_K)(z - x) &\leq (T_Y^{(K)}(a) + T_Y^{(K)}(b))(z - x) \\ \xrightarrow{K \rightarrow \infty} 0 < R(x) - R(z) &\leq (T_Y(a) + T_Y(b))(z - x). \end{aligned} \quad (4.94)$$

□

Corollary 4.3.2. Write $\{\mathcal{E} \in \text{Spec}(H) : \mathcal{P}_{\{\mathcal{E}\}}^{(H)} Y \neq 0\} =: (E_k^{(Y)})_{k=1}^{M_{\max}}$, with $E_1^{(Y)} < E_2^{(Y)} < E_3^{(Y)} < \dots$, where M_{\max} could be finite or infinite. Equation (4.83) then has precisely one solution in each interval $(E_k^{(Y)}, E_{k+1}^{(Y)})$, at most one solution below $E_1^{(Y)}$, and if M_{\max} is finite then at most one solution above $E_{M_{\max}}^{(Y)}$.

Since the spectrum of H' is purely discrete, it follows that for every value $E \in \mathbb{C}$ outside the set of eigenvalues of H' derived above, the resolvent operator $(E - H')^{-1}$ is well-defined. In §A.1 of the Appendix, explicit formulae are derived for the resolvent operators of H' .

4.3.2 Comparison with Eigenvalues and Eigenfunctions of the Delta Potential

Now comparing the eigenvalues and eigenfunctions of the rank-one-perturbation operator H' with those of the delta potential operator H_Θ , an orthonormal eigenbasis for H_Θ can be constructed in a similar way to that described above for H' , as follows:

- (i) Start off with the orthonormal eigenbasis $\{\Psi_j\}_{j=1}^\infty$ of H . Note here that with this choice of eigenbasis, for each eigenspace $\Lambda_E^{(H)}$ with $\mathcal{P}_{\{E\}}^{(H)} \delta_p := \sum_{j: \mathcal{E}_j = E} \overline{\Psi_j(p)} \Psi_j \neq 0$, the basis $\{\Psi_j : \mathcal{E}_j = E\}$ for this eigenspace has one member in $\text{span}\{\mathcal{P}_{\{E\}}^{(H)} \delta_p\}$, namely the only one whose value at p is nonzero. Obviously if $\mathcal{P}_{\{E\}}^{(H)} \delta_p = 0$ then $\Psi_j(p) = 0 \forall j$ with $\mathcal{E}_j = E$.
- (ii) Then for each eigenvalue E of H with $\mathcal{P}_{\{E\}}^{(H)} \delta_p \neq 0$, delete the corresponding eigenfunction whose value at p is nonzero.

(iii) Find all $E \in \mathbb{R} \setminus \{\mathcal{E} \in \text{Spec}(H) : \mathcal{P}_{\{\mathcal{E}\}}^{(H)} \delta_p \neq 0\}$ that solve the equation

$$S(E) := \sum_{j: \Psi_j(p) \neq 0} \left(\frac{|\Psi_j(p)|^2}{E - \mathcal{E}_j} + \frac{|\Psi_j(p)|^2 \mathcal{E}_j}{1 + \mathcal{E}_j^2} \right) = F(\Theta), \quad (4.95)$$

where $F(\Theta) := -\text{RHS}(2.111)$, noting that here $S(E) = -\text{LHS}(2.111)$ (interchanging “ E ” and “ λ ”).

(iv) For each E that solves (4.95), insert the function

$$\widehat{\psi}_E^\delta := \frac{\psi_E^\delta}{\|\psi_E^\delta\|}, \quad (4.96)$$

where

$$\psi_E^\delta := \sum_{j: \Psi_j(p) \neq 0} \frac{\overline{\Psi_j(p)}}{E - \mathcal{E}_j} \Psi_j \in L^2(\mathcal{M}). \quad (4.97)$$

Note that here, $\psi_E^\delta = -g_E$ as given by (2.75) (in the case where $E \notin \text{Spec}(H)$).

Again, for each eigenfunction that we have after step (ii), the corresponding eigenvalue is the same as the corresponding eigenvalue of H . For each eigenfunction $\widehat{\psi}_E^\delta$ introduced in step (iv), the corresponding eigenvalue is E .

By analogy with Lemma 4.3.1, we have

Lemma 4.3.3. $S : \mathbb{R} \setminus \{\mathcal{E} \in \text{Spec}(H) : \mathcal{P}_{\{\mathcal{E}\}}^{(H)} \delta_p \neq 0\} \rightarrow \mathbb{R}$ has the following properties:

- (i) It is strictly decreasing on every interval whose intersection with $\{\mathcal{E} \in \text{Spec}(H) : \mathcal{P}_{\{\mathcal{E}\}}^{(H)} \delta_p \neq 0\}$ is empty.
- (ii) For each $\mathcal{E} \in \text{Spec}(H)$ with $\mathcal{P}_{\{\mathcal{E}\}}^{(H)} \delta_p \neq 0$, $\lim_{E \rightarrow \mathcal{E}^-} S(E) = -\infty$ and $\lim_{E \rightarrow \mathcal{E}^+} S(E) = +\infty$.
- (iii) It is Lipschitz continuous on every compact interval whose intersection with $\{\mathcal{E} \in \text{Spec}(H) : \mathcal{P}_{\{\mathcal{E}\}}^{(H)} \delta_p \neq 0\}$ is empty.

Proof. Let

$$S^{(M)}(E) := \sum_{j \in \{1, \dots, M\} : \Psi_j(p) \neq 0} \left(\frac{|\Psi_j(p)|^2}{E - \mathcal{E}_j} + \frac{|\Psi_j(p)|^2 \mathcal{E}_j}{1 + \mathcal{E}_j^2} \right), \quad (4.98)$$

$$\widetilde{S}^{(M)}(E) := \sum_{j \in \{1, \dots, M\} : \Psi_j(p) \neq 0} \frac{|\Psi_j(p)|^2}{E - \mathcal{E}_j}, \quad (4.99)$$

for each finite $M \in \mathbb{N}$. Note then that

$$S^{(M)}(a) - S^{(M)}(b) = \widetilde{S}^{(M)}(a) - \widetilde{S}^{(M)}(b) \quad (4.100)$$

$\forall a, b \in \mathbb{R} \setminus \{\mathcal{E}_j : j \in \{1, \dots, M\}, \Psi_j(p) \neq 0\}$, and so

$$S(a) - S(b) = \lim_{M \rightarrow \infty} (S^{(M)}(a) - S^{(M)}(b)) = \lim_{M \rightarrow \infty} (\tilde{S}^{(M)}(a) - \tilde{S}^{(M)}(b)) \quad (4.101)$$

$\forall a, b \in \mathbb{R} \setminus \{\mathcal{E} \in \text{Spec}(H) : \mathcal{P}_{\{\mathcal{E}\}}^{(H)} \delta_p \neq 0\}$.

Similar to $R^{(M)}$, $\tilde{S}^{(M)}$ has a singularity at each \mathcal{E}_j with $j \in \{1, \dots, M\}$ and $\Psi_j(p) \neq 0$, tending to $-\infty$ from the left and $+\infty$ from the right, and is smooth and strictly decreasing on every interval which does not intersect one of the singularities (assuming M is large enough that $\{j \in \{1, \dots, M\} : \Psi_j(p) \neq 0\} \neq \emptyset$). The same is true for $S^{(M)}$, since $S^{(M)}$ and $\tilde{S}^{(M)}$ differ only by a constant function.

Define

$$T_\delta(E) := \sum_{j: \Psi_j(p) \neq 0} \frac{|\Psi_j(p)|^2}{(E - \mathcal{E}_j)^2} = \|\psi_E^\delta\|^2, \quad T_\delta^{(M)}(E) := \sum_{j \in \{1, \dots, M\}: \Psi_j(p) \neq 0} \frac{|\Psi_j(p)|^2}{(E - \mathcal{E}_j)^2}, \quad (4.102)$$

and note that

$$\frac{d}{dE} S^{(M)}(E) = \frac{d}{dE} \tilde{S}^{(M)}(E) = -T_\delta^{(M)}(E). \quad (4.103)$$

Lemma 4.3.3 can then be proven by directly adapting the proof of Lemma 4.3.1, replacing e.g. R , $R^{(M)}$, T_Y and $T_Y^{(M)}$ with S , $\tilde{S}^{(M)}$, T_δ and $T_\delta^{(M)}$ respectively. \square

Observe that Corollary 4.3.2, with $\{\mathcal{E} \in \text{Spec}(H) : \mathcal{P}_{\{\mathcal{E}\}}^{(H)} Y \neq 0\} = (E_k^{(Y)})_{k=1}^{M_{\max}}$ replaced with $\{\mathcal{E} \in \text{Spec}(H) : \mathcal{P}_{\{\mathcal{E}\}}^{(H)} \delta_p \neq 0\} = (E_k)_{k=1}^\infty$ and the reference to equation (4.83) replaced with equation (4.95), then follows.

On the basis of these analogous features between the eigenvalues and eigenfunctions of the rank-one perturbed operator H' and those of the delta-perturbed operator H_Θ , there are some interesting further analogies that can be drawn. In §A.2 a particular method of constructing the family of operators $\{H + \nu \langle \cdot, Y \rangle Y : \nu \in \mathbb{R} \setminus \{0\}\}$, for some fixed $Y \in L^2(\mathcal{M}) \setminus \{0\}$, is given. It is then pointed out that the family of operators $\{H_\Theta : \Theta \in (0, 2\pi)\}$ can be constructed in a similar manner, which in essence merely involves replacing Y in the construction of $\{H + \nu \langle \cdot, Y \rangle Y : \nu \in \mathbb{R} \setminus \{0\}\}$ with δ_p .

4.4 Approximation of Eigenvalues and Eigenfunctions to those of the Delta Potential

We are now interested in a sequence of operators

$$H^N := H + \nu_N \langle \cdot, Y_N \rangle Y_N, \quad (4.104)$$

with $(Y_N)_{N=1}^\infty \subset C_0^\infty(\mathcal{M}^\circ) \setminus \{0\}$, $(\nu_N)_{N=1}^\infty \subset \mathbb{R} \setminus \{0\}$, whose eigenvalues and eigenfunctions would approach those of the delta potential operator H_Θ as $N \rightarrow \infty$. To begin with, we shall impose the following requirement: writing $Y_N = \sum_{j=1}^\infty y_j^N \Psi_j$, so $y_j^N = \langle Y_N, \Psi_j \rangle$, we have

$$y_j^N \rightarrow \overline{\Psi_j(p)} \text{ as } N \rightarrow \infty \forall j \in \mathbb{N}. \quad (4.105)$$

Lemma 4.4.1. $\exists (Y_N)_{N=1}^\infty \subset C_0^\infty(\mathcal{M}^\circ) \setminus \{0\}$ such that (4.105) holds.

Proof. Take some $(\tilde{Y}_N)_{N=1}^\infty \subset L^2(\mathcal{M})$ satisfying $\tilde{y}_j^N \rightarrow \overline{\Psi_j(p)}$ as $N \rightarrow \infty \forall j \in \mathbb{N}$, e.g. $\tilde{Y}_N = \sum_{j=1}^N \overline{\Psi_j(p)} \Psi_j$. Since $C_0^\infty(\mathcal{M}^\circ)$ is dense in $L^2(\mathcal{M})$, and so $C_0^\infty(\mathcal{M}^\circ) \setminus \{0\}$ is dense in $L^2(\mathcal{M})$, take a sequence $(\epsilon_N)_{N=1}^\infty \subset (0, \infty)$ with $\epsilon_N \rightarrow 0$, and a sequence $(Y_N)_{N=1}^\infty \subset C_0^\infty(\mathcal{M}^\circ) \setminus \{0\}$ with $\|Y_N - \tilde{Y}_N\| \leq \epsilon_N \forall N \in \mathbb{N}$. Then for each $N \in \mathbb{N}$,

$$\sum_{j=1}^\infty |y_j^N - \tilde{y}_j^N|^2 \leq \epsilon_N^2 \Rightarrow |y_j^N - \tilde{y}_j^N|^2 \leq \epsilon_N^2 \forall j \in \mathbb{N} \Rightarrow |y_j^N - \tilde{y}_j^N| \leq \epsilon_N \forall j \in \mathbb{N}. \quad (4.106)$$

Thus

$$|y_j^N - \overline{\Psi_j(p)}| \leq |y_j^N - \tilde{y}_j^N| + |\tilde{y}_j^N - \overline{\Psi_j(p)}| \xrightarrow{N \rightarrow \infty} 0 \forall j \in \mathbb{N}. \quad (4.107)$$

□

Note that an example of such $(Y_N)_{N=1}^\infty \subset C_0^\infty(\mathcal{M}^\circ)$ with (4.105) holding is given in (4.57), taking $Z_N := A\mathcal{F}^{-1}\{\chi_N\}$ with χ_N given by (4.9). (4.105) in this case is then a reiteration of (4.67). Regarding the $Y_N \neq 0$ requirement, (4.105) is itself clearly sufficient for $Y_N \neq 0$ for all sufficiently large N , since it must hold that $\Psi_j(p) \neq 0$ for some $j \in \mathbb{N}$. As an aside, the result that with this example, $Y_N \neq 0 \forall N \in \mathbb{N}$, can also be obtained by observing that $Z_N \neq 0$ is an analytic function, being the inverse Fourier transform of a nonzero compactly supported function. It then follows that Z_N is everywhere supported.

However, for the sake of what is to follow, it would still be useful to have a proof of Lemma 4.4.1 like the one given directly above, rather than just referencing (4.57) with (4.9) as an example.

4.4.1 Approximation of Eigenfunctions in common with the Unperturbed Operator

Here we shall consider whether the eigenfunctions output upon Steps (i) and (ii) of the construction of an eigenbasis of H^N , as described in §4.3.1, can be made to approach those for H_Θ (construction of eigenbasis described in §4.3.2). Note that all eigenfunctions

relevant here are also eigenfunctions of the unperturbed operator H , with the same eigenvalue.

Consider an eigenvalue \mathcal{E} of H with multiplicity $m \geq 2$ and $\mathcal{P}_{\{\mathcal{E}\}}^{(H)}\delta_p \neq 0$, so we can write $\mathcal{E} = E_k$, $\Phi_k = \Psi_l$. Then since $y_l^N \rightarrow \overline{\Phi_k(p)}$ as $N \rightarrow \infty$, it follows that for all sufficiently large N , $y_l^N \neq 0$ and so $\mathcal{P}_{\{\mathcal{E}\}}^{(H)}Y_N \neq 0$. Thus for H_Θ and also for H^N with sufficiently large N , \mathcal{E} is an eigenvalue with multiplicity $m - 1$, and the eigenspaces $\Lambda_{\{\mathcal{E}\}}^{(H_\Theta)}$ and $\Lambda_{\{\mathcal{E}\}}^{(H^N)}$ are subspaces of $\Lambda_{\{\mathcal{E}\}}^{(H)}$ orthogonal to $\mathcal{P}_{\{\mathcal{E}\}}^{(H)}\delta_p$ (equivalently Φ_k) and $\mathcal{P}_{\{\mathcal{E}\}}^{(H)}Y_N$ respectively. It is then of interest to select an orthonormal basis of $\Lambda_{\{\mathcal{E}\}}^{(H^N)}$ for each sufficiently large N , such that the basis members approach the orthonormal basis $\{\Psi_j : \mathcal{E}_j = \mathcal{E}, j \neq l\}$ of $\Lambda_{\{\mathcal{E}\}}^{(H_\Theta)}$.

To begin with, we shall state that given any finite-dimensional complex Hilbert space \mathcal{H} of dimension $m \geq 2$, and given any $u, v \in \mathcal{H}$ with $\|u\| = \|v\| = 1$, the following results hold:

Lemma 4.4.2.

$$\min_{\theta \in [0, 2\pi)} \|e^{i\theta}v - u\| = \sqrt{2(1 - |\langle u, v \rangle|)}, \quad (4.108)$$

with the minimum occurring at

$$e^{i\theta} = \frac{\langle u, v \rangle}{|\langle u, v \rangle|} \quad (4.109)$$

for $\langle u, v \rangle \neq 0$. $\|e^{i\theta}v - u\| = \sqrt{2} \forall \theta$ when $\langle u, v \rangle = 0$.

Proof.

$$\begin{aligned} \|e^{i\theta}v - u\|^2 &= \langle e^{i\theta}v, e^{i\theta}v \rangle - \langle e^{i\theta}v, u \rangle - \langle u, e^{i\theta}v \rangle + \langle u, u \rangle \\ &= 2(1 - \operatorname{Re}(e^{i\theta} \langle v, u \rangle)) = 2(1 - \operatorname{Re}(\langle v, u \rangle) \cos \theta + \operatorname{Im}(\langle v, u \rangle) \sin \theta) \\ &= 2(1 + |\langle v, u \rangle| \sin(\theta + \alpha)) \quad \forall \theta \in \mathbb{R}, \end{aligned} \quad (4.110)$$

where

$$\sin \alpha = -\frac{\operatorname{Re}(\langle v, u \rangle)}{|\langle v, u \rangle|}, \quad \cos \alpha = \frac{\operatorname{Im}(\langle v, u \rangle)}{|\langle v, u \rangle|}, \quad (4.111)$$

provided $\langle v, u \rangle \neq 0$. If $\langle v, u \rangle = 0$ then clearly $\|e^{i\theta}v - u\|^2 = 2 \forall \theta \in \mathbb{R}$.

Thus

$$\min_{\theta \in \mathbb{R}} \|e^{i\theta}v - u\|^2 = 2(1 - |\langle v, u \rangle|), \quad (4.112)$$

and if $\langle v, u \rangle \neq 0$ this minimum occurs at

$$\theta_{\min} = -\left(\alpha + \frac{\pi}{2}\right) \bmod 2\pi. \quad (4.113)$$

So then,

$$\cos \theta_{\min} = -\sin \alpha = \frac{\operatorname{Re}(\langle v, u \rangle)}{|\langle v, u \rangle|}, \quad \sin \theta_{\min} = -\cos \alpha = -\frac{\operatorname{Im}(\langle v, u \rangle)}{|\langle v, u \rangle|}, \quad (4.114)$$

and so

$$e^{i\theta_{\min}} = \frac{\operatorname{Re}(\langle v, u \rangle) - i\operatorname{Im}(\langle v, u \rangle)}{|\langle v, u \rangle|} = \frac{\langle u, v \rangle}{|\langle u, v \rangle|}. \quad (4.115)$$

Double-checking:

$$\begin{aligned} \|e^{i\theta_{\min}}v - u\|^2 &= \langle e^{i\theta_{\min}}v, e^{i\theta_{\min}}v \rangle - \langle e^{i\theta_{\min}}v, u \rangle - \langle u, e^{i\theta_{\min}}v \rangle + \langle u, u \rangle \\ &= 1 - \frac{\langle u, v \rangle}{|\langle u, v \rangle|} \langle v, u \rangle - \frac{\langle v, u \rangle}{|\langle u, v \rangle|} \langle u, v \rangle + 1 = 1 - \frac{|\langle u, v \rangle|^2}{|\langle u, v \rangle|} - \frac{|\langle u, v \rangle|^2}{|\langle u, v \rangle|} + 1 \\ &= 2(1 - |\langle u, v \rangle|). \end{aligned} \quad (4.116)$$

□

Lemma 4.4.3. *There exists a unitary operator $U : \mathcal{H} \rightarrow \mathcal{H}$ such that*

$$Uu = v, \quad (4.117)$$

$$\|U - I\| = \|v - u\| = \sqrt{2(1 - \operatorname{Re}(\langle u, v \rangle))}, \quad (4.118)$$

where I is the identity map and the notation $\|\cdot\|$ is being used to represent operator norm as well as Hilbert space norm.

Proof. Take an orthonormal basis $\{w_1, \dots, w_m\}$ of \mathcal{H} with

$$w_1 = u, \quad w_2 = \frac{v - \langle v, u \rangle u}{\|v - \langle v, u \rangle u\|} \text{ if } v \notin \operatorname{span}\{u\}. \quad (4.119)$$

Note that if $v \in \operatorname{span}\{u\}$ then writing $v = e^{i\theta}u$, we have $\langle v, u \rangle u = \langle e^{i\theta}u, u \rangle u = e^{i\theta} \langle u, u \rangle u = e^{i\theta}u = v$. If $v \notin \operatorname{span}\{u\}$ then clearly $\langle v, u \rangle u \neq v$. In either case we have

$$\begin{aligned} \|v - \langle v, u \rangle u\|^2 &= \langle v, v \rangle - \langle v, \langle v, u \rangle u \rangle - \langle \langle v, u \rangle u, v \rangle + \langle \langle v, u \rangle u, \langle v, u \rangle u \rangle \\ &= 1 - |\langle v, u \rangle|^2 - |\langle v, u \rangle|^2 + |\langle v, u \rangle|^2 = 1 - |\langle v, u \rangle|^2. \end{aligned} \quad (4.120)$$

With $v \notin \operatorname{span}\{u\}$, clearly w_1 and w_2 as given in (4.119) are normalised. Verifying that they are orthogonal:

$$\langle w_1, w_2 \rangle = \frac{\langle u, v - \langle v, u \rangle u \rangle}{\|v - \langle v, u \rangle u\|} = \frac{\langle u, v \rangle - \langle u, v \rangle \langle u, u \rangle}{\|v - \langle v, u \rangle u\|} = 0. \quad (4.121)$$

Rearranging the formula for w_2 in (4.119) gives

$$v = \langle v, u \rangle u + \|v - \langle v, u \rangle u\| w_2 = \langle v, u \rangle w_1 + \sqrt{1 - |\langle v, u \rangle|^2} w_2. \quad (4.122)$$

Observe that (4.122) also holds in the case where $v \in \operatorname{span}\{u\}$. In this case, $v = \langle v, u \rangle u = \langle v, u \rangle w_1$ and $\|v - \langle v, u \rangle u\| = \sqrt{1 - |\langle v, u \rangle|^2} = 0$ (here we still specify that $w_1 = u$, but allow w_2 to be an arbitrary normalised vector orthogonal to u).

Now representing vectors in \mathcal{H} as column vectors in \mathbb{C}^m through their expansion into the basis $\{w_1, \dots, w_m\}$, let U be the operator represented by pre-multiplication by the $m \times m$ matrix

$$U_{m \times m} = \left(\begin{array}{cc|c} \langle v, u \rangle & -\sqrt{1 - |\langle v, u \rangle|^2} & 0_{2 \times (m-2)} \\ \sqrt{1 - |\langle v, u \rangle|^2} & \langle u, v \rangle & \\ \hline 0_{(m-2) \times 2} & & I_{(m-2) \times (m-2)} \end{array} \right). \quad (4.123)$$

This is a unitary matrix, since the columns are clearly orthogonal and normalised (likewise the rows), from which it follows that U is a unitary operator (furthermore $\det U_{m \times m} = 1$). Noting that u is represented by the vector $(1 \ 0 \ \dots \ 0)^T$, it follows from comparison between the first column of $U_{m \times m}$ and the expression for v in (4.122) that $Uu = v$.

Since $U_{m \times m}$ is unitary, we have

$$U_{m \times m}^{-1} = U_{m \times m}^* = \left(\begin{array}{cc|c} \langle u, v \rangle & \sqrt{1 - |\langle v, u \rangle|^2} & 0_{2 \times (m-2)} \\ -\sqrt{1 - |\langle v, u \rangle|^2} & \langle v, u \rangle & \\ \hline 0_{(m-2) \times 2} & & I_{(m-2) \times (m-2)} \end{array} \right), \quad (4.124)$$

where $*$ here means complex conjugate of the transpose.

The operator norm of $U - I$ can then be calculated by finding the square root of the largest eigenvalue of the matrix

$$\begin{aligned} (U_{m \times m} - I)^*(U_{m \times m} - I) &= U_{m \times m}^* U_{m \times m} - U_{m \times m}^* - U_{m \times m} + I = 2I - U_{m \times m} - U_{m \times m}^* \\ &= \left(\begin{array}{cc|c} 2(1 - \operatorname{Re}(\langle v, u \rangle)) & 0 & 0_{2 \times (m-2)} \\ 0 & 2(1 - \operatorname{Re}(\langle v, u \rangle)) & \\ \hline 0_{(m-2) \times 2} & & 0_{(m-2) \times (m-2)} \end{array} \right). \end{aligned} \quad (4.125)$$

Clearly the eigenvalues of this matrix are $2(1 - \operatorname{Re}(\langle v, u \rangle))$, with corresponding eigenspace $\operatorname{span}\{w_1, w_2\}$, and 0, with corresponding eigenspace $\operatorname{span}\{w_3, \dots, w_m\}$ (or just $2(1 - \operatorname{Re}(\langle v, u \rangle))$ with eigenspace \mathcal{H} if either $m = 2$ or $2(1 - \operatorname{Re}(\langle v, u \rangle)) = 0$). Note that $|\operatorname{Re}(\langle v, u \rangle)| \leq |\langle v, u \rangle| \leq \|v\| \|u\| = 1$, and so $2(1 - \operatorname{Re}(\langle v, u \rangle)) \geq 0$. Hence

$$\|U - I\| = \sqrt{2(1 - \operatorname{Re}(\langle v, u \rangle))}. \quad (4.126)$$

Now

$$\begin{aligned} \|(U - I)u\| &= \|v - u\| = \sqrt{\langle v, v \rangle - \langle v, u \rangle - \langle u, v \rangle + \langle u, u \rangle} \\ &= \sqrt{2(1 - \operatorname{Re}(\langle v, u \rangle))} \end{aligned} \quad (4.127)$$

also. Hence U satisfies (4.117) and (4.118). \square

Corollary 4.4.4. *Let*

$$\mathcal{U}_u^v := \{\text{unitary } U \text{ on } \mathcal{H} : Uu \in \text{span}\{v\}\}. \quad (4.128)$$

Then

$$\min\{\|U - I\| : U \in \mathcal{U}_u^v\} = \sqrt{2(1 - |\langle u, v \rangle|)}. \quad (4.129)$$

Proof. For each $U \in \mathcal{U}_u^v$, since U is unitary, so $\|Uu\| = \|u\| = 1$, and since $Uu \in \text{span}\{v\}$, we can write $Uu = e^{i\theta_U}v$ for some $\theta_U \in [0, 2\pi)$. So then, applying Lemma 4.4.2,

$$\|U - I\| \geq \|(U - I)u\| = \|e^{i\theta_U}v - u\| \geq \|e^{i\theta_{\min}}v - u\| = \sqrt{2(1 - |\langle u, v \rangle|)}, \quad (4.130)$$

where $e^{i\theta_{\min}} = \frac{\langle u, v \rangle}{|\langle u, v \rangle|}$ (or if $\langle u, v \rangle = 0$ then $e^{i\theta_{\min}}$ may take any value on the unit circle in the complex plane). Then by Lemma 4.4.3 (applying Lemma 4.4.3 with $e^{i\theta_{\min}}v$ in place of v), there exists a unitary operator $U_{\min} : \mathcal{H} \rightarrow \mathcal{H}$ such that

$$U_{\min}u = e^{i\theta_{\min}}v \quad (\text{so } U_{\min} \in \mathcal{U}_u^v), \quad (4.131)$$

$$\|U_{\min} - I\| = \|e^{i\theta_{\min}}v - u\| = \sqrt{2(1 - |\langle u, v \rangle|)}. \quad (4.132)$$

This proves (4.129). \square

We now return to the issue of selecting an orthonormal basis of $\Lambda_{\{\mathcal{E}\}}^{(H^N)}$ for each sufficiently large N , where \mathcal{E} is an eigenvalue of H with multiplicity $m \geq 2$ and $\mathcal{P}_{\{\mathcal{E}\}}^{(H)}\delta_p \neq 0$. Write therefore $\mathcal{E} = E_k$, $\Phi_k = \Psi_l$. We shall take ‘‘sufficiently large N ’’ to be $N \geq N_0$, where $N_0 \in \mathbb{N}$ is a value for which it holds that $\mathcal{P}_{\{\mathcal{E}\}}^{(H)}Y_N \neq 0 \forall N \in \mathbb{N} \cap [N_0, \infty)$. Letting

$$\mathcal{U}_k^N := \{\text{unitary } U \text{ on } \Lambda_{\{\mathcal{E}\}}^{(H)} : U\Phi_k \in \text{span}\{\mathcal{P}_{\{\mathcal{E}\}}^{(H)}Y_N\}\}, \quad (4.133)$$

the collection of all possible choices of orthonormal basis of $\Lambda_{\{\mathcal{E}\}}^{(H^N)}$ is

$$\{\{U\Psi_j : \mathcal{E}_j = \mathcal{E}, j \neq l\} : U \in \mathcal{U}_k^N\}. \quad (4.134)$$

Then applying here the existence of a unitary operator satisfying (4.131) and (4.132) in the proof of Corollary 4.4.4, we can select $U_k^N \in \mathcal{U}_k^N$ such that

$$U_k^N\Phi_k = \frac{\overline{y_l^N}\mathcal{P}_{\{\mathcal{E}\}}^{(H)}Y_N}{\left\|\overline{y_l^N}\mathcal{P}_{\{\mathcal{E}\}}^{(H)}Y_N\right\|} \quad \text{if } y_l^N \neq 0, \quad (4.135)$$

and

$$\|U_k^N - I\| = \|(U_k^N - I)\Phi_k\| = \sqrt{2\left(1 - \frac{|y_l^N|}{\|\mathcal{P}_{\{\mathcal{E}\}}^{(H)}Y_N\|}\right)}. \quad (4.136)$$

If $y_l^N = 0$ then just having $U_k^N \Phi_k \in \text{span}\{\mathcal{P}_{\{\mathcal{E}\}}^{(H)} Y_N\}$ in place of (4.135) will do.

[We could require N_0 to be sufficiently large that $y_l^N \neq 0 \forall N \in \mathbb{N} \cap [N_0, \infty)$ rather than just $\mathcal{P}_{\{\mathcal{E}\}}^{(H)} Y_N \neq 0 \forall N \in \mathbb{N} \cap [N_0, \infty)$. However, this kind of discrepancy may in principle make a non-trivial difference when considering behaviour not just for *each individual* eigenvalue \mathcal{E} satisfying certain specifications, but for *infinitely many* such eigenvalues *simultaneously*.]

It then follows that for each $j \in \mathbb{N}$ with $\mathcal{E}_j = \mathcal{E}$, $j \neq l$, we have

$$\|(U_k^N - I)\Psi_j\| \leq \|(U_k^N - I)\Phi_k\| = \sqrt{2 \left(1 - \frac{|y_l^N|}{\|\mathcal{P}_{\{\mathcal{E}\}}^{(H)} Y_N\|}\right)}. \quad (4.137)$$

Note also that

$$\|U_k^N - I\| = \min\{\|U - I\| : U \in \mathcal{U}_k^N\}. \quad (4.138)$$

Since $y_j^N \xrightarrow{N \rightarrow \infty} \overline{\Psi_j(p)}$ for each j with $\mathcal{E}_j = \mathcal{E}$, and $\Psi_l(p) \neq 0$ while $\Psi_j(p) = 0$ for each j with $\mathcal{E}_j = \mathcal{E}$ other than l , it follows that

$$\frac{|y_l^N|}{\|\mathcal{P}_{\{\mathcal{E}\}}^{(H)} Y_N\|} = \frac{|y_l^N|}{\sqrt{\sum_{j:\mathcal{E}_j=\mathcal{E}} |y_j^N|^2}} \xrightarrow{N \rightarrow \infty} \frac{|\Psi_l(p)|}{\sqrt{|\Psi_l(p)|^2}} = 1, \quad (4.139)$$

and so

$$\|U_k^N - I\| = \|(U_k^N - I)\Phi_k\| \xrightarrow{N \rightarrow \infty} 0. \quad (4.140)$$

Observe also that $\mathcal{P}_{\{\mathcal{E}\}}^{(H)} Y_N \xrightarrow{N \rightarrow \infty} \mathcal{P}_{\{\mathcal{E}\}}^{(H)} \delta_p = \overline{\Phi_k(p)} \Phi_k$, and so

$$U_k^N \Phi_k = \frac{\overline{y_l^N} \mathcal{P}_{\{\mathcal{E}\}}^{(H)} Y_N}{\left\| \overline{y_l^N} \mathcal{P}_{\{\mathcal{E}\}}^{(H)} Y_N \right\|} \xrightarrow{N \rightarrow \infty} \frac{\Phi_k(p) \overline{\Phi_k(p)} \Phi_k}{\|\Phi_k(p) \overline{\Phi_k(p)} \Phi_k\|} = \Phi_k, \quad (4.141)$$

again proving that $\|(U_k^N - I)\Phi_k\| \xrightarrow{N \rightarrow \infty} 0$.

Hence by (4.134), (4.137) and (4.140), if for each $N \in \mathbb{N} \cap [N_0, \infty)$, we take the orthonormal basis $\{U_k^N \Psi_j : \mathcal{E}_j = \mathcal{E}, j \neq l\}$ of $\Lambda_{\{\mathcal{E}\}}^{(H^N)}$, these orthonormal bases will then approach the orthonormal basis $\{\Psi_j : \mathcal{E}_j = \mathcal{E}, j \neq l\}$ of $\Lambda_{\{\mathcal{E}\}}^{(H_\Theta)}$.

As for the case of an eigenvalue \mathcal{E} of H with $\mathcal{P}_{\{\mathcal{E}\}}^{(H)} \delta_p = 0$, in which case $\Lambda_{\{\mathcal{E}\}}^{(H)} \subset \Lambda_{\{\mathcal{E}\}}^{(H_\Theta)}$, normally $\Lambda_{\{\mathcal{E}\}}^{(H_\Theta)} = \Lambda_{\{\mathcal{E}\}}^{(H)}$ (the exception being when \mathcal{E} happens to be a solution of (4.95)), here we do not necessarily have $\mathcal{P}_{\{\mathcal{E}\}}^{(H)} Y_N = 0$ for all sufficiently large N .

In the case where it does hold that $\mathcal{P}_{\{\mathcal{E}\}}^{(H)} Y_N = 0$ for all sufficiently large N , in which case $\Lambda_{\{\mathcal{E}\}}^{(H)} \subset \Lambda_{\{\mathcal{E}\}}^{(H^N)}$ for each such N , we can choose the orthonormal eigenbases of both H_Θ and H^N to include $\{\Psi_j : \mathcal{E}_j = \mathcal{E}\}$. In the case where this does not hold, there exists a strictly increasing sequence $(N_n)_{n=1}^\infty \subset \mathbb{N}$ such that $\mathcal{P}_{\{\mathcal{E}\}}^{(H)} Y_{N_n} \neq 0 \forall n \in \mathbb{N}$. For each n ,

the number of eigenfunctions of H^{N_n} with eigenvalue \mathcal{E} output upon Steps (i) and (ii) is one fewer than those for H_Θ .

Thus the approximation of eigenfunctions of H^N from Steps (i) and (ii) to those of H_Θ does not fully work for eigenvalues \mathcal{E} that satisfy $\mathcal{P}_{\{\mathcal{E}\}}^{(H)}\delta_p = 0$ but not $\mathcal{P}_{\{\mathcal{E}\}}^{(H)}Y_N = 0 \forall$ suff. large N , as it does for eigenvalues \mathcal{E} satisfying both $\mathcal{P}_{\{\mathcal{E}\}}^{(H)}\delta_p = 0$ and $\mathcal{P}_{\{\mathcal{E}\}}^{(H)}Y_N = 0 \forall$ suff. large N , and also for degenerate (multiplicity ≥ 2) eigenvalues \mathcal{E} of H satisfying $\mathcal{P}_{\{\mathcal{E}\}}^{(H)}\delta_p \neq 0$.

One could still though consider the possibility of partial success in the approximation of eigenfunctions of H^N from Steps (i) and (ii) to those of H_Θ , in the case where \mathcal{E} satisfies $\mathcal{P}_{\{\mathcal{E}\}}^{(H)}\delta_p = 0$ but not $\mathcal{P}_{\{\mathcal{E}\}}^{(H)}Y_N = 0 \forall$ suff. large N . For example, with \mathcal{E} being degenerate, letting $(N_n)_{n=1}^\infty \subset \mathbb{N}$ be the strictly increasing sequence consisting of all $N \in \mathbb{N}$ with $\mathcal{P}_{\{\mathcal{E}\}}^{(H)}Y_N \neq 0$, we can address this question: does there exist $(\theta_n)_{n=1}^\infty \subset [0, 2\pi)$ such that

$$e^{i\theta_n} \frac{\mathcal{P}_{\{\mathcal{E}\}}^{(H)}Y_{N_n}}{\|\mathcal{P}_{\{\mathcal{E}\}}^{(H)}Y_{N_n}\|} \quad (4.142)$$

converges in $\Lambda_{\{\mathcal{E}\}}^{(H)} \subset L^2(\mathcal{M})$ as $n \rightarrow \infty$? If so, call the limit $\tilde{\Phi}_\mathcal{E}$, and take an orthonormal basis $\{\tilde{\Psi}_j : \mathcal{E}_j = \mathcal{E}\}$ of $\Lambda_{\{\mathcal{E}\}}^{(H)}$ with one of the members being $\tilde{\Phi}_\mathcal{E}$ ($= \tilde{\Psi}_l$). Although in Step (i) of the eigenbasis construction for H_Θ , it was specified that we take the original eigenbasis $\{\Psi_j\}_{j=1}^\infty$ of H , it would be reasonable here to modify the specification by allowing the orthonormal basis of $\Lambda_{\{\mathcal{E}\}}^{(H)}$ within our chosen eigenbasis of H to be $\{\tilde{\Psi}_j : \mathcal{E}_j = \mathcal{E}\}$ rather than $\{\Psi_j : \mathcal{E}_j = \mathcal{E}\}$.

So then, since $\Lambda_{\{\mathcal{E}\}}^{(H)} \subset \Lambda_{\{\mathcal{E}\}}^{(H_\Theta)}$ and $\Lambda_{\{\mathcal{E}\}}^{(H)} \subset \Lambda_{\{\mathcal{E}\}}^{(H^{N_n})}$ for each N with $\mathcal{P}_{\{\mathcal{E}\}}^{(H)}Y_N = 0$, let the chosen eigenbases of H_Θ and of each such H^{N_n} include $\{\tilde{\Psi}_j : \mathcal{E}_j = \mathcal{E}\}$. As for each H^{N_n} , since $\Lambda_{\{\mathcal{E}\}}^{(H^{N_n})}$ is the orthogonal complement of $\text{span}\{\mathcal{P}_{\{\mathcal{E}\}}^{(H)}Y_{N_n}\}$ in $\Lambda_{\{\mathcal{E}\}}^{(H)}$, let the orthonormal basis of $\Lambda_{\{\mathcal{E}\}}^{(H^{N_n})}$ within the chosen eigenbasis of H^{N_n} be $\{\tilde{U}_\mathcal{E}^{N_n}\tilde{\Psi}_j : \mathcal{E}_j = \mathcal{E}, j \neq l\}$, where

$$\tilde{U}_\mathcal{E}^{N_n}\tilde{\Phi}_\mathcal{E} = e^{i\theta_n} \frac{\mathcal{P}_{\{\mathcal{E}\}}^{(H)}Y_{N_n}}{\|\mathcal{P}_{\{\mathcal{E}\}}^{(H)}Y_{N_n}\|}, \quad (4.143)$$

with

$$e^{i\theta_n} = \frac{\langle \tilde{\Phi}_\mathcal{E}, Y_{N_n} \rangle}{|\langle \tilde{\Phi}_\mathcal{E}, Y_{N_n} \rangle|} \quad \text{if } \langle \tilde{\Phi}_\mathcal{E}, Y_{N_n} \rangle \neq 0, \quad (4.144)$$

and

$$\|\tilde{U}_\mathcal{E}^{N_n} - I\| = \|(\tilde{U}_\mathcal{E}^{N_n} - I)\tilde{\Phi}_\mathcal{E}\| \quad (4.145)$$

(by analogy with (4.135) and (4.136)). We then have, for each j with $\mathcal{E}_j = \mathcal{E}$,

$$\|(\tilde{U}_\mathcal{E}^{N_n} - I)\tilde{\Psi}_j\| \leq \|(\tilde{U}_\mathcal{E}^{N_n} - I)\tilde{\Phi}_\mathcal{E}\| \leq \left\| e^{i\theta_n} \frac{\mathcal{P}_{\{\mathcal{E}\}}^{(H)}Y_{N_n}}{\|\mathcal{P}_{\{\mathcal{E}\}}^{(H)}Y_{N_n}\|} - \tilde{\Phi}_\mathcal{E} \right\| \xrightarrow{n \rightarrow \infty} 0. \quad (4.146)$$

For each $N \in \mathbb{N}$ with $\mathcal{P}_{\{\mathcal{E}\}}^{(H)} Y_N = 0$, let $\tilde{U}_{\mathcal{E}}^N = I$.

What we end up with is this: for each j with $\mathcal{E}_j = \mathcal{E}$, $\tilde{U}_{\mathcal{E}}^N \tilde{\Psi}_j \rightarrow \tilde{\Psi}_j$ as $N \rightarrow \infty$. Now every $\tilde{\Psi}_j$ with $\mathcal{E}_j = \mathcal{E}$ belongs to the orthonormal basis of $\Lambda_{\{\mathcal{E}\}}^{(H_\Theta)}$ within the chosen eigenbasis of H_Θ . However, while each $\tilde{U}_{\mathcal{E}}^N \tilde{\Psi}_j$ with $\mathcal{E}_j = \mathcal{E}$ other than $\tilde{U}_{\mathcal{E}}^N \tilde{\Phi}_{\mathcal{E}}$ belongs to the orthonormal basis of $\Lambda_{\{\mathcal{E}\}}^{(H^N)}$ for all $N \in \mathbb{N}$, $\tilde{U}_{\mathcal{E}}^N \tilde{\Phi}_{\mathcal{E}}$ only belongs to the orthonormal basis of $\Lambda_{\{\mathcal{E}\}}^{(H^N)}$ when $\mathcal{P}_{\{\mathcal{E}\}}^{(H)} Y_N = 0$.

4.4.2 Approximation of New Eigenvalues

Given the definitions of functions R , T_Y , S , and T_δ in LHS(4.83), (4.91), (4.95) and (4.102) respectively, define R_N , T_N , S and T_δ here in exactly the same way respectively, where we now have H^N for each $N \in \mathbb{N}$ in place of H' . As before, we may also add a superscript (M) for some $M \in \mathbb{N}$ to represent a partial sum (as in e.g. (4.86)).

Lemma 4.4.5. *For each $E \in \mathbb{R} \setminus \text{Spec}(H)$, and also for each $E \in \text{Spec}(H)$ with $\mathcal{P}_{\{E\}}^{(H)} Y_N = 0$ for all sufficiently large N ,*

$$R_N(E) := \sum_{j: y_j^N \neq 0} \frac{|y_j^N|^2}{E - \mathcal{E}_j} \rightarrow -\infty \quad \text{as } N \rightarrow \infty. \quad (4.147)$$

Proof. Note firstly that by Lemma 2.2.8,

$$\tilde{S}^{(M)}(E) := \sum_{j \in \{1, \dots, M\}: \Psi_j(p) \neq 0} \frac{|\Psi_j(p)|^2}{E - \mathcal{E}_j} \rightarrow -\infty \quad \text{as } M \rightarrow \infty. \quad (4.148)$$

If $E \notin \text{Spec}(H)$ then clearly $\tilde{S}^{(M)}(E)$ is well-defined. If $E \in \text{Spec}(H)$ with $\mathcal{P}_{\{E\}}^{(H)} Y_N = 0$ for all sufficiently large N , then it also follows that $\mathcal{P}_{\{E\}}^{(H)} \delta_p = 0$ so again $\tilde{S}^{(M)}(E)$ is well-defined. Given any $L \in \mathbb{R}$, take some $M_L \in \mathbb{N}$ with $\mathcal{E}_{M_L} > E$ and $\tilde{S}^{(M_L)}(E) \leq L - 1$. It is also the case then that

$$R_N^{(M_L)}(E) \rightarrow \tilde{S}^{(M_L)}(E) \quad \text{as } N \rightarrow \infty, \quad (4.149)$$

so take some $N_L \in \mathbb{N}$ for which $|R_N^{(M_L)}(E) - \tilde{S}^{(M_L)}(E)| \leq 1 \forall N \in \mathbb{N} \cap [N_L, \infty)$. Then

$$R_N(E) \leq R_N^{(M_L)}(E) \leq L \quad \forall N \in \mathbb{N} \cap [N_L, \infty). \quad (4.150)$$

□

Now define

$$\begin{aligned} M_\Theta &:= \{E \in (E_1, \infty) \setminus \{E_j\}_{j \in \mathbb{N}} : \\ S(E) = F(\Theta), \exists N_0 \in \mathbb{N} \text{ s.t. } \forall N \in \mathbb{N} \cap [N_0, \infty) \mathcal{P}_{\{E\}}^{(H)} Y_N = 0\}, \end{aligned} \quad (4.151)$$

so M_Θ is the set of all eigenvalues of H_Θ above E_1 that solve equation (4.95), except those that coincide with an eigenvalue \mathcal{E} of H for which we fail to have $\mathcal{P}_{\{\mathcal{E}\}}^{(H)}Y_N = 0$ for all sufficiently large N (and of course, for any $E \in \mathbb{R} \setminus \text{Spec}(H)$ and $f \in L^2(\mathcal{M}) + \text{span}\{\delta_p\}$ we necessarily have $\mathcal{P}_{\{E\}}^{(H)}f = 0$). Note that fixing p but varying Θ , only for at most countably many values of $\Theta \in (0, 2\pi)$ will there be a solution of (4.95) that coincides with an eigenvalue of H . Thus for almost all values of Θ , M_Θ will simply be the set of solutions of (4.95) above E_1 .

Given some $\mu \in M_\Theta$, let \mathcal{E}^- and \mathcal{E}^+ be the two consecutive values in $\{E_j\}_{j \in \mathbb{N}} = \{\mathcal{E} \in \text{Spec}(H) : \mathcal{P}_{\{\mathcal{E}\}}^{(H)}\delta_p \neq 0\}$ for which $\mu \in (\mathcal{E}^-, \mathcal{E}^+)$. Then choosing some $N_0 \in \mathbb{N}$ for which it holds that $\mathcal{P}_{\{\mathcal{E}^-\}}^{(H)}Y_N \neq 0$, $\mathcal{P}_{\{\mu\}}^{(H)}Y_N = 0$ and $\mathcal{P}_{\{\mathcal{E}^+\}}^{(H)}Y_N \neq 0 \forall N \in \mathbb{N} \cap [N_0, \infty)$, let \mathcal{E}^{N-} and \mathcal{E}^{N+} for each $N \in \mathbb{N} \cap [N_0, \infty)$ be the two consecutive values in $\{\mathcal{E} \in \text{Spec}(H) : \mathcal{P}_{\{\mathcal{E}\}}^{(H)}Y_N \neq 0\}$ for which $\mu \in (\mathcal{E}^{N-}, \mathcal{E}^{N+})$. Finally, for each $N \in \mathbb{N} \cap [N_0, \infty)$, let μ^N be the solution of (4.83) (i.e. $R_N(\mu^N) = \frac{1}{\nu_N}$) lying in the interval $(\mathcal{E}^{N-}, \mathcal{E}^{N+})$, so μ^N is an eigenvalue of H^N . Observe that $\mathcal{E}^- \leq \mathcal{E}^{N-} < \mathcal{E}^{N+} \leq \mathcal{E}^+$.

Now suppose we can vary the parameter $\nu_N \in \mathbb{R} \setminus \{0\}$ for each N , while keeping the function $Y_N \in C_0^\infty(\mathcal{M}^\circ) \setminus \{0\}$ fixed for each N , and also keeping the parameter $\Theta \in (0, 2\pi)$ fixed. If we wish to have $\mu^N \rightarrow \mu$ as $N \rightarrow \infty$ for this particular $\mu \in M_\Theta$, this can be easily achieved by setting $\nu_N = \frac{1}{R_N(\mu)}$ for all sufficiently large N , in which case $\mu^N = \mu$ for sufficiently large N . However, it is obviously in our interest to have $\mu^N \rightarrow \mu$ for more than just one single $\mu \in M_\Theta$.

Proposition 4.4.6. *Given any $\mu \in M_\Theta$, defining \mathcal{E}^- , \mathcal{E}^+ , \mathcal{E}^{N-} , \mathcal{E}^{N+} and μ^N exactly as above, it holds that if*

$$\frac{1}{\nu_N} - R_N(\mu) \rightarrow 0 \quad \text{as } N \rightarrow \infty \quad (4.152)$$

then $\mu^N \rightarrow \mu$ as $N \rightarrow \infty$.

Proof. Let $M^- := \max\{j \in \mathbb{N} : \mathcal{E}_j < \mu\}$ and $M^+ := \min\{j \in \mathbb{N} : \mathcal{E}_j > \mu\}$. Take some $(a_N)_{N=N_0}^\infty, (b_N)_{N=N_0}^\infty \subset (\mathcal{E}_{M^-}, \mathcal{E}_{M^+})$ with $a_N < b_N$ for each N . Take also some $c \in (\mathcal{E}_{M^-}, \infty)$ and $N'_0 \in \mathbb{N} \cap [N_0, \infty)$ for which it holds that $b_N \leq c \forall N \in \mathbb{N} \cap [N'_0, \infty)$. Applying the mean value theorem (exactly as done in (4.93)), and remembering that R_N is a strictly decreasing function on every interval where it does not have a singularity,

$$0 < R_N(a_N) - R_N(b_N) = \lim_{K \rightarrow \infty} (R_N^{(K)}(a_N) - R_N^{(K)}(b_N)) = \lim_{K \rightarrow \infty} T_N^{(K)}(\sigma_N^K)(b_N - a_N) \\ \forall N \in \mathbb{N} \cap [N_0, \infty), \quad (4.153)$$

where $\sigma_N^K \in (a_N, b_N)$. Noting that all terms in the sum T_N are ≥ 0 , and that $T_N^{(M^-)}$ is a strictly decreasing function on $(\mathcal{E}_{M^-}, \infty)$, for each $N \in \mathbb{N} \cap [N'_0, \infty)$ and $K \in \mathbb{N} \cap [M^-, \infty)$

we have

$$T_N^{(K)}(\sigma_N^K) \geq T_N^{(M^-)}(\sigma_N^K) > T_N^{(M^-)}(c), \quad (4.154)$$

and thus in the limit as $K \rightarrow \infty$,

$$R_N(a_N) - R_N(b_N) \geq T_N^{(M^-)}(c)(b_N - a_N) \quad \forall N \in \mathbb{N} \cap [N'_0, \infty). \quad (4.155)$$

Now $T_N^{(M^-)}(c) \xrightarrow{N \rightarrow \infty} T^{(M^-)}(c) > 0$, so take some $L \in (0, T^{(M^-)}(c))$ and $N''_0 \in \mathbb{N} \cap [N'_0, \infty)$ for which $T_N^{(M^-)}(c) \geq L \forall N \in \mathbb{N} \cap [N''_0, \infty)$. Then

$$R_N(a_N) - R_N(b_N) \geq L(b_N - a_N) \quad \forall N \in \mathbb{N} \cap [N''_0, \infty). \quad (4.156)$$

So now, suppose it is the case that (4.152) holds. Take some $L' \in (0, T^{(M^-)}(\mu))$ and some $(\epsilon_N)_{N=N_0}^\infty \subset (0, \min\{\mu - \mathcal{E}_{M^-}, \mathcal{E}_{M^+} - \mu\})$ with $\epsilon_N \xrightarrow{N \rightarrow \infty} 0$ and

$$\epsilon_N \geq \frac{\left| \frac{1}{\nu_N} - R_N(\mu) \right|}{L'} \quad (4.157)$$

for all sufficiently large N .

With this, first of all take

$$a_N = \mu - \epsilon_N, \quad b_N = c = \mu, \quad L = L'. \quad (4.158)$$

Then by (4.156) combined with (4.157),

$$R_N(\mu - \epsilon_N) - R_N(\mu) \geq L'\epsilon_N \geq \frac{1}{\nu_N} - R_N(\mu) \Rightarrow R_N(\mu - \epsilon_N) \geq \frac{1}{\nu_N} \quad (4.159)$$

for all sufficiently large N .

Next, take

$$a_N = \mu, \quad b_N = \mu + \epsilon_N, \quad c \in (\mu, (T^{(M^-)} \upharpoonright_{(\mathcal{E}^-, \infty)})^{-1}(L')), \quad L = L', \quad (4.160)$$

noting that $T^{(M^-)}$ is a strictly decreasing function on the interval (\mathcal{E}^-, ∞) , whose image on this interval is $(0, \infty)$. Then, again by (4.156) combined with (4.157),

$$R_N(\mu) - R_N(\mu + \epsilon_N) \geq L'\epsilon_N \geq R_N(\mu) - \frac{1}{\nu_N} \Rightarrow R_N(\mu + \epsilon_N) \leq \frac{1}{\nu_N} \quad (4.161)$$

for all sufficiently large N .

In conclusion, for all sufficiently large N ,

$$R_N(\mu - \epsilon_N) \geq \frac{1}{\nu_N} = R_N(\mu^N) \geq R_N(\mu + \epsilon_N) \Rightarrow \mu - \epsilon_N \leq \mu^N \leq \mu + \epsilon_N. \quad (4.162)$$

□

Corollary 4.4.7. Keeping $(Y_N)_{N \in \mathbb{N}} \subset C_0^\infty(\mathcal{M}^\circ) \setminus \{0\}$ and $\Theta \in (0, 2\pi)$ fixed, suppose we can vary $(\nu_N)_{N \in \mathbb{N}} \subset \mathbb{R} \setminus \{0\}$. Taking any non-empty set $X \subset M_\Theta$, it holds that if

$$R_N(\mu) - R_N(\mu') \xrightarrow{N \rightarrow \infty} 0 \quad \forall \mu, \mu' \in X \quad (4.163)$$

then $(\nu_N)_{N \in \mathbb{N}}$ can be chosen in such a way that $\mu^N \xrightarrow{N \rightarrow \infty} \mu \quad \forall \mu \in X$, namely by selecting any $\mu \in X$ and imposing (4.152) for that μ .

Proof. Suppose (4.163) holds. Select some $\mu \in X$, and set $(\nu_N)_{N \in \mathbb{N}}$ in such a way that (4.152) holds for this particular μ (e.g. $\nu_N = \frac{1}{R_N(\mu)} \quad \forall$ suff. large N). Then given any $\mu' \in X$,

$$\left| \frac{1}{\nu_N} - R_N(\mu') \right| \leq \left| \frac{1}{\nu_N} - R_N(\mu) \right| + |R_N(\mu) - R_N(\mu')| \xrightarrow{N \rightarrow \infty} 0, \quad (4.164)$$

and so by Proposition 4.4.6, $\mu^N \xrightarrow{N \rightarrow \infty} \mu'$. □

Now observe that for any $\mu, \mu' \in M_\Theta$, we have $S(\mu) = S(\mu')$. Thus

$$\begin{aligned} S(\mu) - S(\mu') &= \lim_{M \rightarrow \infty} (\tilde{S}^{(M)}(\mu) - \tilde{S}^{(M)}(\mu')) = \lim_{M \rightarrow \infty} \lim_{N \rightarrow \infty} (R_N^{(M)}(\mu) - R_N^{(M)}(\mu')) \\ &= 0. \end{aligned} \quad (4.165)$$

By comparison, the condition expressed in (4.163) (only now fixing $\mu, \mu' \in M_\Theta$) can be re-expressed as follows:

$$\lim_{N \rightarrow \infty} (R_N(\mu) - R_N(\mu')) = \lim_{N \rightarrow \infty} \lim_{M \rightarrow \infty} (R_N^{(M)}(\mu) - R_N^{(M)}(\mu')) = 0. \quad (4.166)$$

Since (4.165) necessarily holds, we can then arrive at (4.166) if the order of the limits $\lim_{M \rightarrow \infty}$ and $\lim_{N \rightarrow \infty}$ in (4.165) can validly be swapped round.

Lemma 4.4.8. Given an $\mathbb{N} \times \mathbb{N}$ array $(x_{mn})_{m,n \in \mathbb{N}} \subset \mathbb{C}$ with

$$x_{mn} \xrightarrow{n \rightarrow \infty} y_m \in \mathbb{C} \quad \forall m, \quad x_{mn} \xrightarrow{m \rightarrow \infty} z_n \in \mathbb{C} \quad \forall n, \quad (4.167)$$

for any $a \in \mathbb{C}$ the following are equivalent:

- (i) $\lim_{m,n \rightarrow \infty} x_{mn} = a$, meaning that $\forall \epsilon > 0 \exists M_\epsilon, N_\epsilon \in \mathbb{N}$ s.t. $\forall m \in \mathbb{N} \cap [M_\epsilon, \infty), n \in \mathbb{N} \cap [N_\epsilon, \infty) \quad |x_{mn} - a| \leq \epsilon$,
- (ii) $\forall (m_k)_{k \in \mathbb{N}}, (n_k)_{k \in \mathbb{N}} \subset \mathbb{N}$ with $m_k \xrightarrow{k \rightarrow \infty} \infty$ and $n_k \xrightarrow{k \rightarrow \infty} \infty$ it holds that $x_{m_k n_k} \xrightarrow{k \rightarrow \infty} a$,
- (iii) $\lim_{n \rightarrow \infty} \lim_{m \rightarrow \infty} x_{mn} = a$ and $x_{mn} \xrightarrow{n \rightarrow \infty} y_m$ uniformly over m ,

(iv) $\lim_{m \rightarrow \infty} \lim_{n \rightarrow \infty} x_{mn} = a$ and $x_{mn} \xrightarrow{n \rightarrow \infty} y_m$ uniformly over m ,

(v) $\lim_{m \rightarrow \infty} \lim_{n \rightarrow \infty} x_{mn} = a$ and $x_{mn} \xrightarrow{m \rightarrow \infty} z_n$ uniformly over n ,

(vi) $\lim_{n \rightarrow \infty} \lim_{m \rightarrow \infty} x_{mn} = a$ and $x_{mn} \xrightarrow{m \rightarrow \infty} z_n$ uniformly over n .

Proof. (i) \Rightarrow (ii): If (i) holds true, then given any $(m_k)_{k \in \mathbb{N}}, (n_k)_{k \in \mathbb{N}} \subset \mathbb{N}$ with $m_k \xrightarrow{k \rightarrow \infty} \infty$ and $n_k \xrightarrow{k \rightarrow \infty} \infty$, for each $\epsilon > 0$ there exist $M_\epsilon, N_\epsilon, K_\epsilon \in \mathbb{N}$ such that

$$(a) \quad \forall m \in \mathbb{N} \cap [M_\epsilon, \infty), n \in \mathbb{N} \cap [N_\epsilon, \infty) \quad |x_{mn} - a| \leq \epsilon,$$

$$(b) \quad \forall k \in \mathbb{N} \cap [K_\epsilon, \infty) \quad m_k \geq M_\epsilon \text{ and } n_k \geq N_\epsilon,$$

$$\text{and thus } |x_{m_k n_k} - a| \leq \epsilon \quad \forall k \in \mathbb{N} \cap [K_\epsilon, \infty).$$

$\neg(i) \Rightarrow \neg(ii)$: Suppose (i) is not true. Then $\exists \epsilon_0 > 0$ s.t. $\forall M, N \in \mathbb{N} \exists m_{MN} \in \mathbb{N} \cap [M, \infty), n_{MN} \in \mathbb{N} \cap [N, \infty)$ s.t. $|x_{m_{MN} n_{MN}} - a| > \epsilon_0$. So considering then the sequence $(x_{m_{kk} n_{kk}})_{k \in \mathbb{N}}$, since $|x_{m_{kk} n_{kk}} - a| > \epsilon_0 \quad \forall k \in \mathbb{N}$ it follows that $x_{m_{kk} n_{kk}} \not\xrightarrow{k \rightarrow \infty} a$, while $m_{kk} \geq k \xrightarrow{k \rightarrow \infty} \infty$ and $n_{kk} \geq k \xrightarrow{k \rightarrow \infty} \infty$.

(i) \Rightarrow (iii): Suppose (i) holds true. Then given any $\epsilon > 0$, for each $n \in \mathbb{N} \cap [N_\epsilon, \infty)$ it holds that $|x_{mn} - a| \leq \epsilon \quad \forall m \in \mathbb{N} \cap [M_\epsilon, \infty)$, and thus $|z_n - a| \leq \epsilon$. Hence $\lim_{n \rightarrow \infty} \lim_{m \rightarrow \infty} x_{mn} = \lim_{n \rightarrow \infty} z_n = a$. Now note also that for each $m \in \mathbb{N} \cap [M_{\epsilon/2}, \infty)$ it holds that $|x_{mn} - a| \leq \frac{\epsilon}{2} \quad \forall n \in \mathbb{N} \cap [N_{\epsilon/2}, \infty)$, and so $|y_m - a| \leq \frac{\epsilon}{2}$. Thus for each $m \in \mathbb{N} \cap [M_{\epsilon/2}, \infty), n \in \mathbb{N} \cap [N_{\epsilon/2}, \infty)$ $|x_{mn} - y_m| \leq |x_{mn} - a| + |a - y_m| \leq \epsilon$. Then for each $m \in \{1, \dots, M_{\epsilon/2} - 1\}$ define $N_\epsilon^{(m)} \in \mathbb{N}$ such that $|x_{mn} - y_m| \leq \epsilon \quad \forall n \in \mathbb{N} \cap [N_\epsilon^{(m)}, \infty)$, and then take $\tilde{N}_\epsilon := \max\{N_\epsilon^{(1)}, \dots, N_\epsilon^{(M_{\epsilon/2} - 1)}, N_{\epsilon/2}\}$. It follows then that $|x_{mn} - y_m| \leq \epsilon \quad \forall m \in \mathbb{N}, n \in \mathbb{N} \cap [\tilde{N}_\epsilon, \infty)$. Hence $x_{mn} \xrightarrow{n \rightarrow \infty} y_m$ uniformly over $m \in \mathbb{N}$.

(iii) \Rightarrow (iv): Suppose (iii) holds true. Then for each $\epsilon > 0$ take some $N^{(\epsilon/3)} \in \mathbb{N}$ for which $|x_{mN^{(\epsilon/3)}} - y_m| \leq \frac{\epsilon}{3} \quad \forall m \in \mathbb{N}$ and also $|z_{N^{(\epsilon/3)}} - a| \leq \frac{\epsilon}{3}$. Take also some $M^{(\epsilon/3)} \in \mathbb{N}$ for which $|x_{mN^{(\epsilon/3)}} - z_{N^{(\epsilon/3)}}| \leq \frac{\epsilon}{3} \quad \forall m \in \mathbb{N} \cap [M^{(\epsilon/3)}, \infty)$. Then for each $m \in \mathbb{N} \cap [M^{(\epsilon/3)}, \infty), |y_m - a| \leq |y_m - x_{mN^{(\epsilon/3)}}| + |x_{mN^{(\epsilon/3)}} - z_{N^{(\epsilon/3)}}| + |z_{N^{(\epsilon/3)}} - a| \leq \epsilon$. Hence $\lim_{m \rightarrow \infty} \lim_{n \rightarrow \infty} x_{mn} = \lim_{m \rightarrow \infty} y_m = a$.

(iv) \Rightarrow (i): Suppose (iv) holds true. Then for each $\epsilon > 0$, take some $M_{(\epsilon/2)} \in \mathbb{N}$ for which $|y_m - a| \leq \frac{\epsilon}{2} \quad \forall m \in \mathbb{N} \cap [M_{(\epsilon/2)}, \infty)$, and some $N_{(\epsilon/2)} \in \mathbb{N}$ for which $|x_{mn} - y_m| \leq \frac{\epsilon}{2} \quad \forall m \in \mathbb{N}, n \in \mathbb{N} \cap [N_{(\epsilon/2)}, \infty)$. Then $|x_{mn} - a| \leq |x_{mn} - y_m| + |y_m - a| \leq \epsilon \quad \forall m \in \mathbb{N} \cap [M_{(\epsilon/2)}, \infty), n \in \mathbb{N} \cap [N_{(\epsilon/2)}, \infty)$. Hence $\lim_{m, n \rightarrow \infty} x_{mn} = a$.

(i) \Rightarrow (v) \Rightarrow (vi) \Rightarrow (i) can then be proved in exactly the same way as (i) \Rightarrow (iii) \Rightarrow (iv) \Rightarrow (i), only swapping round the roles of m and n (but still keeping x_{mn} as x_{mn} rather than replacing it with x_{nm}).

□

Lemma 4.4.9. *Again, given an $\mathbb{N} \times \mathbb{N}$ array $(x_{mn})_{m,n \in \mathbb{N}} \subset \mathbb{C}$ with*

$$x_{mn} \xrightarrow{n \rightarrow \infty} y_m \in \mathbb{C} \quad \forall m, \quad x_{mn} \xrightarrow{m \rightarrow \infty} z_n \in \mathbb{C} \quad \forall n, \quad (4.168)$$

suppose it furthermore holds that

(i) *Either $|x_{mn} - y_m|$ is non-increasing in n for each m or $|x_{mn} - z_n|$ is non-increasing in m for each n ,*

(ii) $\lim_{m \rightarrow \infty} \lim_{n \rightarrow \infty} x_{mn} = \lim_{n \rightarrow \infty} \lim_{m \rightarrow \infty} x_{mn} = a$.

Then $\lim_{m,n \rightarrow \infty} x_{mn} = a$.

Proof. Suppose $|x_{mn} - y_m|$ is non-increasing in n for each m and $\lim_{m \rightarrow \infty} \lim_{n \rightarrow \infty} x_{mn} = \lim_{n \rightarrow \infty} \lim_{m \rightarrow \infty} x_{mn} = a$. Then given any $\epsilon > 0$ take some $N^{(\epsilon/4)} \in \mathbb{N}$ for which $|z_{N^{(\epsilon/4)}} - a| \leq \frac{\epsilon}{4}$, and some $M^{(\epsilon/4)} \in \mathbb{N}$ for which $|x_{mN^{(\epsilon/4)}} - z_{N^{(\epsilon/4)}}| \leq \frac{\epsilon}{4} \quad \forall m \in \mathbb{N} \cap [M^{(\epsilon/4)}, \infty)$ and also $|y_m - a| \leq \frac{\epsilon}{4} \quad \forall m \in \mathbb{N} \cap [M^{(\epsilon/4)}, \infty)$. Then for each $m \in \mathbb{N} \cap [M^{(\epsilon/4)}, \infty), n \in \mathbb{N} \cap [N^{(\epsilon/4)}, \infty)$

$$\begin{aligned} |x_{mn} - a| &\leq |x_{mn} - y_m| + |y_m - a| \leq |x_{mN^{(\epsilon/4)}} - y_m| + |y_m - a| \\ &\leq |x_{mN^{(\epsilon/4)}} - z_{N^{(\epsilon/4)}}| + |z_{N^{(\epsilon/4)}} - a| + 2|y_m - a| \leq \epsilon. \end{aligned} \quad (4.169)$$

Hence $\lim_{m,n \rightarrow \infty} x_{mn} = a$. In order to prove this starting from $|x_{mn} - z_n|$ being non-increasing in m for each n (and again $\lim_{m \rightarrow \infty} \lim_{n \rightarrow \infty} x_{mn} = \lim_{n \rightarrow \infty} \lim_{m \rightarrow \infty} x_{mn} = a$), simply swap round the roles of m and n . □

Corollary 4.4.10. *Given $(x_{mn})_{m,n \in \mathbb{N}} \subset \mathbb{C}$ with (4.167), suppose it is known that $\lim_{m \rightarrow \infty} \lim_{n \rightarrow \infty} x_{mn}$ converges or that $\lim_{n \rightarrow \infty} \lim_{m \rightarrow \infty} x_{mn}$ converges. Then a sufficient condition for being able to swap round the order of the two limits without changing the resulting value is that either the convergence of x_{mn} as $n \rightarrow \infty$ is uniform over m or the convergence as $m \rightarrow \infty$ is uniform over n . In this case it would also result that this uniform convergence holds in both of these two directions.*

Now suppose it is known not only that $\lim_{m \rightarrow \infty} \lim_{n \rightarrow \infty} x_{mn}$ converges or that $\lim_{n \rightarrow \infty} \lim_{m \rightarrow \infty} x_{mn}$ converges, but it is also known that $|x_{mn} - y_m|$ is non-increasing in n for each m or that $|x_{mn} - z_n|$ is non-increasing in m for each n . Then this sufficient

condition for being able to swap round the order of these limits is also a necessary condition for this. In fact, for each of the two possible directions of uniform convergence, uniform convergence in that direction is both sufficient and necessary.

Proof. The first claim follows straightforwardly from the equivalence of (iii) - (vi) in Lemma 4.4.8. Then for the second claim, where we suppose it is known that

- (i) Either $|x_{mn} - y_m|$ is non-increasing in n for each m or $|x_{mn} - z_n|$ is non-increasing in m for each n ,
- (ii) $\lim_{m \rightarrow \infty} \lim_{n \rightarrow \infty} x_{mn}$ converges or $\lim_{n \rightarrow \infty} \lim_{m \rightarrow \infty} x_{mn}$ converges,

let a be the value of the limit in (ii) here which we know to be convergent. Anything that must result from (i) and (ii) in Lemma 4.4.9 would clearly be a necessary condition here for being able to swap the order of the limits. Thus by Lemma 4.4.9, $\lim_{m,n \rightarrow \infty} x_{mn} = a$ is a necessary condition here, and then by Lemma 4.4.8, uniform convergence of x_{mn} over m as $n \rightarrow \infty$ is a necessary condition. Likewise uniform convergence of x_{mn} over n as $m \rightarrow \infty$ is also a necessary condition. \square

Remark. Regarding the condition that either $|x_{mn} - y_m|$ is non-increasing in n for each m or $|x_{mn} - z_n|$ is non-increasing in m for each n , a simple example of this would be the case where $x_{mn} \in \mathbb{R}$ and either x_{mn} is non-increasing/non-decreasing in n for each m or x_{mn} is non-increasing/non-decreasing in m for each n .

So then, taking some $\mu, \mu' \in M_\Theta$ with $\mu < \mu'$, choose $N_0 \in \mathbb{N}$ so as to satisfy the specification for N_0 given earlier, for both μ and μ' . M_Θ again is defined in (4.151). Let $M_0 := \min\{j \in \mathbb{N} : \mathcal{E}_j > \mu'\}$. Then

- (i) $R_N^{(M)}(\mu) - R_N^{(M)}(\mu') \xrightarrow{M \rightarrow \infty} R_N(\mu) - R_N(\mu') \quad \forall N \in \mathbb{N} \cap [N_0, \infty)$,
- (ii) $R_N^{(M+1)}(\mu) - R_N^{(M+1)}(\mu') = R_N^{(M)}(\mu) - R_N^{(M)}(\mu') + \frac{|y_{M+1}^N|^2}{\mu - \mathcal{E}_{M+1}} - \frac{|y_{M+1}^N|^2}{\mu' - \mathcal{E}_{M+1}}$
 $\geq R_N^{(M)}(\mu) - R_N^{(M)}(\mu') \quad \forall M \in \mathbb{N} \cap [M_0, \infty), N \in \mathbb{N} \cap [N_0, \infty)$,
- (iii) $R_N^{(M)}(\mu) - R_N^{(M)}(\mu') \xrightarrow{N \rightarrow \infty} S^{(M)}(\mu) - S^{(M)}(\mu') \quad \forall M \in \mathbb{N}$,
- (iv) $\lim_{M \rightarrow \infty} \lim_{N \rightarrow \infty} (R_N^{(M)}(\mu) - R_N^{(M)}(\mu')) = 0$.

Hence by Corollary 4.4.10 (with $M = M_0$ and $N = N_0$ in place of $m = 1$ and $n = 1$), the following are equivalent:

- (a) $\lim_{N \rightarrow \infty} \lim_{M \rightarrow \infty} (R_N^{(M)}(\mu) - R_N^{(M)}(\mu')) = \lim_{N \rightarrow \infty} (R_N(\mu) - R_N(\mu')) = 0$ (swapping the order of limits in (iv) above),

- (b) the convergence in (i) above is uniform,
(c) the convergence in (iii) above is uniform.

Proposition 4.4.11. *The following are equivalent, provided M_Θ contains at least two elements:*

- (i) $\exists \mu, \mu' \in M_\Theta$ with $\mu \neq \mu'$ such that $R_N(\mu) - R_N(\mu') \xrightarrow{N \rightarrow \infty} 0$,
(ii) $R_N(\mu) - R_N(\mu') \xrightarrow{N \rightarrow \infty} 0 \forall \mu, \mu' \in M_\Theta$,
(iii) $\exists E \in \mathbb{R}$ s.t. $\sum_{j=M}^{\infty} \frac{|y_j^N|^2}{(E - \mathcal{E}_j)^2} \xrightarrow{M \rightarrow \infty} 0$ uniformly over $N \in \mathbb{N}$,
(iv) $\forall E \in \mathbb{R}$ $\sum_{j=M}^{\infty} \frac{|y_j^N|^2}{(E - \mathcal{E}_j)^2} \xrightarrow{M \rightarrow \infty} 0$ uniformly over $N \in \mathbb{N}$,
(v) $\exists E \in \mathbb{R}$ with $\mathcal{P}_{\{E\}}^{(H)} Y_N = 0 \forall$ suff. large $N \in \mathbb{N}$ s.t. $T_N(E) \xrightarrow{N \rightarrow \infty} T_\delta(E)$,
(vi) $T_N(E) \xrightarrow{N \rightarrow \infty} T_\delta(E) \forall E \in \mathbb{R}$ with $\mathcal{P}_{\{E\}}^{(H)} Y_N = 0 \forall$ suff. large $N \in \mathbb{N}$.

Proof. Proving first the equivalence of (i) - (iv), given any $\mu, \mu' \in M_\Theta$ with $\mu \neq \mu'$, supposing w.l.o.g. that $\mu < \mu'$, $R_N(\mu) - R_N(\mu') \xrightarrow{N \rightarrow \infty} 0$ if and only if

$$(R_N(\mu) - R_N(\mu')) - (R_N^{(M)}(\mu) - R_N^{(M)}(\mu')) \xrightarrow{M \rightarrow \infty} 0 \quad (4.170)$$

uniformly over $N \in \mathbb{N} \cap [N_0, \infty)$ (N_0 being defined as above, given our chosen μ, μ'). For each $M \in \mathbb{N} \cap [M_0, \infty)$, $N \in \mathbb{N} \cap [N_0, \infty)$,

$$\begin{aligned} (R_N(\mu) - R_N(\mu')) - (R_N^{(M)}(\mu) - R_N^{(M)}(\mu')) &= \sum_{j=M+1}^{\infty} \frac{|y_j^N|^2}{\mu - \mathcal{E}_j} - \sum_{j=M+1}^{\infty} \frac{|y_j^N|^2}{\mu' - \mathcal{E}_j} \\ &= \lim_{M' \rightarrow \infty} (\mu' - \mu) \sum_{j=M+1}^{M'} \frac{|y_j^N|^2}{(\sigma_N^{MM'} - \mathcal{E}_j)^2}, \end{aligned} \quad (4.171)$$

where $\sigma_N^{MM'} \in (\mu, \mu')$. Note also that

$$\sum_{j=M+1}^{M'} \frac{|y_j^N|^2}{(\mu - \mathcal{E}_j)^2} \leq \sum_{j=M+1}^{M'} \frac{|y_j^N|^2}{(\sigma_N^{MM'} - \mathcal{E}_j)^2} \leq \sum_{j=M+1}^{M'} \frac{|y_j^N|^2}{(\mu' - \mathcal{E}_j)^2} \quad (4.172)$$

$\forall M' \in \mathbb{N} \cap [M+1, \infty)$, so

$$\begin{aligned} (\mu' - \mu) \sum_{j=M+1}^{\infty} \frac{|y_j^N|^2}{(\mu - \mathcal{E}_j)^2} &\leq \sum_{j=M+1}^{\infty} \frac{|y_j^N|^2}{\mu - \mathcal{E}_j} - \sum_{j=M+1}^{\infty} \frac{|y_j^N|^2}{\mu' - \mathcal{E}_j} \\ &\leq (\mu' - \mu) \sum_{j=M+1}^{\infty} \frac{|y_j^N|^2}{(\mu' - \mathcal{E}_j)^2}. \end{aligned} \quad (4.173)$$

Thus if $(\mu' - \mu) \sum_{j=M+1}^{\infty} \frac{|y_j^N|^2}{(\mu' - \mathcal{E}_j)^2} \xrightarrow{M \rightarrow \infty} 0$ uniformly over $N \in \mathbb{N} \cap [N_0, \infty)$ then so does $\sum_{j=M+1}^{\infty} \frac{|y_j^N|^2}{\mu - \mathcal{E}_j} - \sum_{j=M+1}^{\infty} \frac{|y_j^N|^2}{\mu' - \mathcal{E}_j}$, and if $\sum_{j=M+1}^{\infty} \frac{|y_j^N|^2}{\mu - \mathcal{E}_j} - \sum_{j=M+1}^{\infty} \frac{|y_j^N|^2}{\mu' - \mathcal{E}_j} \xrightarrow{M \rightarrow \infty} 0$ uniformly over $N \in \mathbb{N} \cap [N_0, \infty)$ then so does $(\mu' - \mu) \sum_{j=M+1}^{\infty} \frac{|y_j^N|^2}{(\mu - \mathcal{E}_j)^2}$.

Note that the statement “ $(\mu' - \mu) \sum_{j=M+1}^{\infty} \frac{|y_j^N|^2}{(\mu - \mathcal{E}_j)^2} \xrightarrow{M \rightarrow \infty} 0$ uniformly over $N \in \mathbb{N} \cap [N_0, \infty)$ ” is equivalent to the simpler statement “ $\sum_{j=M}^{\infty} \frac{|y_j^N|^2}{(\mu - \mathcal{E}_j)^2} \xrightarrow{M \rightarrow \infty} 0$ uniformly over $N \in \mathbb{N}$ ”, and likewise with μ' in place of μ in “ $\frac{|y_j^N|^2}{(\mu - \mathcal{E}_j)^2}$ ”. Recall also that $\sum_{j=M+1}^{\infty} \frac{|y_j^N|^2}{\mu - \mathcal{E}_j} - \sum_{j=M+1}^{\infty} \frac{|y_j^N|^2}{\mu' - \mathcal{E}_j} \xrightarrow{M \rightarrow \infty} 0$ uniformly over $N \in \mathbb{N} \cap [N_0, \infty)$ if and only if $R_N(\mu) - R_N(\mu') \xrightarrow{N \rightarrow \infty} 0$.

Now given any $E \in \mathbb{R}$, suppose $\sum_{j=M}^{\infty} \frac{|y_j^N|^2}{(E - \mathcal{E}_j)^2} \xrightarrow{M \rightarrow \infty} 0$ uniformly over $N \in \mathbb{N}$. Then given any $E' \in \mathbb{R}$, $\frac{(E - \mathcal{E}_j)^2}{(E' - \mathcal{E}_j)^2} = \left(1 + \frac{E - E'}{E' - \mathcal{E}_j}\right)^2 \xrightarrow{j \rightarrow \infty} 1$, so taking some $C > 1$ and $M_C \in \mathbb{N}$ for which $\mathcal{E}_{M_C} > \max\{E, E'\}$ and $\frac{(E - \mathcal{E}_j)^2}{(E' - \mathcal{E}_j)^2} \leq C \forall j \in \mathbb{N} \cap [M_C, \infty)$, it holds that

$$\sum_{j=M}^{\infty} \frac{|y_j^N|^2}{(E' - \mathcal{E}_j)^2} = \sum_{j=M}^{\infty} \frac{|y_j^N|^2}{(E - \mathcal{E}_j)^2} \frac{(E - \mathcal{E}_j)^2}{(E' - \mathcal{E}_j)^2} \leq C \sum_{j=M}^{\infty} \frac{|y_j^N|^2}{(E - \mathcal{E}_j)^2} \quad (4.174)$$

$\forall M \in \mathbb{N} \cap [M_C, \infty), N \in \mathbb{N}$. Thus $\sum_{j=M}^{\infty} \frac{|y_j^N|^2}{(E' - \mathcal{E}_j)^2} \xrightarrow{M \rightarrow \infty} 0$ uniformly over $N \in \mathbb{N}$ also. This proves the equivalence of (iii) and (iv).

So now going back to our $\mu, \mu' \in M_{\Theta}$, it holds that $R_N(\mu) - R_N(\mu') \xrightarrow{N \rightarrow \infty} 0$ if and only if (iii), or equivalently (iv), holds. This likewise holds for any other choice of $\mu, \mu' \in M_{\Theta}$ with $\mu \neq \mu'$. Hence (i) - (iv) are all equivalent, assuming M_{Θ} contains at least two elements (note though that the proof that (iii) and (iv) are equivalent clearly does not have any requirement on M_{Θ}).

Now moving on to prove the equivalence of (iii) - (vi), take some $E \in \mathbb{R}$ for which, for some $N_0^{(E)} \in \mathbb{N}$ we have $\mathcal{P}_{\{E\}}^{(H)} Y_N = 0 \forall N \in \mathbb{N} \cap [N_0^{(E)}, \infty)$, and so $\mathcal{P}_{\{E\}}^{(H)} \delta_p = 0$ also (note of course that if $E \notin \text{Spec}(H)$ then trivially $\mathcal{P}_{\{E\}}^{(H)} Y_N = 0 \forall N \in \mathbb{N}$ and $\mathcal{P}_{\{E\}}^{(H)} \delta_p = 0$). Then

- (a) $T_N^{(M)}(E) \xrightarrow{M \rightarrow \infty} T_N(E) \forall N \in \mathbb{N} \cap [N_0^{(E)}, \infty)$,
- (b) $T_N^{(M)}(E)$ is non-decreasing in M for each $N \in \mathbb{N} \cap [N_0^{(E)}, \infty)$,
- (c) $T_N^{(M)}(E) \xrightarrow{N \rightarrow \infty} T_{\delta}^{(M)}(E) \forall M \in \mathbb{N}$,
- (d) $\lim_{M \rightarrow \infty} \lim_{N \rightarrow \infty} T_N^{(M)}(E) = \lim_{M \rightarrow \infty} T_{\delta}^{(M)}(E) = T_{\delta}(E)$.

So then by Corollary 4.4.10, $\lim_{N \rightarrow \infty} \lim_{M \rightarrow \infty} T_N^{(M)}(E) = \lim_{N \rightarrow \infty} T_N(E) = T_{\delta}(E)$ if and

only if $T_N^{(M)}(E) \xrightarrow{M \rightarrow \infty} T_N(E)$ uniformly over $N \in \mathbb{N} \cap [N_0^{(E)}, \infty)$, equivalently

$$T_N(E) - T_N^{(M)}(E) = \sum_{j=M+1}^{\infty} \frac{|y_j^N|^2}{(E - \mathcal{E}_j)^2} \xrightarrow{M \rightarrow \infty} 0 \quad (4.175)$$

uniformly over $N \in \mathbb{N} \cap [N_0^{(E)}, \infty)$, or more simply $\sum_{j=M}^{\infty} \frac{|y_j^N|^2}{(E - \mathcal{E}_j)^2} \xrightarrow{M \rightarrow \infty} 0$ uniformly over $N \in \mathbb{N}$. This is then equivalent to (iii)/(iv). Since this likewise holds for any other choice of $E \in \mathbb{R}$ with $\mathcal{P}_{\{E\}}^{(H)} Y_N = 0 \forall$ suff. large $N \in \mathbb{N}$, it follows that (iii) - (vi) are all equivalent. \square

Remark. The equivalence of (iii) - (vi) in Prop. 4.4.11 does not require M_Θ to contain at least two elements.

Proposition 4.4.12. *Suppose $(Y_N)_{N=1}^\infty \subset C_0^\infty(\mathcal{M}^\circ) \setminus \{0\}$ satisfies*

$$(i) \quad y_j^N \xrightarrow{N \rightarrow \infty} \overline{\Psi_j(p)} \quad \forall j \in \mathbb{N},$$

$$(ii) \quad \sum_{j=M}^{\infty} \frac{|y_j^N|^2}{\mathcal{E}_j^2} \xrightarrow{M \rightarrow \infty} 0 \quad \text{uniformly over } N \in \mathbb{N}.$$

Then fixing $\Theta \in (0, 2\pi)$, if $M_\Theta \neq \emptyset$ and $(\nu_N)_{N=1}^\infty \subset \mathbb{R} \setminus \{0\}$ is chosen in such a way that $\exists \mu \in M_\Theta$ s.t.

$$\frac{1}{\nu_N} - R_N(\mu) \xrightarrow{N \rightarrow \infty} 0, \quad (4.176)$$

then (4.176) holds $\forall \mu \in M_\Theta$ and $\mu^N \xrightarrow{N \rightarrow \infty} \mu \forall \mu \in M_\Theta$. If on the other hand, $\nexists \mu \in M_\Theta$ s.t. (4.176) holds, then $\nexists \mu \in M_\Theta$ s.t. $\mu^N \xrightarrow{N \rightarrow \infty} \mu$.

Proof. Clearly requirement (ii) for $(Y_N)_{N=1}^\infty$ here implies statement (iii) in Proposition 4.4.11, thus giving statement (ii) in Prop. 4.4.11 (note that (ii) in Prop. 4.4.11 is automatic if $\#M_\Theta \leq 1$). Hence if $\exists \mu \in M_\Theta$ s.t. (4.176) holds then (4.176) holds $\forall \mu \in M_\Theta$, and thus by Proposition 4.4.6, $\mu^N \xrightarrow{N \rightarrow \infty} \mu \forall \mu \in M_\Theta$.

Next, suppose $(Y_N)_{N=1}^\infty$ satisfies (i) and (ii) here, and suppose $\exists \mu \in M_\Theta$ s.t. $\mu^N \xrightarrow{N \rightarrow \infty} \mu$. Then $\exists (\epsilon_N)_{N=N_0}^\infty \subset (0, \infty)$ with $\epsilon_N \xrightarrow{N \rightarrow \infty} 0$ s.t. $\mu^N \in [\mu - \epsilon_N, \mu + \epsilon_N] \forall N \in \mathbb{N} \cap [N_0, \infty)$, and so for sufficiently large N ,

$$R_N(\mu - \epsilon_N) \geq R_N(\mu^N) = \frac{1}{\nu_N} \geq R_N(\mu + \epsilon_N). \quad (4.177)$$

Now take some $\epsilon > 0$ for which $[\mu - \epsilon, \mu + \epsilon] \cap \text{Spec}(H) \setminus \{\mu\} = \emptyset$, take some $C > T_\delta(\mu - \epsilon) + T_\delta(\mu + \epsilon)$, and then given (iii) \Rightarrow (vi) in Prop. 4.4.11, take some $N'_0 \in \mathbb{N} \cap [N_0, \infty)$ for which $\epsilon_N \leq \epsilon \forall N \in \mathbb{N} \cap [N'_0, \infty)$ and $T_N(\mu - \epsilon) + T_N(\mu + \epsilon) \leq C \forall N \in \mathbb{N} \cap [N'_0, \infty)$. Then applying (4.94),

$$\begin{aligned} R_N(\mu - \epsilon_N) - R_N(\mu + \epsilon_N) &\leq 2\epsilon_N(T_N(\mu - \epsilon) + T_N(\mu + \epsilon)) \\ &\leq 2C\epsilon_N \quad \forall N \in \mathbb{N} \cap [N'_0, \infty). \end{aligned} \quad (4.178)$$

Hence

$$\left| \frac{1}{\nu_N} - R_N(\mu) \right| \leq R_N(\mu - \epsilon_N) - R_N(\mu + \epsilon_N) \xrightarrow{N \rightarrow \infty} 0. \quad (4.179)$$

From this it is concluded that if $\# \mu \in M_\Theta$ s.t. (4.176) holds then $\# \mu \in M_\Theta$ s.t. $\mu^N \xrightarrow{N \rightarrow \infty} \mu$. \square

Observe that in light of Lemma 4.4.5, if the sequence (ν_N) satisfies (4.176) then $\nu_N < 0$ for all suff. large N and $\nu_N \rightarrow 0$. This matches earlier observations on ν_N in (4.11), (4.48) and (4.52), when reviewing [Zor80], [AK00] and [GN12] respectively. Again, the setting in (4.11) and (4.48) is \mathbb{R}^3 , and the setting in (4.48) is \mathbb{R}^2 . The setting here however is the two-dimensional compact manifold \mathcal{M} . This observation also further supports the suggestion in §2.2.4 that the delta potential intuitively speaking has negative infinitesimal strength.

Lemma 4.4.13.

$$|x + y|^2 \leq 2(|x|^2 + |y|^2) \quad \forall x, y \in \mathbb{C}. \quad (4.180)$$

Proof.

$$\begin{aligned} |x + y|^2 &\leq (|x| + |y|)^2 \leq (|x| + |y|)^2 + (|x| - |y|)^2 \\ &= |x|^2 + 2|x||y| + |y|^2 + |x|^2 - 2|x||y| + |y|^2 = 2(|x|^2 + |y|^2). \end{aligned} \quad (4.181)$$

\square

Lemma 4.4.14. $\exists (Y_N)_{N=1}^\infty \subset C_0^\infty(\mathcal{M}^\circ) \setminus \{0\}$ such that both (i) and (ii) in Proposition 4.4.12 hold.

Proof. Proving firstly that $\exists (\tilde{Y}_N)_{N=1}^\infty \subset L^2(\mathcal{M})$ such that both (i) and (ii) hold, take the example $\tilde{Y}_N = \sum_{j=1}^N \overline{\Psi_j(p)} \Psi_j$, just like in the proof of Lemma 4.4.1. This clearly satisfies (i). To show that it also satisfies (ii), note that clearly $|\tilde{y}_j^N|^2 \leq |\Psi_j(p)|^2 \forall j, N \in \mathbb{N}$, and so for every $N \in \mathbb{N}$,

$$\sum_{j=M}^\infty \frac{|\tilde{y}_j^N|^2}{\mathcal{E}_j^2} \leq \sum_{j=M}^\infty \frac{|\Psi_j(p)|^2}{\mathcal{E}_j^2} \xrightarrow{M \rightarrow \infty} 0, \quad (4.182)$$

since $\sum_{j=M}^\infty \frac{|\Psi_j(p)|^2}{\mathcal{E}_j^2}$ is a convergent sum for any $M \in \mathbb{N}$ with $\mathcal{E}_M > 0$. This proves that (ii) is also satisfied.

Now given any $(\tilde{Y}_N)_{N=1}^\infty \subset L^2(\mathcal{M})$ for which both (i) and (ii) hold, we can then take some $(Y_N)_{N=1}^\infty \subset C_0^\infty(\mathcal{M}^\circ) \setminus \{0\}$ for which $\|Y_N - \tilde{Y}_N\| \xrightarrow{N \rightarrow \infty} 0$, in which case $(Y_N)_{N=1}^\infty$

also satisfies (i), as demonstrated in the proof of Lemma 4.4.1. It remains then to show that $(Y_N)_{N=1}^\infty$ also satisfies (ii).

Let $Y'_N := Y_N - \tilde{Y}_N$. Then $y_j^N = \tilde{y}_j^N + y'^N_j$ for each $j, N \in \mathbb{N}$, and so by Lemma 4.4.13, $|y_j^N|^2 \leq 2|\tilde{y}_j^N|^2 + 2|y'^N_j|^2$. Thus

$$\sum_{j=M}^{\infty} \frac{|y_j^N|^2}{\mathcal{E}_j^2} \leq 2 \sum_{j=M}^{\infty} \frac{|\tilde{y}_j^N|^2}{\mathcal{E}_j^2} + 2 \sum_{j=M}^{\infty} \frac{|y'^N_j|^2}{\mathcal{E}_j^2} \quad (4.183)$$

for each $N \in \mathbb{N}$ and $M \in \mathbb{N}$ with $\mathcal{E}_M > 0$. For each $\epsilon > 0$ we can take some $\tilde{M}_{\epsilon/4} \in \mathbb{N}$ for which

$$\sum_{j=\tilde{M}_{\epsilon/4}}^{\infty} \frac{|\tilde{y}_j^N|^2}{\mathcal{E}_j^2} \leq \frac{\epsilon}{4} \quad \forall N \in \mathbb{N}. \quad (4.184)$$

We can also take some $N'_{\epsilon/4} \in \mathbb{N}$ for which $\|Y'_N\|^2 \leq \frac{\epsilon}{4} \quad \forall N \in \mathbb{N} \cap [N'_{\epsilon/4}, \infty)$. It then follows that for each $N \in \mathbb{N} \cap [N'_{\epsilon/4}, \infty)$ and $M \in \mathbb{N}$ with $\mathcal{E}_M \geq 1$,

$$\sum_{j=M}^{\infty} \frac{|y'^N_j|^2}{\mathcal{E}_j^2} \leq \sum_{j=M}^{\infty} |y'^N_j|^2 \leq \|Y'_N\|^2 \leq \frac{\epsilon}{4}. \quad (4.185)$$

If $N'_{\epsilon/4} \geq 2$ then for each $N \in \{1, \dots, N'_{\epsilon/4} - 1\}$ we can take some $M'^{(N)}_{\epsilon/4} \in \mathbb{N}$ for which $\sum_{j=M'^{(N)}_{\epsilon/4}}^{\infty} \frac{|y'^N_j|^2}{\mathcal{E}_j^2} \leq \frac{\epsilon}{4}$. Then taking some $M'_{\epsilon/4} \in \mathbb{N}$ with $M'_{\epsilon/4} \geq \max_{N \in \{1, \dots, N'_{\epsilon/4} - 1\}} M'^{(N)}_{\epsilon/4}$ if $N'_{\epsilon/4} \geq 2$ and $\mathcal{E}_{M'_{\epsilon/4}} \geq 1$, it follows that

$$\sum_{j=M'_{\epsilon/4}}^{\infty} \frac{|y'^N_j|^2}{\mathcal{E}_j^2} \leq \frac{\epsilon}{4} \quad \forall N \in \mathbb{N}. \quad (4.186)$$

Finally, letting $M_\epsilon := \max\{\tilde{M}_{\epsilon/4}, M'_{\epsilon/4}\}$, it follows from (4.183), (4.184) and (4.186) that

$$\sum_{j=M_\epsilon}^{\infty} \frac{|y_j^N|^2}{\mathcal{E}_j^2} \leq \epsilon \quad \forall N \in \mathbb{N}. \quad (4.187)$$

Hence (ii) is satisfied by $(Y_N)_{N=1}^\infty$. \square

Now we may wish to bring into this discussion consideration of the following condition on $(Y_N)_{N=1}^\infty$:

$$\langle \phi, Y_N \rangle \xrightarrow{N \rightarrow \infty} \phi(p) \quad \forall \phi \in \text{Dom}(H). \quad (4.188)$$

Note that this is clearly stronger than the condition $y_j^N \xrightarrow{N \rightarrow \infty} \overline{\Psi_j(p)} \quad \forall j \in \mathbb{N}$, since $y_j^N = \overline{\langle \Psi_j, Y_N \rangle}$.

Lemma 4.4.15. *If $(Y_N)_{N=1}^\infty \subset C_0^\infty(\mathcal{M}^\circ) \setminus \{0\}$ satisfies both (i) and (ii) in Proposition 4.4.12 then (4.188) is also satisfied.*

Proof. Let $\phi = \sum_{j=1}^{\infty} a_j \Psi_j \in \text{Dom}(H)$. Then

$$\langle \phi, Y_N \rangle = \lim_{M \rightarrow \infty} \sum_{j=1}^M a_j \overline{y_j^N}, \quad (4.189)$$

and by Corollary 2.2.2,

$$\phi(p) = \lim_{M \rightarrow \infty} \sum_{j=1}^M a_j \Psi_j(p) = \lim_{M \rightarrow \infty} \lim_{N \rightarrow \infty} \sum_{j=1}^M a_j \overline{y_j^N}. \quad (4.190)$$

Thus we wish to obtain

$$\lim_{N \rightarrow \infty} \lim_{M \rightarrow \infty} \sum_{j=1}^M a_j \overline{y_j^N} = \lim_{M \rightarrow \infty} \lim_{N \rightarrow \infty} \sum_{j=1}^M a_j \overline{y_j^N}, \quad (4.191)$$

which by Corollary 4.4.10, will hold if

$$\sum_{j=M}^{\infty} a_j \overline{y_j^N} \xrightarrow[\text{unif.}]{M \rightarrow \infty} 0. \quad (4.192)$$

Now observe that by the Cauchy-Schwartz inequality, together with Lemma 2.1.1,

$$\left| \sum_{j=M}^{\infty} a_j \overline{y_j^N} \right| = \left| \sum_{j=M}^{\infty} (\mathcal{E}_j a_j) \left(\frac{\overline{y_j^N}}{\mathcal{E}_j} \right) \right| \leq \sqrt{\left(\sum_{j=M}^{\infty} \mathcal{E}_j^2 |a_j|^2 \right) \left(\sum_{k=M}^{\infty} \frac{|y_k^N|^2}{\mathcal{E}_k^2} \right)} < \infty. \quad (4.193)$$

With $\sum_{k=M}^{\infty} \frac{|y_k^N|^2}{\mathcal{E}_k^2} \xrightarrow{M \rightarrow \infty} 0$ uniformly over N , it follows that RHS(4.193) $\xrightarrow{M \rightarrow \infty} 0$ uniformly over N , and hence (4.192) holds. \square

4.4.3 Approximation of New Eigenfunctions

Throughout §4.4.3 it shall be assumed that $(Y_N)_{N=1}^{\infty} \subset C_0^{\infty}(\mathcal{M}^{\circ}) \setminus \{0\}$ satisfies conditions (i) and (ii) in Proposition 4.4.12, $M_{\Theta} \neq \emptyset$ and $\exists \mu \in M_{\Theta}$ for which (4.176) holds, in which case (4.176) holds $\forall \mu \in M_{\Theta}$ and $\mu^N \xrightarrow{N \rightarrow \infty} \mu \forall \mu \in M_{\Theta}$.

For each $\mu \in M_{\Theta}$, with μ being an eigenvalue of H_{Θ} , it has an associated eigenfunction

$$\psi_{\mu}^{\delta} := \sum_{j: \mathcal{E}_j \neq \mu} \frac{\overline{\Psi_j(p)}}{\mu - \mathcal{E}_j} \Psi_j. \quad (4.194)$$

Likewise μ^N is an eigenvalue of H^N for each $N \in \mathbb{N} \cap [N_0, \infty)$, with corresponding eigenfunction

$$\psi_{\mu^N}^N := \sum_{j: \mathcal{E}_j \neq \mu^N} \frac{y_j^N}{\mu^N - \mathcal{E}_j} \Psi_j. \quad (4.195)$$

Let $\widehat{\psi}_\mu^\delta$ and $\widehat{\psi}_{\mu^N}^N$ be the respective normalisations of these eigenfunctions.

Note that since $\mu^N \xrightarrow{N \rightarrow \infty} \mu$, we can take some $N'_0 \in \mathbb{N} \cap [N_0, \infty)$ for which $\forall N \in \mathbb{N} \cap [N'_0, \infty)$ we have $[\mu^N, \mu] \cap \text{Spec}(H) = \emptyset$ if $\mu^N < \mu$, $(\mu, \mu^N] \cap \text{Spec}(H) = \emptyset$ if $\mu^N > \mu$. Note also then that for $N \in \mathbb{N} \cap [N'_0, \infty)$, we can replace the appearance of “ $\sum_{j: \mathcal{E}_j \neq \mu^N}$ ” in (4.195) with “ $\sum_{j: \mathcal{E}_j \neq \mu}$ ”, since every $\mathcal{E}_j \neq \mu$ is also not equal to μ^N , and for any j with $\mathcal{E}_j = \mu$ we have $y_j^N = 0$.

Proposition 4.4.16. *For each $\mu \in M_\Theta$,*

$$\|\psi_{\mu^N}^N - \psi_\mu^\delta\| \xrightarrow{N \rightarrow \infty} 0. \quad (4.196)$$

Proof. Let

$$U_{MN} := \sum_{j \in \{1, \dots, M\}: \mathcal{E}_j \neq \mu} \left| \frac{y_j^N}{\mu^N - \mathcal{E}_j} - \frac{\overline{\Psi_j(p)}}{\mu - \mathcal{E}_j} \right|^2 \quad \forall M \in \mathbb{N}, N \in \mathbb{N} \cap [N'_0, \infty). \quad (4.197)$$

Then

- (i) $U_{MN} \xrightarrow{M \rightarrow \infty} \|\psi_{\mu^N}^N - \psi_\mu^\delta\|^2 \forall N \in \mathbb{N} \cap [N'_0, \infty)$,
- (ii) U_{MN} is non-decreasing in M for each $N \in \mathbb{N} \cap [N'_0, \infty)$,
- (iii) $U_{MN} \xrightarrow{N \rightarrow \infty} 0 \forall M \in \mathbb{N}$,
- (iv) so then $\lim_{M \rightarrow \infty} \lim_{N \rightarrow \infty} U_{MN} = 0$.

Hence by Corollary 4.4.10, $\|\psi_{\mu^N}^N - \psi_\mu^\delta\|^2 \xrightarrow{N \rightarrow \infty} 0$ if and only if $U_{MN} \xrightarrow{M \rightarrow \infty} \|\psi_{\mu^N}^N - \psi_\mu^\delta\|^2$ uniformly over $N \in \mathbb{N} \cap [N'_0, \infty)$, equivalently

$$\sum_{j=M}^{\infty} \left| \frac{y_j^N}{\mu^N - \mathcal{E}_j} - \frac{\overline{\Psi_j(p)}}{\mu - \mathcal{E}_j} \right|^2 \xrightarrow{M \rightarrow \infty} 0 \quad (4.198)$$

uniformly over $N \in \mathbb{N} \cap [N'_0, \infty)$.

Now take some $\epsilon > 0$ for which $[\mu - \epsilon, \mu + \epsilon] \cap \text{Spec}(H) \setminus \{\mu\} = \emptyset$, and some $N_\epsilon \in \mathbb{N} \cap [N'_0, \infty)$ for which $|\mu^N - \mu| \leq \epsilon \forall N \in \mathbb{N} \cap [N_\epsilon, \infty)$. Then for each $N \in \mathbb{N} \cap [N_\epsilon, \infty)$ and $j \in \mathbb{N}$ with $\mathcal{E}_j > \mu$ we have by Lemma 4.4.13,

$$\begin{aligned} \left| \frac{y_j^N}{\mu^N - \mathcal{E}_j} - \frac{\overline{\Psi_j(p)}}{\mu - \mathcal{E}_j} \right|^2 &\leq 2 \left| \frac{y_j^N}{\mu - \mathcal{E}_j} - \frac{\overline{\Psi_j(p)}}{\mu - \mathcal{E}_j} \right|^2 + 2 \left| \frac{y_j^N}{\mu^N - \mathcal{E}_j} - \frac{y_j^N}{\mu - \mathcal{E}_j} \right|^2 \\ &\leq 4 \frac{|y_j^N|^2}{(\mu - \mathcal{E}_j)^2} + 4 \frac{|\overline{\Psi_j(p)}|^2}{(\mu - \mathcal{E}_j)^2} + 2|y_j^N|^2 \left| \frac{1}{\mu^N - \mathcal{E}_j} - \frac{1}{\mu - \mathcal{E}_j} \right|^2. \end{aligned} \quad (4.199)$$

Furthermore by the mean value theorem,

$$\left| \frac{1}{\mu^N - \mathcal{E}_j} - \frac{1}{\mu - \mathcal{E}_j} \right|^2 = \left| -\frac{\mu^N - \mu}{(\sigma_j^N - \mathcal{E}_j)^2} \right|^2 = \frac{|\mu^N - \mu|^2}{(\sigma_j^N - \mathcal{E}_j)^4} \leq \frac{\epsilon^2}{(\mu + \epsilon - \mathcal{E}_j)^4}. \quad (4.200)$$

Hence for each $N \in \mathbb{N} \cap [N_\epsilon, \infty)$ and $M \in \mathbb{N}$ with $\mathcal{E}_M > \mu$,

$$\begin{aligned} \sum_{j=M}^{\infty} \left| \frac{y_j^N}{\mu^N - \mathcal{E}_j} - \frac{\overline{\Psi_j(p)}}{\mu - \mathcal{E}_j} \right|^2 &\leq 4 \sum_{j=M}^{\infty} \frac{|y_j^N|^2}{(\mu - \mathcal{E}_j)^2} + 4 \sum_{j=M}^{\infty} \frac{|\Psi_j(p)|^2}{(\mu - \mathcal{E}_j)^2} \\ &\quad + 2\epsilon^2 \sum_{j=M}^{\infty} \frac{|y_j^N|^2}{(\mu + \epsilon - \mathcal{E}_j)^4}. \end{aligned} \quad (4.201)$$

In RHS(4.201), the first term converges to zero as $M \rightarrow \infty$ uniformly over $N \in \mathbb{N} \cap [N_\epsilon, \infty)$, by (iii) \Rightarrow (iv) in Proposition 4.4.11. The second term is independent of N , and so being a convergent sum for each M , it follows trivially that it converges to zero as $M \rightarrow \infty$ uniformly over $N \in \mathbb{N} \cap [N_\epsilon, \infty)$. The third term also converges to zero as $M \rightarrow \infty$ uniformly over $N \in \mathbb{N} \cap [N_\epsilon, \infty)$, because $\sum_{j=M}^{\infty} \frac{|y_j^N|^2}{(\mu + \epsilon - \mathcal{E}_j)^4} \leq \sum_{j=M}^{\infty} \frac{|y_j^N|^2}{(\mu + \epsilon - \mathcal{E}_j)^2}$ when $\mathcal{E}_M \geq \mu + \epsilon + 1$, and $\sum_{j=M}^{\infty} \frac{|y_j^N|^2}{(\mu + \epsilon - \mathcal{E}_j)^2} \xrightarrow{M \rightarrow \infty} 0$ uniformly over N by (iii) \Rightarrow (iv) in Proposition 4.4.11.

Hence LHS(4.201) converges to zero as $M \rightarrow \infty$ uniformly over $N \in \mathbb{N} \cap [N_\epsilon, \infty)$, from which it follows immediately that LHS(4.201) converges to zero as $M \rightarrow \infty$ uniformly also over $N \in \mathbb{N} \cap [N'_0, \infty)$. Thus $\|\psi_{\mu^N}^N - \psi_{\mu}^\delta\| \xrightarrow{N \rightarrow \infty} 0$. \square

Lemma 4.4.17. For each $\mu \in M_\Theta$,

$$T_N(\mu^N) \xrightarrow{N \rightarrow \infty} T_\delta(\mu). \quad (4.202)$$

Proof. Firstly, $T_N(\mu) - T_\delta(\mu) \xrightarrow{N \rightarrow \infty} 0$ by (iii) \Rightarrow (vi) in Proposition 4.4.11. We then wish to show that $T_N(\mu^N) - T_N(\mu) \xrightarrow{N \rightarrow \infty} 0$.

By the mean value theorem,

$$\begin{aligned} |T_N(\mu^N) - T_N(\mu)| &= \left| \lim_{M \rightarrow \infty} \left(\sum_{j \in \{1, \dots, M\}: \mathcal{E}_j \neq \mu} \frac{|y_j^N|^2}{(\mu^N - \mathcal{E}_j)^2} - \sum_{j \in \{1, \dots, M\}: \mathcal{E}_j \neq \mu} \frac{|y_j^N|^2}{(\mu - \mathcal{E}_j)^2} \right) \right| \\ &= \left| -2(\mu^N - \mu) \lim_{M \rightarrow \infty} \sum_{j \in \{1, \dots, M\}: \mathcal{E}_j \neq \mu} \frac{|y_j^N|^2}{(\sigma_N^{(M)} - \mathcal{E}_j)^3} \right| \\ &= 2|\mu^N - \mu| \lim_{M \rightarrow \infty} \left| \sum_{j \in \{1, \dots, M\}: \mathcal{E}_j \neq \mu} \frac{|y_j^N|^2}{(\sigma_N^{(M)} - \mathcal{E}_j)^3} \right| \\ &\quad \forall N \in \mathbb{N} \cap [N'_0, \infty). \end{aligned} \quad (4.203)$$

Let

$$W_N(E) := \sum_{j:y_j^N \neq 0} \frac{|y_j^N|^2}{(E - \mathcal{E}_j)^3}, \quad W_N^{(M)}(E) := \sum_{j \in \{1, \dots, M\}: y_j^N \neq 0} \frac{|y_j^N|^2}{(E - \mathcal{E}_j)^3}. \quad (4.204)$$

Like R_N and T_N , $W_N(E)$ is a convergent sum for each $E \in \mathbb{R} \setminus \{\mathcal{E} \in \text{Spec}(H) : \mathcal{P}_{\{\mathcal{E}\}}^{(H)} Y_N \neq 0\}$.

Given any compact interval I with $I \cap \{\mathcal{E} \in \text{Spec}(H) : \mathcal{P}_{\{\mathcal{E}\}}^{(H)} Y_N \neq 0\} = \emptyset$, with M being sufficiently large that $\{j \in \{1, \dots, M\} : y_j^N \neq 0\} \neq \emptyset$, $W_N^{(M)}$ is a smooth, strictly decreasing function on I . Thus $|W_N^{(M)}|$ is either everywhere decreasing on I , everywhere increasing on I or decreasing to the left of some $c \in I^\circ$ and increasing to the right of c . In all three of these cases, the maximum of $|W_N^{(M)}|$ on I is clearly at an end-point of I .

More precisely, letting a be the left end-point and b be the right end-point, $|W_N^{(M)}|$ has a maximum on I only at a if $W_N^{(M)}(a) + W_N^{(M)}(b) > 0$, at both a and b if $W_N^{(M)}(a) + W_N^{(M)}(b) = 0$, and only at b if $W_N^{(M)}(a) + W_N^{(M)}(b) < 0$. To see this, remembering that $W_N^{(M)}(a) > W_N^{(M)}(b)$, if $W_N^{(M)}(a) + W_N^{(M)}(b) > 0$ then $W_N^{(M)}(a) > -W_N^{(M)}(b)$ as well as $W_N^{(M)}(a) > W_N^{(M)}(b)$, so $|W_N^{(M)}(a)| > |W_N^{(M)}(b)|$. If $W_N^{(M)}(a) + W_N^{(M)}(b) = 0$ then $W_N^{(M)}(a) = -W_N^{(M)}(b)$, so $|W_N^{(M)}(a)| = |W_N^{(M)}(b)|$. If $W_N^{(M)}(a) + W_N^{(M)}(b) < 0$ then $W_N^{(M)}(b) < -W_N^{(M)}(a)$ as well as $W_N^{(M)}(b) < W_N^{(M)}(a)$, so $|W_N^{(M)}(b)| > |W_N^{(M)}(a)|$.

As M increases, when $\mathcal{E}_M > b$, $W_N^{(M)}(a) + W_N^{(M)}(b)$ is non-increasing, and converges to $W_N(a) + W_N(b)$. Thus if $W_N(a) + W_N(b) \geq 0$ then $|W_N^{(M)}|$ has a maximum on I at a for all sufficiently large M , and if $W_N(a) + W_N(b) < 0$ then $|W_N^{(M)}|$ has a maximum on I at b for all sufficiently large M .

Now as before, take some $\epsilon > 0$ for which $[\mu - \epsilon, \mu + \epsilon] \cap \text{Spec}(H) \setminus \{\mu\} = \emptyset$, and some $N_\epsilon \in \mathbb{N} \cap [N'_0, \infty)$ for which $|\mu^N - \mu| \leq \epsilon \forall N \in \mathbb{N} \cap [N_\epsilon, \infty)$. Then for each $N \in \mathbb{N} \cap [N_\epsilon, \infty)$, taking $\eta_N = 1$ if $W_N(\mu - \epsilon) + W_N(\mu + \epsilon) < 0$ and $\eta_N = -1$ if $W_N(\mu - \epsilon) + W_N(\mu + \epsilon) \geq 0$,

$$\begin{aligned} |W_N^{(M)}(\sigma_N^{(M)})| &\leq |W_N^{(M)}(\mu + \eta_N \epsilon)| \quad \forall s.l. \ M \in \mathbb{N} \\ \xrightarrow[(4.203)]{M \rightarrow \infty} |T_N(\mu^N) - T_N(\mu)| &\leq 2|\mu^N - \mu| |W_N(\mu + \eta_N \epsilon)|. \end{aligned} \quad (4.205)$$

Now for each $E \in \mathbb{R}$ and $N \in \mathbb{N}$ we have

$$\begin{aligned} -\frac{|y_j^N|^2}{(E - \mathcal{E}_j)^2} &\leq \frac{|y_j^N|^2}{(E - \mathcal{E}_j)^3} \leq 0 \quad \forall j \in \mathbb{N} \text{ with } \mathcal{E}_j \geq E + 1 \quad \Rightarrow \\ \left| \sum_{j=M}^{\infty} \frac{|y_j^N|^2}{(E - \mathcal{E}_j)^3} \right| &= \sum_{j=M}^{\infty} \frac{|y_j^N|^2}{|E - \mathcal{E}_j|^3} \leq \sum_{j=M}^{\infty} \frac{|y_j^N|^2}{(E - \mathcal{E}_j)^2} \quad \forall M \in \mathbb{N} \text{ with } \mathcal{E}_M \geq E + 1. \end{aligned} \quad (4.206)$$

It thus follows from the uniform convergence over N of $\sum_{j=M}^{\infty} \frac{|y_j^N|^2}{(E - \mathcal{E}_j)^2}$ to zero as $M \rightarrow \infty$ that $\sum_{j=M}^{\infty} \frac{|y_j^N|^2}{(E - \mathcal{E}_j)^3}$ likewise converges to zero as $M \rightarrow \infty$ uniformly over N . Note that

(4.206) also holds if $|y_j^N|^2$ is replaced with $|\Psi_j(p)|^2$, and thus

$$W_\delta(E) := \sum_{j:\Psi_j(p) \neq 0} \frac{|\Psi_j(p)|^2}{(E - \mathcal{E}_j)^3} \quad (4.207)$$

is a convergent sum for each $E \in \mathbb{R} \setminus \{E_j\}_{j=1}^\infty$. Then, by the same argument as the proof of (iv) \Rightarrow (vi) in Prop. 4.4.11, it follows that $W_N(E) \xrightarrow{N \rightarrow \infty} W_\delta(E) \forall E \in \mathbb{R}$ with $\mathcal{P}_{\{E\}}^{(H)} Y_N = 0 \forall$ suff. large N .

So now taking some $C > \max\{|W_\delta(\mu - \epsilon)|, |W_\delta(\mu + \epsilon)|\}$, it follows from (4.205) that for sufficiently large N ,

$$|T_N(\mu^N) - T_N(\mu)| \leq 2C|\mu^N - \mu| \xrightarrow{N \rightarrow \infty} 0. \quad (4.208)$$

Finally then,

$$|T_N(\mu^N) - T_\delta(\mu)| \leq |T_N(\mu^N) - T_N(\mu)| + |T_N(\mu) - T_\delta(\mu)| \xrightarrow{N \rightarrow \infty} 0. \quad (4.209)$$

□

Proposition 4.4.18. *For each $\mu \in M_\Theta$,*

$$\|\widehat{\psi}_{\mu^N}^N - \widehat{\psi}_\mu^\delta\| \xrightarrow{N \rightarrow \infty} 0. \quad (4.210)$$

Proof. For each $N \in \mathbb{N} \cap [N'_0, \infty)$,

$$\|\widehat{\psi}_{\mu^N}^N - \widehat{\psi}_\mu^\delta\|^2 = \sum_{j:\mathcal{E}_j \neq \mu} \left| \frac{\left(\frac{y_j^N}{\mu^N - \mathcal{E}_j}\right)}{\sqrt{T_N(\mu^N)}} - \frac{\left(\frac{\overline{\Psi_j(p)}}{\mu - \mathcal{E}_j}\right)}{\sqrt{T_\delta(\mu)}} \right|^2. \quad (4.211)$$

For each j with $\mathcal{E}_j \neq \mu$, by Lemma 4.4.13,

$$\begin{aligned} \left| \frac{\left(\frac{y_j^N}{\mu^N - \mathcal{E}_j}\right)}{\sqrt{T_N(\mu^N)}} - \frac{\left(\frac{\overline{\Psi_j(p)}}{\mu - \mathcal{E}_j}\right)}{\sqrt{T_\delta(\mu)}} \right|^2 &\leq 2 \left| \frac{\left(\frac{y_j^N}{\mu^N - \mathcal{E}_j}\right)}{\sqrt{T_\delta(\mu)}} - \frac{\left(\frac{\overline{\Psi_j(p)}}{\mu - \mathcal{E}_j}\right)}{\sqrt{T_\delta(\mu)}} \right|^2 + 2 \left| \frac{\left(\frac{y_j^N}{\mu^N - \mathcal{E}_j}\right)}{\sqrt{T_N(\mu^N)}} - \frac{\left(\frac{y_j^N}{\mu^N - \mathcal{E}_j}\right)}{\sqrt{T_\delta(\mu)}} \right|^2 \\ &= \frac{2}{T_\delta(\mu)} \left| \frac{y_j^N}{\mu^N - \mathcal{E}_j} - \frac{\overline{\Psi_j(p)}}{\mu - \mathcal{E}_j} \right|^2 + 2 \frac{|y_j^N|^2}{(\mu^N - \mathcal{E}_j)^2} \left| \frac{1}{\sqrt{T_N(\mu^N)}} - \frac{1}{\sqrt{T_\delta(\mu)}} \right|^2. \end{aligned} \quad (4.212)$$

Then summing over all j with $\mathcal{E}_j \neq \mu$,

$$\|\widehat{\psi}_{\mu^N}^N - \widehat{\psi}_\mu^\delta\|^2 \leq \frac{2}{T_\delta(\mu)} \|\psi_{\mu^N}^N - \psi_\mu^\delta\|^2 + 2 \left| 1 - \sqrt{\frac{T_N(\mu^N)}{T_\delta(\mu)}} \right|^2. \quad (4.213)$$

In RHS(4.213), as $N \rightarrow \infty$ the first term tends to zero by Proposition 4.4.16 and the second term tends to zero by Lemma 4.4.17. □

4.4.4 Convergence of All Eigenvalues within an Interval and Corresponding Eigenfunctions

Theorem 4.4.19. *Given the operator H_Θ for some $\Theta \in (0, 2\pi)$, take a sequence of operators $H^N = H + \nu_N \langle \cdot, Y_N \rangle Y_N$, with $(Y_N)_{N=1}^\infty \subset C_0^\infty(\mathcal{M}^\circ) \setminus \{0\}$ and $(\nu_N)_{N=1}^\infty \subset \mathbb{R} \setminus \{0\}$, for which the following are satisfied:*

- (i) $y_j^N := \langle Y_N, \Psi_j \rangle \xrightarrow{N \rightarrow \infty} \overline{\Psi_j(p)} \quad \forall j \in \mathbb{N}$,
- (ii) $\sum_{j=M}^\infty \frac{|y_j^N|^2}{\varepsilon_j^2} \xrightarrow{M \rightarrow \infty} 0$ uniformly over $N \in \mathbb{N}$,
- (iii) $M_\Theta \neq \emptyset$ and $\exists \mu \in M_\Theta$ s.t. $\frac{1}{\nu_N} - R_N(\mu) \xrightarrow{N \rightarrow \infty} 0$.

Then there exists an orthonormal eigenbasis of H_Θ and of each H^N such that for any $K, L \in \mathbb{N}$ with $K \leq L$ satisfying

(*) $\forall \mathcal{E} \in \text{Spec}(H) \cap [E_K, E_L]$ if $\mathcal{P}_{\{\mathcal{E}\}}^{(H)} \delta_p = 0$ then $\mathcal{P}_{\{\mathcal{E}\}}^{(H)} Y_N = 0$ for all suff. large N ,

we obtain the following:

Labelling the functions in the H_Θ eigenbasis with eigenvalue in $[E_K, E_L]$ as $\{\phi_1^\delta, \dots, \phi_n^\delta\}$, and labelling the corresponding eigenvalues $\{\lambda_1^\delta, \dots, \lambda_n^\delta\} \subset [E_K, E_L]$, the same can then be done with H^N for each suff. large N , having eigenfunctions $\{\phi_1^N, \dots, \phi_n^N\}$ and eigenvalues $\{\lambda_1^N, \dots, \lambda_n^N\} \subset [E_K, E_L]$, in such a way that

$$\lambda_k^N \xrightarrow{N \rightarrow \infty} \lambda_k^\delta, \quad \phi_k^N \xrightarrow[L^2]{N \rightarrow \infty} \phi_k^\delta \quad \forall k \in \{1, \dots, n\}. \quad (4.214)$$

Proof. Assuming (i) - (iii) here are satisfied, for the eigenbasis of H_Θ follow the construction given in §4.3.2, and for the eigenbasis of H^N follow the construction given in §4.3.1, only in the case of H^N , add the following requirements into Step (i) of the construction:

- (a) For each $\mathcal{E} \in \text{Spec}(H)$ with both $\mathcal{P}_{\{\mathcal{E}\}}^{(H)} Y_N \neq 0$ and $\mathcal{P}_{\{\mathcal{E}\}}^{(H)} \delta_p \neq 0$, take the orthonormal basis of $\Lambda_{\mathcal{E}}^{(H)}$ to be $\{U_{\mathcal{E}}^N \Psi_j : \mathcal{E}_j = \mathcal{E}\}$, where $U_{\mathcal{E}}^N$ is some chosen unitary operator on $\Lambda_{\mathcal{E}}^{(H)}$ satisfying

$$U_{\mathcal{E}}^N \Psi_l \in \text{span}\{\mathcal{P}_{\{\mathcal{E}\}}^{(H)} Y_N\}, \quad \|U_{\mathcal{E}}^N - I\| = \sqrt{2 \left(1 - \frac{|y_l^N|}{\|\mathcal{P}_{\{\mathcal{E}\}}^{(H)} Y_N\|} \right)}, \quad (4.215)$$

with Ψ_l being the member of the original basis of $\Lambda_{\mathcal{E}}^{(H)}$ for which $\Psi_l(p) \neq 0$. Such a unitary operator exists according to the arguments given in §4.4.1.

- (b) For each $\mathcal{E} \in \text{Spec}(H)$ with $\mathcal{P}_{\{\mathcal{E}\}}^{(H)} Y_N = 0$, take the orthonormal basis of $\Lambda_{\mathcal{E}}^{(H)}$ to be the original one, namely $\{\Psi_j : \mathcal{E}_j = \mathcal{E}\}$.

Observe that since $y_j^N \xrightarrow{N \rightarrow \infty} \overline{\Psi_j(p)} \forall j \in \mathbb{N}$, it therefore follows that for each $\mathcal{E} \in \text{Spec}(H)$ for which $\mathcal{P}_{\{\mathcal{E}\}}^{(H)} \delta_p \neq 0$, it also holds that $\mathcal{P}_{\{\mathcal{E}\}}^{(H)} Y_N \neq 0$ for all suff. large N . Now take an interval $[E_K, E_L]$ for which it also holds that for each $\mathcal{E} \in \text{Spec}(H) \cap [E_K, E_L]$ with $\mathcal{P}_{\{\mathcal{E}\}}^{(H)} \delta_p = 0$ we have $\mathcal{P}_{\{\mathcal{E}\}}^{(H)} Y_N = 0$ for all suff. large N . Then we can take some $N_0 \in \mathbb{N}$ for which, for each $\mathcal{E} \in \text{Spec}(H) \cap [E_K, E_L]$, we have either $\mathcal{P}_{\{\mathcal{E}\}}^{(H)} \delta_p \neq 0$ and $\mathcal{P}_{\{\mathcal{E}\}}^{(H)} Y_N \neq 0 \forall N \in \mathbb{N} \cap [N_0, \infty)$, or $\mathcal{P}_{\{\mathcal{E}\}}^{(H)} \delta_p = 0$ and $\mathcal{P}_{\{\mathcal{E}\}}^{(H)} Y_N = 0 \forall N \in \mathbb{N} \cap [N_0, \infty)$.

Now partitioning the interval $[E_K, E_L]$ into the following sets - $\{E_K\}, \{E_{K+1}\}, \dots, \{E_L\}, (E_K, E_{K+1}), (E_{K+1}, E_{K+2}), \dots, (E_{L-1}, E_L)$ - for each $E_k \in [E_K, E_L]$ the multiplicity of E_k as an eigenvalue of H_Θ is one less than its multiplicity as an eigenvalue of H , and the same holds with E_k as an eigenvalue of H^N for each $N \in \mathbb{N} \cap [N_0, \infty)$. As discussed in §4.4.1, provided E_k is indeed an eigenvalue of H_Θ (which will be so if and only if E_k as an eigenvalue of H is not simple), $\|U_{E_k}^N - I\| \xrightarrow{N \rightarrow \infty} 0$, and so the H^N eigenbasis members in $\Lambda_{E_k}^{(H^N)}$ will converge to the H_Θ eigenbasis members in $\Lambda_{E_k}^{(H_\Theta)}$ as $N \rightarrow \infty$.

For each $(E_k, E_{k+1}) \subset [E_K, E_L]$, every Ψ_j with $\mathcal{E}_j \in (E_k, E_{k+1})$ will be in the eigenbasis of H_Θ and of H^N for each $N \in \mathbb{N} \cap [N_0, \infty)$, with eigenvalue \mathcal{E}_j . On top of this, H_Θ will have one more eigenbasis member with eigenvalue in (E_k, E_{k+1}) . This eigenvalue (call it μ) will be in M_Θ , and the eigenfunction will be $\widehat{\psi}_\mu^\delta$ (the normalisation of ψ_μ^δ as defined in (4.97) and (4.194)). Likewise H^N will have one more eigenbasis member (namely $\widehat{\psi}_{\mu^N}^N$) with eigenvalue (namely μ^N) in (E_k, E_{k+1}) for each $N \in \mathbb{N} \cap [N_0, \infty)$. By Proposition 4.4.12, $\mu^N \xrightarrow{N \rightarrow \infty} \mu$, and by Proposition 4.4.18, $\widehat{\psi}_{\mu^N}^N \xrightarrow[L^2]{N \rightarrow \infty} \widehat{\psi}_\mu^\delta$. \square

Remarks. (a) Again, M_Θ is a subset of the set of eigenvalues of H_Θ , defined in (4.151).

(b) The set of eigenfunctions $\{\phi_1^\delta, \dots, \phi_n^\delta\}$ of H_Θ with eigenvalue in $[E_K, E_L]$ will be non-empty unless $E_K = E_L$ and E_K is a simple eigenvalue of H .

(c) It is not required that the eigenvalues $\{\lambda_1^N, \dots, \lambda_n^N\} \subset [E_K, E_L]$ of H_N necessarily be numbered in increasing order.

(d) Recall from Lemma 4.4.15 that with (Y_N) satisfying (i) and (ii) here, it follows that

$$\langle \phi, Y_N \rangle \xrightarrow{N \rightarrow \infty} \phi(p) \quad \forall \phi \in \text{Dom}(H). \quad (4.216)$$

This parallels (4.45) in the review of [Zor80].

(e) Recall that with (ν_N) satisfying (iii) here, it follows from Lemma 4.4.5 that $\nu_N < 0$ for all suff. large N and $\nu_N \rightarrow 0$. Again this matches earlier observations on ν_N in (4.11), (4.48) and (4.52), when reviewing [Zor80], [AK00] and [GN12] respectively, with (4.11) and (4.48) set in \mathbb{R}^3 and (4.48) set in \mathbb{R}^2 .

If wishing to apply the above theorem in the study of high-energy limits, it may then be useful to address the question of whether $\exists (Y_N)_{N=1}^\infty \subset C_0^\infty(\mathcal{M}^\circ) \setminus \{0\}$ which as well as satisfying conditions (i) and (ii) in the statement of the above theorem, also satisfies the following:

$$\begin{aligned} \exists J \in \mathbb{N} \text{ s.t. } \forall \mathcal{E} \in \text{Spec}(H) \cap (E_J, \infty) \setminus \{E_j\}_{j=J}^\infty \exists N_0^{(\mathcal{E})} \in \mathbb{N} \text{ s.t.} \\ \forall N \in \mathbb{N} \cap [N_0^{(\mathcal{E})}, \infty) \quad \mathcal{P}_{\mathcal{E}}^{(H)} Y_N = 0. \end{aligned} \quad (4.217)$$

If this is satisfied then all solutions of the equation $S(E) = F(\Theta)$ above E_J are contained in M_Θ , so $M_\Theta \neq \emptyset$, and thus $(\nu_N)_{N=1}^\infty$ can be chosen so as to satisfy condition (iii) in the statement of Thm. 4.4.19. Furthermore, for every choice of $K, L \in \mathbb{N} \cap [J, \infty)$ with $K \leq L$ the condition within Thm. 4.4.19 that “ $\forall \mathcal{E} \in \text{Spec}(H) \cap [E_K, E_L]$ if $\mathcal{P}_{\{\mathcal{E}\}}^{(H)} \delta_p = 0$ then $\mathcal{P}_{\{\mathcal{E}\}}^{(H)} Y_N = 0$ for all suff. large N ” will be satisfied.

It could be even more useful though if the following stronger condition is satisfied:

$$\exists J \in \mathbb{N} \text{ s.t. } \quad \forall \mathcal{E} \in \{E_j\}_{j=J}^\infty \quad \forall N \in \mathbb{N} \quad \mathcal{P}_{\{\mathcal{E}\}}^{(H)} Y_N \neq 0, \quad (4.218)$$

$$\forall \mathcal{E} \in \text{Spec}(H) \cap (E_J, \infty) \setminus \{E_j\}_{j=J}^\infty \quad \forall N \in \mathbb{N} \quad \mathcal{P}_{\{\mathcal{E}\}}^{(H)} Y_N = 0. \quad (4.219)$$

Proposition 4.4.20. *If \mathcal{M} is without boundary then $\exists (Y_N)_{N=1}^\infty \subset C_0^\infty(\mathcal{M}^\circ) \setminus \{0\} = C^\infty(\mathcal{M}) \setminus \{0\}$ such that the following are satisfied:*

- (i) $y_j^N \xrightarrow{N \rightarrow \infty} \overline{\Psi_j(p)} \quad \forall j \in \mathbb{N}$,
- (ii) $\sum_{j=M}^\infty \frac{|y_j^N|^2}{\mathcal{E}_j^2} \xrightarrow{M \rightarrow \infty} 0$ uniformly over $N \in \mathbb{N}$,
- (iii) $\forall j, N \in \mathbb{N}$ it holds that $y_j^N = 0$ if and only if $\Psi_j(p) = 0$.

Proof. Try

$$Y_N = \sum_{j=1}^N \overline{\Psi_j(p)} \Psi_j + \sum_{j=N+1}^\infty e^{-\mathcal{E}_j} \overline{\Psi_j(p)} \Psi_j. \quad (4.220)$$

Firstly by Corollary 2.1.2, we have $Y_N \in C^\infty(\mathcal{M})$ if

$$\sum_{j=1}^\infty \mathcal{E}_j^n e^{-2\mathcal{E}_j} |\Psi_j(p)|^2 < \infty \quad \forall n \in \mathbb{N} \cup \{0\}. \quad (4.221)$$

By Lemma 2.1.7, sufficient for (4.221) to hold is that for every $n \in \mathbb{N} \cup \{0\}$, the following converge:

$$\lim_{s \rightarrow \infty} s^n e^{-2s} N_p(s), \quad \int_0^\infty (nt^{n-1} - 2t^n) e^{-2t} N_p(t) dt. \quad (4.222)$$

Via Weyl's law (Lemma 2.1.5 or Corollary 2.1.6), it can then be shown from standard mathematics that these indeed converge, and thus $Y_N \in C^\infty(\mathcal{M})$ for every $N \in \mathbb{N}$ (and clearly $Y_N \neq 0$).

Next, it is clear that statements (i) and (iii) are satisfied. Observe also that for every $N \in \mathbb{N}$,

$$\sum_{j=M}^\infty \frac{|y_j^N|^2}{\mathcal{E}_j^2} \leq \sum_{j=M}^\infty \frac{|\Psi_j(p)|^2}{\mathcal{E}_j^2} \xrightarrow{M \rightarrow \infty} 0 \quad (4.223)$$

by Lemma 2.2.5, and thus statement (ii) is also satisfied. \square

Observe that statement (iii) within the statement of the above proposition is stronger than (4.218), (4.219).

We shall now suppose for the small remainder of this Chapter that we are at liberty to vary the positioning on \mathcal{M}° of the point p at which the delta potential is concentrated. By allowing $p \in \mathcal{M}^\circ$ to vary, this obviously will not affect $\text{Spec}(H) = \{\mathcal{E}_j\}_{j=1}^\infty$, but it may nevertheless affect $\{E_j\}_{j=1}^\infty = \{\mathcal{E} \in \text{Spec}(H) : \mathcal{P}_{\{\mathcal{E}\}}^{(H)} \delta_p := \sum_{j:\mathcal{E}_j=\mathcal{E}} \overline{\Psi_j(p)} \Psi_j \neq 0\}$.

In either case of \mathcal{M} being with or without boundary, we have the following:

Lemma 4.4.21. *Given any eigenfunction u of H , the nodal set \mathcal{N}_u of u on \mathcal{M}° , defined as $\mathcal{N}_u := \{x \in \mathcal{M}^\circ : u(x) = 0\}$, has zero (2D area) measure.*

Proof. According to [DF90], the nodal set of a real eigenfunction is the union of a 1-dimensional manifold with a finite set of ‘‘singular’’ points, and this 1D manifold has finite 1D measure. It obviously follows then that the 2D measure of this nodal set is zero. Now if u is an eigenfunction of H then so is \bar{u} , having the same eigenvalue, and thus so are the real and imaginary parts of u . Since $\mathcal{N}_{\text{Re}(u)}$ and $\mathcal{N}_{\text{Im}(u)}$ are zero measure sets, it follows that $\mathcal{N}_u = \mathcal{N}_{\text{Re}(u)} \cap \mathcal{N}_{\text{Im}(u)}$ is a zero measure set. \square

Corollary 4.4.22. *Concerning the selection of the point $p \in \mathcal{M}^\circ$ at which to place the point scatterer, there is a full measure subset of \mathcal{M}° for which, if p is taken to lie in this subset, then $\mathcal{P}_{\{\mathcal{E}\}}^{(H)} \delta_p \neq 0 \forall \mathcal{E} \in \text{Spec}(H)$, or in other words, $\text{Spec}(H) = \{E_j\}_{j \in \mathbb{N}}$.*

Proof. For each $\mathcal{E} \in \text{Spec}(H)$, take an eigenfunction $u_\mathcal{E} \in \Lambda_\mathcal{E}^{(H)} \setminus \{0\}$. Let $\mathcal{N} := \bigcup_{\mathcal{E} \in \text{Spec}(H)} \mathcal{N}_{u_\mathcal{E}} \subset \mathcal{M}^\circ$. Then by countable additivity of measure, \mathcal{N} is a zero measure set, and so $\mathcal{M}^\circ \setminus \mathcal{N}$ is a full measure set in \mathcal{M} . If p is then selected to be contained in $\mathcal{M}^\circ \setminus \mathcal{N}$, it follows that $u_\mathcal{E}(p) \neq 0 \forall \mathcal{E} \in \text{Spec}(H)$, and thus $\mathcal{P}_{\{\mathcal{E}\}}^{(H)} \delta_p \neq 0 \forall \mathcal{E} \in \text{Spec}(H)$. \square

With $\mathcal{P}_{\{\mathcal{E}\}}^{(H)} \delta_p \neq 0 \forall \mathcal{E} \in \text{Spec}(H)$, (4.217) is automatically satisfied.

Chapter 5

Equidistribution in Position Space

5.1 Systems where Work has Already Been Done

5.1.1 Classical Behaviour Leading to Position Space

Equidistribution in the Unperturbed System

Concerning the unperturbed system, the *Quantum Ergodicity Theorem* states that if the classical dynamical system is *ergodic*, then the quantum system is *quantum ergodic* (proved in [Sni74], [Ver85] and [Zel87] for the boundaryless case; [GL93] and [ZZ96] for the case with boundary).

A set $V \subset S^*\mathcal{M}$ (for which we'll say every point in V , if taken as an initial state, gives rise to a fully determined trajectory) is *invariant* under the classical flow if for every $(x, \xi) \in V$, the whole trajectory stemming from (x, ξ) as an initial state is contained within V , i.e. $\Phi^t(x, \xi) \in V \ \forall t \in \mathbb{R}$, equivalently $\Phi^t(V) = V \ \forall t \in \mathbb{R}$ (noting that with the dynamical system being autonomous, if every trajectory which is in V at time $t = 0$ remains in V for all time, then every trajectory which is in V at *any* moment in time remains in V for all time). The classical system is then *ergodic* if every invariant measurable subset of $S^*\mathcal{M}$ has either zero measure or full measure.

The quantum system is *quantum ergodic* for a given choice of orthonormal eigenbasis of H (arranging the eigenbasis members in order of non-decreasing eigenvalue), if this eigenbasis sequence has a density-one subsequence which *equidistributes* (in phase space). Equidistribution (that is, *phase space* equidistribution) is a certain type of limiting behaviour (see for example, the Theorem in [ZZ96]), which in particular implies *position space equidistribution*. A subsequence $\{\Psi_{j_n}\}_{n=1}^{\infty}$ equidistributes in position space if, for

every measurable subset $A \subset \mathcal{M}$ whose boundary has (2D area) measure zero [MR12],

$$\lim_{n \rightarrow \infty} \int_A |\Psi_{j_n}(x)|^2 dx = \frac{\text{area}(A)}{\text{area}(\mathcal{M})}. \quad (5.1)$$

A subsequence $(x_{j_n})_{n=1}^\infty$ of a sequence $(x_j)_{j=1}^\infty$ is said to have density $d \in [0, 1]$ if

$$\lim_{N \rightarrow \infty} \frac{\#\{n : j_n \leq N\}}{N} = d. \quad (5.2)$$

Note that in general, it is possible for some choices of orthonormal eigenbasis to give quantum ergodicity while others do not. For an example of this, see [Zel92], in which it is proved that for the $-\Delta$ operator on the 2-sphere, “almost all” choices of orthonormal eigenbasis possess quantum ergodicity, even though the usual basis consisting of spherical harmonics does not. However, if the classical system is ergodic then the quantum system will be quantum ergodic regardless of what orthonormal eigenbasis is chosen.

In [MR12], it is proved that if \mathcal{M} is a *rational polygon* then in the quantum system, any orthonormal eigenbasis of H (arranged in order of non-decreasing eigenvalue) will have a density-one subsequence that equidistributes in position space. The classical flow is not ergodic, but it can be broken down into what is referred to in [MR12] as *directional flows*, and almost all of these directional flows are ergodic (in fact, *uniquely ergodic*), as proved in [KMS86]. The key property of the classical flow, from which this behaviour in the quantum system is derived, is:

$$\lim_{T \rightarrow \infty} \int_{S^*\mathcal{M}} |a^T(x, \xi) - \langle a \rangle|^2 d\mu(x, \xi) = 0 \quad \forall a \in C^\infty(\mathcal{M}), \quad (5.3)$$

where

$$a^T(x, \xi) := \frac{1}{2T} \int_{-T}^T (\pi^* a) \circ \Phi^t(x, \xi) dt, \quad (5.4)$$

$$\langle a \rangle := \frac{1}{\text{area}(\mathcal{M})} \int_{\mathcal{M}} a(x) dx = \int_{S^*\mathcal{M}} (\pi^* a)(x, \xi) d\mu(x, \xi), \quad (5.5)$$

$(\pi^* a)(x, \xi) := a(x)$, and μ is the standard normalised measure on $S^*\mathcal{M}$. Describing this in words, $\langle a \rangle$ is the *spatial* average of a over \mathcal{M} and $a^T(x, \xi)$ is the *temporal* average of a over time interval $[-T, T]$ for a trajectory passing through x with unit velocity in the direction of ξ at time 0. (5.3) then tells us that the mean square deviation over phase space of this temporal average a^T from this spatial average $\langle a \rangle$ tends to zero as $T \rightarrow \infty$.

Observe that in (5.3), a is dependent on position only. One can also consider a stronger version of (5.3) where a is a general smooth (or more generally L^2) function on the phase space $S^*\mathcal{M}$. According to von Neumann’s Ergodic Theorem, this stronger “phase space version” of (5.3) is satisfied if the system is ergodic. Thus (5.3) can be seen as a kind of “position space version” of ergodicity.

It can already be established (by e.g. extending the arguments in §3 of [MR12] beyond just rational polygons and similar systems) that in general, if the classical system satisfies (5.3) then the *unperturbed* quantum system has a density-one subsequence of functions in the eigenbasis that equidistributes in position space, i.e. satisfies (5.1). It is now in our interest to extend this result to the *delta-perturbed* quantum system (remembering that the classical system is considered to be unaffected by this perturbation).

5.1.2 The Unperturbed and Delta-Perturbed Flat Torus

Work on position space equidistribution when a delta potential is added has already been carried out for the case of the rectangular flat torus in [RU12]. It is proved that the sequence of new eigenfunctions (i.e. $(\widehat{\phi}_j)_{j=0}^\infty$ as defined in §2.2.5) has a density-one subsequence that equidistributes in position space.

Now like the rational polygon, the flow (on $S^*\mathcal{M}$) in the case of the flat torus $\mathcal{M} = \mathbb{T}^2$ can be broken down into directional flows (where in this case, each directional flow is simply the restriction of the flow to a surface in $S^*\mathbb{T}^2 \simeq \mathbb{T}^2 \times S^1$ of constant covector ξ , representing direction of motion), and again almost all of these directional flows are ergodic (and uniquely ergodic). This follows from e.g. Thm. 1 in [Mao88], part of which states that for a flow on a 1×1 flat torus (this flow here being defined just on the 2D torus itself, not the (co)tangent or (co)sphere bundle), given by a C^1 velocity vector field that is everywhere non-zero, if the flow has no periodic orbits then it is uniquely ergodic. Unique ergodicity here means that there is a unique Borel measure, with total measure 1, under which the flow is measure-preserving, in which case the flow is also ergodic with respect to this measure.

Each directional flow for the 1×1 flat torus would then be represented by a *constant* velocity vector field, with the norm of the vector being 1. If this vector \mathbf{v} is in $\mathbb{R}\mathbb{Z}^2 := \left\{ \begin{pmatrix} sk \\ sl \end{pmatrix} : s \in \mathbb{R}, k, l \in \mathbb{Z} \right\}$ then all trajectories are periodic with period $\min\{t > 0 : \mathbf{v}t \in \mathbb{Z}^2\}$, and if $\mathbf{v} \notin \mathbb{R}\mathbb{Z}^2$ then no trajectory is periodic. Now \mathbb{Z}^2 is countable, and so $S^1 \cap \mathbb{R}\mathbb{Z}^2$ is only a countable subset of S^1 . Thus almost all directional flows have no periodic orbits, and hence are uniquely ergodic. Furthermore, all of these directional flows clearly preserve the Lebesgue measure, and so the uniquely ergodic directional flows are ergodic with respect to the Lebesgue measure. Finally, for a general $a \times b$ flat torus, this torus can be matched to the 1×1 torus by the simple coordinate transformations $\tilde{x} = \frac{x}{a}$, $\tilde{y} = \frac{y}{b}$. This will then match the directional flows in such a way that, although speed rescalings and angle distortions would in general be involved, it

would nevertheless still hold that only countably many directional flows are periodic, and the rest are uniquely ergodic and ergodic under the (normalised) Lebesgue measure (note that this transformation will preserve the *normalised* Lebesgue measure).

It thus follows that geodesic flow for the flat torus (taking the whole flow on $S^*\mathbb{T}^2$) satisfies (5.3), by the same arguments that unique ergodicity of almost all directional flows on a rational polygon leads to its whole flow satisfying (5.3). In short, this can be obtained firstly by deriving, from unique ergodicity of almost all directional flows, that $a^T(x, \xi) \xrightarrow{T \rightarrow \infty} \langle a \rangle$ for almost all $(x, \xi) \in S^*\mathcal{M}$ (noting that $\langle a \rangle$ is also the average of a on the domain of each directional flow), so $\lim_{T \rightarrow \infty} |a^T(x, \xi) - \langle a \rangle|^2 = 0$ for almost all $(x, \xi) \in S^*\mathcal{M}$, and then applying the dominated convergence theorem to obtain $\lim_{T \rightarrow \infty} \int_{S^*\mathcal{M}} |a^T - \langle a \rangle|^2 d\mu = 0$.

It also follows then that for the flat torus, the unperturbed quantum system has a density-one subsequence of functions in the eigenbasis that equidistributes in position space (regardless of choice of orthonormal eigenbasis). Indeed, it is remarked in [MR12] that the position space equidistribution result presented applies not only to rational billiards with a Dirichlet $-\Delta$, but also to those with a Neumann $-\Delta$, and furthermore to the $-\Delta$ operator on any *translation surface* (which would include the flat torus; see e.g. Ch. 1, 17 and 18 of [Sch11] for discussion on what translation surfaces are and their properties). [Since in general, we only state this position space equidistribution on the torus to hold for a density-one subsequence, one can also consider the possibility of other limiting behaviours in position space of eigenfunction subsequences, and these are investigated in [Jak97]].

For the flat torus then, combining the position space equidistribution of almost all (i.e. full density subsequence of) eigenbasis functions in the unperturbed system (regardless of choice of orthonormal eigenbasis), with the position space equidistribution of almost all “new eigenfunctions” in the perturbed system, it follows that, taking the full eigenbasis in the perturbed system, almost all eigenbasis functions equidistribute in position space, whichever orthonormal eigenbasis is chosen.

To see this, note firstly that one particular choice of unperturbed eigenbasis consists purely of functions whose modulus is spatially constant, and only the argument/phase varies (see [RU12]). Hence every eigenspace includes functions that are non-vanishing at p , and so using our own notation from §2.2.5, $\text{Spec}(H) = \{E_j\}_{j=1}^\infty$ and $\text{Spec}(H) \cap \{\lambda_j\}_{j=0}^\infty = \emptyset$. Thus an arbitrary orthonormal eigenbasis for the perturbed system can be constructed as follows: firstly take an orthonormal eigenbasis $\{\tilde{\Psi}_j\}_{j \in \mathbb{N}}$ for which the first member in each eigenspace is nonzero at p and the rest are zero at p , and then replace the first

member in each eigenspace $\Lambda_{E_j}^{(H)}$ with $e^{i\theta_j-1}\widehat{\phi}_{j-1}$, where each $\theta_j \in [0, 2\pi)$ is arbitrary. Note that every unperturbed eigenvalue, except the lowest (zero), has multiplicity ≥ 2 in the unperturbed system, and therefore survives as an eigenvalue of the perturbed system, with 1 less multiplicity.

Now taking a full density subsequence of $\{\widetilde{\Psi}_j\}_{j=1}^\infty$ which equidistributes in position space, and a full density subsequence of $\{\widehat{\phi}_j\}_{j=0}^\infty$, or equivalently $\{e^{i\theta_j}\widehat{\phi}_j\}_{j=0}^\infty$, which equidistributes in position space (multiplication by a phase factor does not affect position space equidistribution), the exceptional members (members of the full sequence that are outside the full density subsequence) in each case form a zero density subset. Thus the exceptional members of $\{\widetilde{\Psi}_j\}_{j=1}^\infty$ which survive into the eigenbasis of the perturbed system form a zero density subset of this perturbed eigenbasis, and likewise the exceptional members of $\{\widehat{\phi}_j\}_{j=0}^\infty$, and so the union of these two zero density subsets of the perturbed eigenbasis is zero density. Thus the complement of this union is a full density subsequence, and is itself the union of two position space equidistributing subsequences, therefore itself being a position space equidistributing subsequence.

5.1.3 Methods of Arriving at Position Space Equidistribution

The method used in [RU12] to prove position space equidistribution of almost all new eigenfunctions in the perturbed system makes use of the behaviour of eigenvalues and eigenfunctions specific to the flat torus. However, the method in [MR12] makes use of more general laws, in particular, a *local Weyl law* (relating quantum averages with classical averages; also known as the *Szegő limit theorem*), and *Egorov's theorem* (about quantisation of observables composed with time evolution under the classical flow). Both of these involve the theory of *pseudodifferential operators*.

There is much literature discussing the theory of pseudodifferential operators, such as [Hör85a], [Sai91], [Tay96b] and [Shu01]. For the sake of ease, here we shall introduce pseudodifferential operators (abbreviated Ψ DOs) using a relatively neat construction of Ψ DOs on \mathbb{R}^n , found in e.g. [Sai91]. A more sophisticated construction of Ψ DOs can be found for example in Ch. 1 of [Shu01].

5.2 Pseudodifferential Operators on \mathbb{R}^n

5.2.1 Associating Ψ DOs with Symbols

Given a *multi-index* $\alpha = (\alpha_1, \dots, \alpha_n) \in (\{0\} \cup \mathbb{N})^n$, define $|\alpha| := \alpha_1 + \dots + \alpha_n$, define the differential operator $\partial^\alpha := \partial_{x_1}^{\alpha_1} \dots \partial_{x_n}^{\alpha_n}$, and define the polynomial $x^\alpha := x_1^{\alpha_1} \dots x_n^{\alpha_n}$ for $x = (x_1, \dots, x_n) \in \mathbb{R}^n$. Define again the *Schwartz space* $\mathcal{S} \subset C^\infty(\mathbb{R}^n)$ to be the space of all C^∞ -smooth functions u on \mathbb{R}^n satisfying the following rule: $x^\alpha \partial^\beta u(x)$ is a bounded function on \mathbb{R}^n for every $\alpha, \beta \in (\{0\} \cup \mathbb{N})^n$. Note that $\mathcal{S} \subset L^p(\mathbb{R}^n)$ for every $p \in [1, \infty) \cup \{\infty\}$.

For each $u \in L^1(\mathbb{R}^n)$, define its Fourier transform $\widehat{u} \in L^\infty(\mathbb{R}^n)$ by

$$\widehat{u}(\xi) := \int_{\mathbb{R}^n} u(x) e^{-ix \cdot \xi} dx. \quad (5.6)$$

On the Schwartz space, the Fourier transform is a linear isomorphism from the Schwartz space to itself, with

$$u(x) = \frac{1}{(2\pi)^n} \int_{\mathbb{R}^n} \widehat{u}(\xi) e^{ix \cdot \xi} d\xi \quad \forall u \in \mathcal{S}, x \in \mathbb{R}^n. \quad (5.7)$$

For each $m \in \mathbb{R}$, define the class of *symbols of order m* , denoted $S^m \subset C^\infty(\mathbb{R}^n \times \mathbb{R}^n)$, to consist of all C^∞ -smooth functions a on $\mathbb{R}^n \times \mathbb{R}^n$, satisfying the following rule: for each $\alpha, \beta \in (\{0\} \cup \mathbb{N})^n$ there exists $C_{\alpha\beta} \geq 0$ such that

$$|\partial_x^\alpha \partial_\xi^\beta a(x, \xi)| \leq C_{\alpha\beta} (1 + \|\xi\|^2)^{(m-|\beta|)/2} \quad \forall (x, \xi) \in \mathbb{R}^n \times \mathbb{R}^n. \quad (5.8)$$

Note that if $l \leq m$ then $S^l \subset S^m$. Thus we also define $S^\infty := \bigcup_{m \in \mathbb{R}} S^m$ and $S^{-\infty} := \bigcap_{m \in \mathbb{R}} S^m$.

Now given some $a \in S^\infty$, let A be the *pseudodifferential operator with symbol a* . Then for every $u \in \mathcal{S}$, it holds that $Au \in \mathcal{S}$, where

$$(Au)(x) := \frac{1}{(2\pi)^n} \int_{\mathbb{R}^n} a(x, \xi) \widehat{u}(\xi) e^{ix \cdot \xi} d\xi \quad \forall x \in \mathbb{R}^n. \quad (5.9)$$

The domain of the operator A can then be extended, by techniques of distribution theory, to the space of *tempered distributions* \mathcal{S}' , and again $L^p(\mathbb{R}^n) \subset \mathcal{S}'$ for every $p \in [1, \infty) \cup \{\infty\}$. If $a \in S^m$ then A is a *pseudodifferential operator of order m* , and we write $A \in \Psi^m$.

Furthermore, given any Ψ DO $A \in \Psi^\infty$, its symbol a can be recovered: for each $\xi \in \mathbb{R}^n$ we have

$$a(x, \xi) = e^{-ix \cdot \xi} (Ae^{i \cdot \xi})(x) \quad \forall x \in \mathbb{R}^n, \quad (5.10)$$

where $e^{i \cdot \xi}$ refers to the function $x \mapsto e^{ix \cdot \xi}$.

5.2.2 Differential Operators and Polyhomogeneous Ψ DOs

Now for each $\alpha \in (\{0\} \cup \mathbb{N})^n$, define the differential operator $D^\alpha := -i^{|\alpha|} \partial^\alpha$. Given some $m \in \{0\} \cup \mathbb{N}$, suppose we have $a \in C^\infty(\mathbb{R}^n \times \mathbb{R}^n)$ of the form:

$$a(x, \xi) = \sum_{|\alpha| \leq m} a_\alpha(x) \xi^\alpha, \quad (5.11)$$

where each $\alpha \in (\{0\} \cup \mathbb{N})^n$, and each $a_\alpha \in C^\infty(\mathbb{R}^n)$ with $\partial^\beta a_\alpha \in L^\infty(\mathbb{R}^n) \quad \forall \beta \in (\{0\} \cup \mathbb{N})^n$. Then $a \in S^m$ and the Ψ DO with symbol a is the differential operator

$$A = \sum_{|\alpha| \leq m} a_\alpha(x) D^\alpha \in \Psi^m. \quad (5.12)$$

A is then said to have *principal symbol*

$$\sum_{|\alpha|=m} a_\alpha(x) \xi^\alpha. \quad (5.13)$$

(For each integer $l > m$ it then also holds that $A \in \Psi^l$ with zero principal symbol).

This notion then has a generalisation to what is referred to as *polyhomogeneous symbols*. For each $m \in \mathbb{R}$, S^m has a particular subclass $S_{\text{phg}}^m \subset S^m$, the class of polyhomogeneous symbols of order m . These are symbols a for which there exists a so-called *asymptotic expansion* of the form:

$$a \sim \sum_{j=0}^{\infty} a_{m-j}, \quad (5.14)$$

where each $a_{m-j} \in C^\infty(\mathbb{R}^n \times (\mathbb{R}^n \setminus \{0\}))$ is positively homogeneous of order $m - j$ in ξ , meaning

$$a_{m-j}(x, r\xi) = r^{m-j} a_{m-j}(x, \xi) \quad \forall (x, \xi) \in \mathbb{R}^n \times (\mathbb{R}^n \setminus \{0\}), r \in (0, \infty). \quad (5.15)$$

If $A \in \Psi_{\text{phg}}^m$ is the Ψ DO of symbol a , then its principal symbol is then a_m .

5.3 Weyl's Law, Egorov's Theorem, Quantum Variance and Position Space Equidistribution

The theory of pseudodifferential operators can be applied to the compact manifold/region \mathcal{M} (or \mathcal{M}°), with every polyhomogeneous Ψ DO of any certain order having a well-defined principal symbol, with this principal symbol being a function on the cotangent bundle. Another property that every Ψ DO has (and this in fact goes beyond just Ψ DOs) is the

Schwartz kernel. If A is a Ψ DO on \mathcal{M}° then the Schwartz kernel K_A is a distribution on $\mathcal{M}^\circ \times \mathcal{M}^\circ$ satisfying

$$\langle Au, v \rangle_{ll}^{\mathcal{M}^\circ} = \langle K_A, (\pi_2^*u)(\pi_1^*v) \rangle_{ll}^{\mathcal{M}^\circ \times \mathcal{M}^\circ} \quad \forall u, v \in C_0^\infty(\mathcal{M}^\circ), \quad (5.16)$$

where π_2^*u is the function $(x, y) \mapsto u(y)$, likewise π_1^*v is the function $(x, y) \mapsto v(x)$ and again the subscript ll means linearity in both arguments. Formally then, we can write

$$Au = \int_{\mathcal{M}^\circ} K_A(\cdot, y)u(y) dy. \quad (5.17)$$

Now when stating the local Weyl law and Egorov's theorem, we shall involve zero-order polyhomogeneous Ψ DOs, taken as bounded linear operators on $L^2(\mathcal{M})$, with principal symbols being functions on the cosphere bundle $S^*\mathcal{M}$ (noting that as functions on the cotangent bundle $T^*\mathcal{M}$, they are dependent only on position on \mathcal{M} and on direction of the non-zero covector, but not on magnitude of the covector).

Lemma 5.3.1 (Local Weyl Law / Szegö Limit Theorem, see e.g. Lemma 4 in [ZZ96], Thm. 2.2.18 in [Sch01], §3 in [MR12]). *Let $A \in \Psi_{\text{phg}}^0(\mathcal{M})$, with Schwartz kernel compactly supported in $\mathcal{M}^\circ \times \mathcal{M}^\circ$. Let $\sigma_0(A)$ denote the zero-order principal symbol of A . Then*

$$\lim_{E \rightarrow \infty} \frac{1}{\#\{j : \mathcal{E}_j \leq E\}} \sum_{j: \mathcal{E}_j \leq E} \langle A\Psi_j, \Psi_j \rangle = \int_{S^*\mathcal{M}} \sigma_0(A) d\mu. \quad (5.18)$$

[In fact it is remarked in [ZZ96] that the requirement of the Schwartz kernel being supported away from the boundary can be eliminated with further (heat equation) techniques beyond what is provided in that paper]. Interpreting $\langle A\Psi_j, \Psi_j \rangle$ to be the expectation value of the quantum observable A under the quantum state Ψ_j , this law says that when we take the average of these expectation values over the first N states in the eigenbasis, as N tends to infinity this average tends to the average of the classical observable $\sigma_0(A)$ over the phase space $S^*\mathcal{M}$.

Next, before stating Egorov's theorem, we define the operators \sqrt{H} and $e^{it\sqrt{H}}$ for every $t \in \mathbb{R}$ as follows:

- (i) \sqrt{H} , as before, is the self-adjoint operator with orthonormal eigenbasis $\{\Psi_j\}_{j \in \mathbb{N}}$ and respective corresponding eigenvalues $\{\sqrt{\mathcal{E}_j}\}_{j \in \mathbb{N}}$. By the same arguments as in the proof of Lemma 2.1.1, we have

$$\sum_{j=1}^{\infty} a_j \Psi_j \in \text{Dom}(\sqrt{H}) \quad \text{iff} \quad \sum_{j=1}^{\infty} \sqrt{\mathcal{E}_j} a_j \Psi_j \in L^2(\mathcal{M}), \quad (5.19)$$

$$\sqrt{H} \left(\sum_{j=1}^{\infty} a_j \Psi_j \right) = \sum_{j=1}^{\infty} \sqrt{\mathcal{E}_j} a_j \Psi_j. \quad (5.20)$$

(ii) $\text{Dom}(e^{it\sqrt{H}})$ is the whole Hilbert space $L^2(\mathcal{M})$ for every $t \in \mathbb{R}$, with

$$e^{it\sqrt{H}} \left(\sum_{j=1}^{\infty} a_j \Psi_j \right) = \sum_{j=1}^{\infty} e^{it\sqrt{\varepsilon_j}} a_j \Psi_j. \quad (5.21)$$

Observe then that $e^{it\sqrt{H}} : L^2(\mathcal{M}) \rightarrow L^2(\mathcal{M})$ is a bijective operator with inverse $e^{-it\sqrt{H}}$. Furthermore, with $f = \sum_{j=1}^{\infty} a_j \Psi_j$, $g = \sum_{j=1}^{\infty} b_j \Psi_j \in L^2(\mathcal{M})$,

$$\left\langle e^{it\sqrt{H}} f, e^{it\sqrt{H}} g \right\rangle = \sum_{j=1}^{\infty} e^{it\sqrt{\varepsilon_j}} a_j e^{-it\sqrt{\varepsilon_j}} \bar{b}_j = \sum_{j=1}^{\infty} a_j \bar{b}_j = \langle f, g \rangle, \quad (5.22)$$

and so $e^{it\sqrt{H}}$ is a unitary operator, with $e^{-it\sqrt{H}}$ being its adjoint as well as its inverse.

Lemma 5.3.2 (Egorov's Theorem). *Taking the case where \mathcal{M} is without boundary, let $A \in \Psi_{\text{phg}}^0(\mathcal{M})$ and let $\sigma_0(B)$ denote the zero-order principal symbol of any $B \in \Psi_{\text{phg}}^0(\mathcal{M})$. Then for every $t \in \mathbb{R}$,*

$$e^{it\sqrt{H}} A e^{-it\sqrt{H}} \in \Psi_{\text{phg}}^0(\mathcal{M}), \quad (5.23)$$

$$\sigma_0(e^{it\sqrt{H}} A e^{-it\sqrt{H}}) = \sigma_0(A) \circ \Phi^t. \quad (5.24)$$

On Egorov's Theorem, see for example [Far81], §4 of [Zel86], §1 of [Zel87], Lemma 5 in [ZZ96], or §2.2.5 in [Sch01]. For simplicity, here it is only stated for the case where \mathcal{M} is without boundary.

A statement of Egorov's theorem in the case where \mathcal{M} is with boundary can be found for example in Lemma 5 of [ZZ96]. In Lemma 5 of [ZZ96], further technicalities are involved, including such concerning the issue of "bad trajectories". When considering a time interval $(-T, T)$, the flow Φ^t is restricted to an open full-measure set $X_T \subset S^*\mathcal{M}$ (where an "open" set here can include boundary points on $S^*\mathcal{M}$) for which $\Phi^t(x, \xi)$ is well-defined for all $(x, \xi) \in X_T$, $t \in [-T, T]$. In accordance with this restriction of the flow to X_T , there is also a restriction on suitable Ψ DOs A .

Now note that the differential operator $-\Delta$, being a 2nd-order linear differential operator, is also then a 2nd-order polyhomogeneous Ψ DO, with principal symbol $(x, \xi) \in T^*\mathcal{M} \mapsto \|\xi\|^2$. Indeed, if we consider the representation of $-\Delta$ in local coordinates (see (2.3)), the sum of the leading-order terms is

$$\sum_{i=1}^n \sum_{j=1}^n g^{ij} D_{x_i} D_{x_j}, \quad (5.25)$$

where n is the dimension (so in our case $n = 2$), and again $D_{x_i} := -i \frac{\partial}{\partial x_i}$. Thus the principal symbol is

$$\sum_{i=1}^n \sum_{j=1}^n g^{ij} \xi_i \xi_j = \|\xi\|^2. \quad (5.26)$$

(Note that when taking principal symbol in local coordinates on a manifold, it is the *cotangent* bundle, not the tangent bundle, that we work with, see e.g. §I.4 of [Shu01]). Then applying Thm. 2.2.13 in [Sch01] (at least for the case where \mathcal{M} is without boundary), it holds that for every $m \in (0, \infty)$, the operator H^m is an order $2m$ polyhomogeneous Ψ DO with principal symbol $\|\xi\|^{2m}$. Thus in particular, \sqrt{H} has principal symbol $\|\xi\|$.

Given a real scalar function G on the cotangent bundle, one can consider the *Hamiltonian flow generated by G* , which in local coordinates is given by

$$\frac{dx_j}{dt} = \frac{\partial G}{\partial \xi_j}, \quad \frac{d\xi_j}{dt} = -\frac{\partial G}{\partial x_j}. \quad (5.27)$$

Lemma 5.3.3. *Given any C^∞ -smooth function $f : I \rightarrow \mathbb{R}$, where $I \subset (0, \infty)$ is an open interval (bounded or unbounded), the Hamiltonian flow Φ_f^t on $\{(x, \xi) \in T^*\mathcal{M} : \|\xi\| \in I\}$ generated by $f(\|\xi\|)$ satisfies the following:*

Each surface of constant $\|\xi\|$ is invariant under the flow Φ_f^t , possibly excluding points giving rise to bad trajectories. Furthermore, on each surface of constant $\|\xi\|$, say $\|\xi\| = \rho \in I$, let $\Phi_{f,\rho}^t$ be the restriction of Φ_f^t to this surface, and let $\Phi_{(\rho)}^t$ be the flow on this surface given by $\Phi_{(\rho)}^t := \iota_\rho \circ \Phi^t \circ \iota_{1/\rho}$, where $\iota_r(x, \xi) := (x, r\xi)$ and Φ^t is our usual flow on $S^\mathcal{M}$. We then have*

$$\Phi_{f,\rho}^t = \Phi_{(\rho)}^{f'(\rho)t}. \quad (5.28)$$

In other words, if $f'(\rho) \neq 0$ then the flow $\Phi_{f,\rho}^t$ consists of geodesic motion in position space with speed $|f'(\rho)|$, and with direction of motion being the direction of the covector if $f'(\rho) > 0$; opposite direction if $f'(\rho) < 0$. If $f'(\rho) = 0$ then the flow $\Phi_{f,\rho}^t$ is static.

If \mathcal{M} is with boundary, then define Φ_f^t in such a way that when a particle in the flow hits the boundary, the normal component of the covector to the boundary is reversed while the tangential component is unchanged. It then follows that as usual, we have specular reflection at the boundary, and (5.28) still holds.

This is proved by performing appropriate mathematical manipulations in local coordinates. This in particular would make use of the standard coordinate representations of vector and covector lengths and of geodesics, as well as making use of the coordinate representation of generated Hamiltonian flows, given by (5.27).

In particular then, the flow generated by $\|\xi\|^2$ is geodesic flow (with specular reflection at the boundary if there is one) with speed $2\|\xi\|$, and the flow generated by $\|\xi\|$ is geodesic

flow with speed 1. It is evident from e.g. §7.8 in [Tay96b] and §2.2.5 in [Sch01] that this is how the appearance of the flow Φ^t in (5.24) is connected with the appearance of the operator \sqrt{H} within the exponents in (5.24).

Now another concept in the study of quantum observables is *quantum variance*. Given some $A \in \Psi_{\text{phg}}^0(\mathcal{M})$, the quantum variance $V(A, E)$ for A relative to the basis $\{\Psi_j\}_{j \in \mathbb{N}}$ is given by the following:

$$V(A, E) := \frac{1}{\#\{j : \mathcal{E}_j \leq E\}} \sum_{j: \mathcal{E}_j \leq E} |\langle A\Psi_j, \Psi_j \rangle - \langle \sigma_0(A) \rangle|^2, \quad (5.29)$$

where $\langle \sigma_0(A) \rangle := \int_{S^*\mathcal{M}} \sigma_0(A) d\mu$.

With the local Weyl law being a law relating quantum averages with classical averages, there is also the following law relating quantum variance with a certain dynamical variance property in the classical system, derived via both the local Weyl law and Egorov's theorem (see §3 of [MR12]):

Lemma 5.3.4. *Given any $A \in \Psi_{\text{phg}}^0(\mathcal{M})$ with Schwartz kernel compactly supported in $\mathcal{M}^\circ \times \mathcal{M}^\circ$, letting a be the principal symbol,*

$$\limsup_{E \rightarrow \infty} V(A, E) \leq \int_{S^*\mathcal{M}} |a^T - \langle a \rangle|^2 d\mu \quad \forall T > 0. \quad (5.30)$$

Here a^T is again as defined in (5.4), only now for a being more generally a function on $S^*\mathcal{M}$ rather than just a function on \mathcal{M} , and so the appearance of “ π^* ” in (5.4) can now be removed.

Now a simple kind of example of $A \in \Psi_{\text{phg}}^0(\mathcal{M})$ with Schwartz kernel compactly supported in $\mathcal{M}^\circ \times \mathcal{M}^\circ$ is A being a multiplication operator by some $a \in C_0^\infty(\mathcal{M}^\circ)$, in which case $\sigma_0(A) = a$. It is easy to show that such a multiplication operator is indeed a bounded linear operator:

Lemma 5.3.5. *Given any $a \in L^\infty(\mathcal{M})$, letting \hat{a} be the multiplication operator by a , i.e. $(\hat{a}f)(x) = a(x)f(x)$, \hat{a} is then a bounded linear operator on $L^2(\mathcal{M})$ whose operator norm is $\|a\|_\infty$.*

Proof. Letting $\mu_{\mathcal{M}}$ be the standard area measure on \mathcal{M} , we have $\mu_{\mathcal{M}}(\text{Im}_{|a|}^{-1}(L, \infty)) = 0$ for $L \geq \|a\|_\infty$, where $\text{Im}_{|a|}^{-1}$ means inverse image under $|a|$, and $\mu_{\mathcal{M}}(\text{Im}_{|a|}^{-1}(L, \infty)) > 0$ for $L < \|a\|_\infty$. In particular then, $|a(x)| \leq \|a\|_\infty$ for almost all $x \in \mathcal{M}$. Given then any $f \in L^2(\mathcal{M})$, we have

$$\int_{\mathcal{M}} |a(x)f(x)|^2 dx \leq \|a\|_\infty^2 \int_{\mathcal{M}} |f(x)|^2 dx, \quad (5.31)$$

and so $\hat{a}f = af \in L^2(\mathcal{M})$, with

$$\|\hat{a}f\|_2^2 \leq \|a\|_\infty^2 \|f\|_2^2 \stackrel{\text{if } f \neq 0}{\implies} \frac{\|\hat{a}f\|_2}{\|f\|_2} \leq \|a\|_\infty. \quad (5.32)$$

Hence \hat{a} is a bounded operator on $L^2(\mathcal{M})$ with $\|\hat{a}\|_2 \leq \|a\|_\infty$ (where we allow $\|\cdot\|_2$ to denote operator norm under L^2 as well as L^2 -norm).

Next, to show that $\|\hat{a}\|_2 = \|a\|_\infty$, first note that this holds trivially when $a = 0$. So then for $a \neq 0$ (in which case $\|a\|_\infty > 0$), taking any $L \in (0, \|a\|_\infty)$, let $f_{a,L}$ be the characteristic function of $\text{Im}_{|a|}^{-1}(L, \infty)$ on \mathcal{M} , i.e.

$$f_{a,L}(x) := \chi_{\text{Im}_{|a|}^{-1}(L, \infty)} = \begin{cases} 1 & \text{for } |a(x)| > L, \\ 0 & \text{for } |a(x)| \leq L. \end{cases} \quad (5.33)$$

It thus follows that $f_{a,L} \in L^2(\mathcal{M})$ with

$$\|f_{a,L}\|_2^2 = \mu_{\mathcal{M}}(\text{Im}_{|a|}^{-1}(L, \infty)) > 0, \quad (5.34)$$

and furthermore,

$$\|\hat{a}f_{a,L}\|_2^2 = \int_{\mathcal{M}} |a(x)|^2 \chi_{\text{Im}_{|a|}^{-1}(L, \infty)}(x) dx > L^2 \mu_{\mathcal{M}}(\text{Im}_{|a|}^{-1}(L, \infty)) = L^2 \|f_{a,L}\|_2^2. \quad (5.35)$$

Hence

$$\frac{\|\hat{a}f_{a,L}\|_2}{\|f_{a,L}\|_2} > L \quad \forall L \in (0, \|a\|_\infty), \quad (5.36)$$

and so $\|\hat{a}\|_2 = \|a\|_\infty$. \square

Applying then Lemma 5.3.4 to multiplication operators, we have the following:

Corollary 5.3.6. *If the classical dynamical system satisfies (5.3) then*

$$\lim_{E \rightarrow \infty} V(\hat{a}, E) = \lim_{E \rightarrow \infty} \frac{1}{\#\{j : \mathcal{E}_j \leq E\}} \sum_{j: \mathcal{E}_j \leq E} \left| \int_{\mathcal{M}} a(x) |\Psi_j(x)|^2 dx - \langle a \rangle \right|^2 = 0 \quad (5.37)$$

$\forall a \in C_0^\infty(\mathcal{M}^\circ)$.

From this the following is then derived (see §3 of [MR12], aided with Thm. 1.20 in §1.7 of [Wal82] and §3 of [ZZ96]):

Lemma 5.3.7. *If the classical dynamical system satisfies (5.3) then the quantum eigenbasis $(\Psi_j)_{j \in \mathbb{N}}$, as a sequence, has a density-one subsequence $(\Psi_{j_n})_{n \in \mathbb{N}}$ for which*

$$\lim_{n \rightarrow \infty} \int_{\mathcal{M}} a(x) |\Psi_{j_n}(x)|^2 dx = \langle a \rangle \quad \forall a \in C_0^\infty(\mathcal{M}^\circ). \quad (5.38)$$

Note in particular that this is a common density-one subsequence for all $a \in C_0^\infty(\mathcal{M}^\circ)$, in other words $(j_n)_{n \in \mathbb{N}}$ is independent of a .

It can then be shown that with $(\Psi_{j_n})_{n \in \mathbb{N}}$ satisfying (5.38), it follows that $(\Psi_{j_n})_{n \in \mathbb{N}}$ equidistributes in position space, as defined in (5.1). Observe that (5.1) is effectively (5.38) but with $a \in C_0^\infty(\mathcal{M}^\circ)$ replaced with the characteristic function χ_A of a measurable set $A \subset \mathcal{M}$ with measure zero boundary.

5.4 Potential Methods of Approach for the Delta-Perturbed System

Again, we are interested in attempting to prove that if the classical dynamical system satisfies (5.3) then not only does the *unperturbed* quantum system have a full-density subsequence of eigenbasis functions that equidistributes in position space (already established), but so does the *delta-perturbed* quantum system. This has already been achieved for the specific case of the flat torus, but we now wish to consider methods of proving this to hold more generally.

5.4.1 Method 1: Computations using Formulae for Perturbed Eigenfunctions

If the classical system satisfies (5.3), then working with the starting point that for every $a \in C_0^\infty(\mathcal{M}^\circ)$ we have

$$\lim_{E \rightarrow \infty} \frac{1}{\#\{j : \mathcal{E}_j \leq E\}} \sum_{j: \mathcal{E}_j \leq E} \langle \hat{a} \Psi_j, \Psi_j \rangle = \langle a \rangle, \quad (5.39)$$

$$\lim_{E \rightarrow \infty} \frac{1}{\#\{j : \mathcal{E}_j \leq E\}} \sum_{j: \mathcal{E}_j \leq E} |\langle \hat{a} \Psi_j, \Psi_j \rangle - \langle a \rangle|^2 = 0, \quad (5.40)$$

we could then attempt to determine whether (5.39) and (5.40) still hold if the unperturbed eigenbasis $\{\Psi_j\}_{j \in \mathbb{N}}$ and corresponding eigenvalues $\{\mathcal{E}_j\}_{j \in \mathbb{N}}$ are replaced with an orthonormal eigenbasis and corresponding eigenvalues for the delta-perturbed system, given the formulae we have for perturbed eigenvalues and eigenfunctions in terms of unperturbed eigenvalues and eigenfunctions.

If employing this method, it would be useful to be able to represent bounded linear operators as $\mathbb{N} \times \mathbb{N}$ matrices. This is enabled by the following:

Lemma 5.4.1. *Given a bounded linear operator $A : L^2(\mathcal{M}) \rightarrow L^2(\mathcal{M})$ and function $f \in L^2(\mathcal{M})$, writing $f = \sum_{j=1}^{\infty} a_j \Psi_j$, it holds that*

$$Af = \sum_{n=1}^{\infty} \left(a_n \sum_{m=1}^{\infty} \langle A \Psi_n, \Psi_m \rangle \Psi_m \right) = \sum_{m=1}^{\infty} \left(\sum_{n=1}^{\infty} a_n \langle A \Psi_n, \Psi_m \rangle \right) \Psi_m. \quad (5.41)$$

In the middle part of this equation, both the m -sum and n -sum converge in L^2 , and in the right-most part of this equation, the n -sum converges in \mathbb{C} and the m -sum converges in L^2 .

Proof. Firstly, applying continuity of A followed by the orthonormal basis expansion formula,

$$\begin{aligned}
Af &= A \left(\lim_{N \rightarrow \infty} \sum_{n=1}^N a_n \Psi_n \right) = \lim_{N \rightarrow \infty} A \sum_{n=1}^N a_n \Psi_n = \lim_{N \rightarrow \infty} \sum_{n=1}^N a_n A \Psi_n \\
&= \lim_{N \rightarrow \infty} \sum_{n=1}^N \left(a_n \sum_{m=1}^{\infty} \langle A \Psi_n, \Psi_m \rangle \Psi_m \right) \\
&= \sum_{n=1}^{\infty} \left(a_n \sum_{m=1}^{\infty} \langle A \Psi_n, \Psi_m \rangle \Psi_m \right), \tag{5.42}
\end{aligned}$$

thus proving the middle part of (5.41).

Continuing on now,

$$\begin{aligned}
\lim_{N \rightarrow \infty} \sum_{n=1}^N \left(a_n \sum_{m=1}^{\infty} \langle A \Psi_n, \Psi_m \rangle \Psi_m \right) &= \lim_{N \rightarrow \infty} \sum_{m=1}^{\infty} \left(\sum_{n=1}^N a_n \langle A \Psi_n, \Psi_m \rangle \right) \Psi_m \\
&=: \sum_{m=1}^{\infty} c_m \Psi_m, \tag{5.43}
\end{aligned}$$

so

$$\begin{aligned}
&\lim_{N \rightarrow \infty} \sum_{m=1}^{\infty} \left(c_m - \sum_{n=1}^N a_n \langle A \Psi_n, \Psi_m \rangle \right) \Psi_m = 0 \\
&\Rightarrow \lim_{N \rightarrow \infty} \sum_{m=1}^{\infty} \left| c_m - \sum_{n=1}^N a_n \langle A \Psi_n, \Psi_m \rangle \right|^2 = 0 \\
&\Rightarrow \lim_{N \rightarrow \infty} \left| c_m - \sum_{n=1}^N a_n \langle A \Psi_n, \Psi_m \rangle \right|^2 = 0 \quad \forall m \in \mathbb{N}, \tag{5.44}
\end{aligned}$$

and thus

$$c_m = \lim_{N \rightarrow \infty} \sum_{n=1}^N a_n \langle A \Psi_n, \Psi_m \rangle = \sum_{n=1}^{\infty} a_n \langle A \Psi_n, \Psi_m \rangle \quad \forall m \in \mathbb{N}. \tag{5.45}$$

This proves the right-most part of (5.41). \square

It therefore follows that just as functions in $L^2(\mathcal{M})$ can be represented by l^2 column vectors through orthonormal basis expansion, a bounded linear operator $A : L^2(\mathcal{M}) \rightarrow L^2(\mathcal{M})$ can similarly be represented by an $\mathbb{N} \times \mathbb{N}$ matrix, with the $(m, n)^{\text{th}}$ element being

$$A_{mn} = \langle A \Psi_n, \Psi_m \rangle. \tag{5.46}$$

(Note of course that Lemma 5.4.1 works not only with the eigenbasis $\{\Psi_j\}_{j \in \mathbb{N}}$ but with any arbitrary orthonormal basis of $L^2(\mathcal{M})$).

When considering then, $\langle \hat{a}\phi, \phi \rangle$ for some eigenfunction ϕ of the perturbed operator H_Θ , one could derive an expression for $\langle \hat{a}\phi, \phi \rangle$ using this matrix representation of \hat{a} with respect to the unperturbed eigenbasis, combined with the expansion of ϕ into the unperturbed eigenbasis.

5.4.2 Method 2: Approximation by Non-Singular Perturbations

So far, we have stated Weyl's law (for Ψ DOs) and Egorov's theorem specifically in the context where the quantum Hamiltonian operator is a $-\Delta$ operator. However, these laws do have more general forms.

Thm. 2.2.18 in §2.2.4 of [Sch01] gives a statement of Weyl's law (referred to there as the Szegő limit theorem), in the case where \mathcal{M} is without boundary, for which the operator playing the role of the quantum Hamiltonian operator can be any self-adjoint polyhomogeneous Ψ DO of positive order with strictly positive principal symbol on $\{(x, \xi) \in T^*\mathcal{M} : \|\xi\| \neq 0\}$ (replacing the appearance of $S^*\mathcal{M}$ within the statement of Weyl's law with the set of all points in $\{(x, \xi) \in T^*\mathcal{M} : \|\xi\| \neq 0\}$ at which the principal symbol of the ‘‘Hamiltonian’’ operator is 1). Furthermore, in [ZZ96], although Weyl's law (Lemma 4) is stated for the self-adjoint $-\Delta$ operator, the proof largely references propositions/theorems in Ch. 29 of [Hör85b], and there again it deals with more general symmetric/self-adjoint Ψ DOs (still with certain conditions).

Similarly, Thm. 2.2.20 in §2.2.5 of [Sch01] gives a statement of Egorov's theorem in which the role of $e^{-it\sqrt{H}}$ in (5.23) and (5.24) here is taken by a general *Fourier integral operator* (FIO) (satisfying certain specified conditions), and the role of Φ^t is taken by the *canonical transformation generated by the FIO's phase function*. Further on in §2.2.5 of [Sch01], operators of the form $e^{-it\mathcal{H}}$, where \mathcal{H} is a first-order elliptic self-adjoint Ψ DO (elliptic meaning that the principal symbol is nonzero at all points in the cotangent bundle with a nonzero covector), are stated to be examples of FIOs, with the canonical transformation generated by the phase function being the Hamiltonian flow generated by the principal symbol of \mathcal{H} (self-adjointness results in the principal symbol being real). Thm. 8.1 in §8 of Ch. 7 in [Tay96b] also gives a statement of Egorov's theorem for which the role of \sqrt{H} in Lemma 5.3.2 here is taken by a more general 1st-order polyhomogeneous Ψ DO, and the flow involved is the Hamiltonian flow generated by the principal symbol. [Note though that §8 of Ch. 7 in [Tay96b] works on Euclidean space \mathbb{R}^n , and in §2.2.5 of [Sch01], some of the discussion is on \mathbb{R}^n and some of it is on a manifold].

In light of this, it seems likely then that if we perturb the operator $H = -\Delta \in \Psi_{\text{phg}}^2(\mathcal{M}^\circ)$ in such a way as to keep it being an appropriate Ψ DO with principal symbol $\|\xi\|^2$, and also if necessary, add a positive multiple of the identity map to keep the operator non-negative so that we can still take its square root (this certainly shouldn't cause a problem, since $-\Delta + cI$ is still a “well-behaved” second-order differential operator with principal symbol $\|\xi\|^2$), then Weyl's law and Egorov's theorem, as stated in Lemmas 5.3.1 and 5.3.2 here (or appropriate modification of Lemma 5.3.2 if \mathcal{M} is with boundary), would still apply.

In turn, it should follow that if the *unperturbed* classical system satisfies (5.3) then the quantum system should still satisfy (5.39) and (5.40) under this perturbation. Note that we could also then “undo” the addition of a multiple of the identity map, and (5.39) and (5.40) would be left unaffected, since the only effect would be a constant shift in the eigenvalues, and the corresponding eigenspaces would remain the same. Position space equidistribution of a full-density subsequence of eigenbasis functions would then follow. It would seem likely that all of this should still work even when \mathcal{M} is with boundary.

We could then consider approximating the delta potential by such perturbations. So then, whereas in Method 1, we consider deriving (5.39) and (5.40) for the delta potential only from the starting point that they hold for the unperturbed system, now we could consider deriving these for the delta potential with the aid of them holding not only for the unperturbed system but also for these perturbations (or we could consider directly deriving the position space equidistribution result, either in the form of Lemma 5.3.7 or (5.1), for the delta potential, given this holding for these perturbations).

Consideration of Rank-One Perturbations

Now in Chapter 4 is discussion on rank-one perturbations of H , and how these could be used to approximate the delta potential. These perturbed operators are specified to take the following form:

$$H' = H + \nu \langle \cdot, Y \rangle Y, \tag{5.47}$$

where $Y \in C_0^\infty(\mathcal{M}^\circ) \setminus \{0\}$ and $\nu \in \mathbb{R} \setminus \{0\}$.

Let us then address this question: If $Y, Z \in C_0^\infty(\mathcal{M}^\circ)$ then is the operator $W := \langle \cdot, Z \rangle Y$ a pseudodifferential operator, and if so, of what order is it?

Firstly, for every $\phi, \psi \in C_0^\infty(\mathcal{M}^\circ)$ we have

$$\begin{aligned}
\langle W\phi, \psi \rangle_u &= \langle \langle \phi, \bar{Z} \rangle_u Y, \psi \rangle_u = \langle \bar{Z}, \phi \rangle_u \langle Y, \psi \rangle_u \\
&= \left(\int_{\mathcal{M}} \overline{Z(y)} \phi(y) \, dy \right) \left(\int_{\mathcal{M}} Y(x) \psi(x) \, dx \right) \\
&= \int_{\mathcal{M}} \int_{\mathcal{M}} \overline{Z(y)} \phi(y) Y(x) \psi(x) \, dy \, dx \\
&= \langle (\pi_1^* Y)(\pi_2^* \bar{Z}), (\pi_2^* \phi)(\pi_1^* \psi) \rangle_u^{\mathcal{M} \times \mathcal{M}}. \tag{5.48}
\end{aligned}$$

Thus W (or at least W restricted to $C_0^\infty(\mathcal{M}^\circ)$), has Schwartz kernel $K_W \in C_0^\infty(\mathcal{M}^\circ \times \mathcal{M}^\circ)$ given by

$$K_W(x, y) = Y(x) \overline{Z(y)}. \tag{5.49}$$

Obviously the image of W is $\text{span}\{Y\} \subset C_0^\infty(\mathcal{M}^\circ)$ (or $\{0\}$ if $Z = 0$), and so K_W can be said to be the Schwartz kernel of $W : C_0^\infty(\mathcal{M}^\circ) \rightarrow C_0^\infty(\mathcal{M}^\circ)$. $W : L^2(\mathcal{M}) \rightarrow L^2(\mathcal{M})$ is then simply the continuous extension of $W : C_0^\infty(\mathcal{M}^\circ) \rightarrow C_0^\infty(\mathcal{M}^\circ)$ under the L^2 -norm.

Considering the case where $\mathcal{M} \subset \mathbb{R}^2$, according to Exercise 2.4 in §2 in Ch. I of [Shu01], a linear operator from $C_0^\infty(\mathcal{M}^\circ)$ to $C^\infty(\mathcal{M}^\circ)$ with C^∞ -smooth kernel on $\mathcal{M}^\circ \times \mathcal{M}^\circ$ is a Ψ DO of order $-\infty$ under the Ψ DO theory constructed in that chapter of [Shu01], which therefore makes this so of W .

Furthermore, if we extend functions on \mathcal{M} to functions on \mathbb{R}^2 by having these extensions be zero everywhere outside \mathcal{M} (in which case functions in $C_0^\infty(\mathcal{M}^\circ)$ obviously become functions in $C_0^\infty(\mathbb{R}^2)$), then considering the extension of W to Schwartz space $\mathcal{S}(\mathbb{R}^2)$, still given by $W = \langle \cdot, Z \rangle Y$ (only this time $\langle \cdot, \cdot \rangle$ is the L^2 inner product on \mathbb{R}^2), we have

$$\begin{aligned}
Wu(x) &= Y(x) \int_{\mathbb{R}^2} u(y) \overline{Z(y)} \, dy = \frac{1}{4\pi^2} Y(x) \int_{\mathbb{R}^2} \widehat{u}(\xi) \overline{\widehat{Z}(\xi)} \, d\xi \\
&= \frac{1}{4\pi^2} \int_{\mathbb{R}^2} \left(Y(x) \overline{\widehat{Z}(\xi)} e^{-ix \cdot \xi} \right) \widehat{u}(\xi) e^{ix \cdot \xi} \, d\xi \quad \forall x \in \mathbb{R}^2 \quad \forall u \in \mathcal{S}(\mathbb{R}^2) \tag{5.50}
\end{aligned}$$

(see Parseval's formula in e.g. Thm. 1.8 in §1.2 of [Sai91] for justification of $\int u \bar{Z} = \frac{1}{4\pi^2} \int \widehat{u} \overline{\widehat{Z}}$, and note that $\widehat{Z} \in \mathcal{S}(\mathbb{R}^2)$). Let then

$$w(x, \xi) := Y(x) \overline{\widehat{Z}(\xi)} e^{-ix \cdot \xi} \quad \forall (x, \xi) \in \mathbb{R}^2 \times \mathbb{R}^2. \tag{5.51}$$

Given any expression $\tilde{w}(x, \xi)$ of the form

$$\tilde{w}(x, \xi) = \sum_{k=1}^M b_k x^{\gamma_k} \xi^{\eta_k} \partial_x^{\rho_k} Y(x) \overline{\partial_\xi^{\sigma_k} \widehat{Z}(\xi)} e^{-ix \cdot \xi} \quad \forall (x, \xi) \in \mathbb{R}^2 \times \mathbb{R}^2, \tag{5.52}$$

where $b_k \in \mathbb{C}$ and $\gamma_k, \eta_k, \rho_k, \sigma_k \in (\{0\} \cup \mathbb{N})^2$ are multi-indices, it is easy to check that for $j \in \{1, 2\}$, $\partial_{x_j} \tilde{w}(x, \xi)$ maintains the same form, as does $\partial_{\xi_j} \tilde{w}(x, \xi)$. Since $w(x, \xi)$ itself

takes this form (with $M = 1$, $b_k = 1$ and $\gamma_k = \eta_k = \rho_k = \sigma_k = (0, 0)$), it follows by induction then that $\partial_x^\alpha \partial_\xi^\beta w(x, \xi)$ takes this form for all multi-indices $\alpha, \beta \in (\{0\} \cup \mathbb{N})^2$. Now for each $l \in \{0\} \cup \mathbb{N}$,

$$\begin{aligned} (1 + \|\xi\|^2)^l |\tilde{w}(x, \xi)| &\leq \sum_{k=1}^M \left| b_k x^{\gamma_k} (1 + \|\xi\|^2)^l \xi^{\eta_k} \partial_x^{\rho_k} Y(x) \partial_\xi^{\sigma_k} \overline{\widehat{Z}(\xi)} \right| \\ &\leq \sum_{k=1}^M |b_k| \|s^{\gamma_k} \partial_s^{\rho_k} Y(s)\|_\infty \|(1 + \|\zeta\|^2)^l \zeta^{\eta_k} \partial_\zeta^{\sigma_k} \widehat{Z}(\zeta)\|_\infty =: \tilde{C}_l < \infty \\ &\quad \forall (x, \xi) \in \mathbb{R}^2 \times \mathbb{R}^2. \end{aligned} \tag{5.53}$$

So then, given any $m \in \mathbb{R}$ and $\alpha, \beta \in (\{0\} \cup \mathbb{N})^2$, since $\partial_x^\alpha \partial_\xi^\beta w(x, \xi)$ takes the form given in (5.52), taking any $l \in \{0\} \cup \mathbb{N}$ for which $-l \leq \frac{m - |\beta|}{2}$, we have

$$|\partial_x^\alpha \partial_\xi^\beta w(x, \xi)| \leq \tilde{C}_l^{(\alpha, \beta)} (1 + \|\xi\|^2)^{-l} \leq \tilde{C}_l^{(\alpha, \beta)} (1 + \|\xi\|^2)^{(m - |\beta|)/2} \quad \forall (x, \xi) \in \mathbb{R}^2 \times \mathbb{R}^2. \tag{5.54}$$

Thus comparing (5.50) and (5.54) with (5.8) and (5.9), it follows that $W : \mathcal{S}(\mathbb{R}^2) \rightarrow \mathcal{S}(\mathbb{R}^2)$ is a Ψ DO of order $-\infty$ under the construction given in §5.2.1.

5.4.3 Method 3: Theory Permitting Singular Behaviour

Whereas with Methods 1 and 2, the approach is to start with the principles relating quantum and classical behaviour for only non-singular systems, and then by employing other techniques, derive desired results for the case of the delta-perturbed system, another approach is to develop or work with a theory for the relationship between quantum and classical behaviour which, at a more fundamental level, accommodates certain permissible singular behaviour.

In [JSSV15], compact manifolds with a metric that is discontinuous on a co-dimension 1 hypersurface are studied. In this case, there is not a straight-forward classical flow, because a trajectory that strikes the wall of discontinuous metric could result in both a reflected and a refracted trajectory. Nevertheless, a dynamical system is developed to describe the classical behaviour, together with a notion of ergodicity, and a quantum ergodicity theorem is proved.

One could then consider adapting the arguments in [JSSV15] to the case of the delta potential, where the singular behaviour is only at a point.

Appendix A

Further Material on Rank-One Perturbations

A.1 Construction of Resolvents

In §4.3.1 an orthonormal eigenbasis was constructed for the operator

$$H' := H + \nu \langle \cdot, Y \rangle Y, \quad (\text{A.1})$$

along with the corresponding eigenvalues. Here $Y \in L^2(\mathcal{M}) \setminus \{0\}$, $\nu \in \mathbb{R} \setminus \{0\}$ and H is the self-adjoint $-\Delta$ operator on \mathcal{M} , with Dirichlet boundary conditions if there is a boundary.

By Prop. 4.2.4, the spectrum of H' (denoted $\text{Spec}(H')$) is purely the set of eigenvalues of H' . Since the full set of eigenvalues of H' has been derived, it follows that associated with every complex value E outside this set of eigenvalues, there is a well-defined resolvent operator $(E - H')^{-1}$. Here we shall further demonstrate this to be true, by deriving explicit formulae for the resolvent operators of H' .

Wishing therefore to obtain the resolvent operator $(E - H')^{-1}$ for every $E \in \mathbb{C} \setminus \text{Spec}(H')$, we shall split the situation into two cases:

- (i) $E \in \mathbb{C} \setminus (\text{Spec}(H') \cup \text{Spec}(H))$,
- (ii) $E \in \text{Spec}(H) \setminus \text{Spec}(H')$, which is the case if and only if E is a *simple* eigenvalue of H (i.e. the eigenspace is 1-dimensional) with $\mathcal{P}_{\{E\}}^{(H)} Y \neq 0$.

Before dealing with these two cases separately, first we shall state that for any $E \in \mathbb{C}$,

$\psi = \sum_{j=1}^{\infty} a_j \Psi_j \in \text{Dom}(H) = \text{Dom}(H')$ and $\phi = \sum_{j=1}^{\infty} b_j \Psi_j \in L^2(\mathcal{M})$, we have

$$\begin{aligned} (E - H')\psi = \phi & \quad \text{iff} \quad (E - H)\psi = \nu \langle \psi, Y \rangle Y + \phi \\ & \quad \text{iff} \quad (E - \mathcal{E}_j)a_j = \nu \langle \psi, Y \rangle y_j + b_j \quad \forall j \in \mathbb{N}. \end{aligned} \quad (\text{A.2})$$

Now tackling case (i), note firstly that since $E \notin \text{Spec}(H)$, $(E - H)^{-1} : L^2(\mathcal{M}) \rightarrow \text{Dom}(H)$ is a well-defined bounded operator. The adjoint of $(E - H)^{-1}$ is $(\bar{E} - H)^{-1}$, since given any $f, g \in L^2(\mathcal{M})$ we have

$$\begin{aligned} \langle (E - H)^{-1}f, g \rangle &= \langle (E - H)^{-1}f, (\bar{E} - H)(\bar{E} - H)^{-1}g \rangle \\ &= \langle (E - H)^{-1}f, \bar{E}(\bar{E} - H)^{-1}g \rangle - \langle (E - H)^{-1}f, H(\bar{E} - H)^{-1}g \rangle \\ &= \langle E(E - H)^{-1}f, (\bar{E} - H)^{-1}g \rangle - \langle H(E - H)^{-1}f, (\bar{E} - H)^{-1}g \rangle \\ &= \langle (E - H)(E - H)^{-1}f, (\bar{E} - H)^{-1}g \rangle = \langle f, (\bar{E} - H)^{-1}g \rangle. \end{aligned} \quad (\text{A.3})$$

Furthermore, since $E \notin \text{Spec}(H')$, letting $\psi_E := (E - H)^{-1}Y$, it must hold that $\langle \psi_E, Y \rangle \neq \frac{1}{\nu}$, so far at least in the case where $E \in \mathbb{R}$. For general $E \in \mathbb{C} \setminus \text{Spec}(H)$, we have

$$\begin{aligned} \langle \psi_E, Y \rangle &= \sum_{j=1}^{\infty} \frac{|y_j|^2}{E - \mathcal{E}_j} = \sum_{j=1}^{\infty} \frac{|y_j|^2(\bar{E} - \mathcal{E}_j)}{|E - \mathcal{E}_j|^2} \\ &= \sum_{j=1}^{\infty} \frac{|y_j|^2(\text{Re}(E) - \mathcal{E}_j)}{|E - \mathcal{E}_j|^2} - i\text{Im}(E) \sum_{j=1}^{\infty} \frac{|y_j|^2}{|E - \mathcal{E}_j|^2}, \end{aligned} \quad (\text{A.4})$$

and so if $E \in \mathbb{C} \setminus \mathbb{R}$ then $\langle \psi_E, Y \rangle \in \mathbb{C} \setminus \mathbb{R} \not\cong \frac{1}{\nu}$.

So then, given some $\psi \in \text{Dom}(H)$ and $\phi \in L^2(\mathcal{M})$, suppose $(E - H')\psi = \phi$. For shorthand notation, let $\phi_E := (E - H)^{-1}\phi$. Then

$$\begin{aligned} \psi = \nu \langle \psi, Y \rangle \psi_E + \phi_E & \Rightarrow \langle \psi, Y \rangle = \nu \langle \psi, Y \rangle \langle \psi_E, Y \rangle + \langle \phi_E, Y \rangle \\ \Rightarrow \langle \psi, Y \rangle (1 - \nu \langle \psi_E, Y \rangle) &= \langle \phi_E, Y \rangle \Rightarrow \langle \psi, Y \rangle = \left\langle \frac{\phi_E}{1 - \nu \langle \psi_E, Y \rangle}, Y \right\rangle \\ & \Rightarrow \psi = \frac{\phi_E}{1 - \nu \langle \psi_E, Y \rangle} + \psi_{\perp}, \end{aligned} \quad (\text{A.5})$$

where $\langle \psi_{\perp}, Y \rangle = 0$. So then

$$\begin{aligned} (E - H)\psi &= \frac{\phi}{1 - \nu \langle \psi_E, Y \rangle} + (E - H)\psi_{\perp} = \nu \langle \psi, Y \rangle Y + \phi = \nu \frac{\langle \phi_E, Y \rangle}{1 - \nu \langle \psi_E, Y \rangle} Y + \phi \\ & \Rightarrow (E - H)\psi_{\perp} = \frac{\nu \langle \phi_E, Y \rangle}{1 - \nu \langle \psi_E, Y \rangle} Y + \left(1 - \frac{1}{1 - \nu \langle \psi_E, Y \rangle}\right) \phi \\ & \Rightarrow \psi_{\perp} = \frac{\nu \langle \phi_E, Y \rangle}{1 - \nu \langle \psi_E, Y \rangle} \psi_E - \frac{\nu \langle \psi_E, Y \rangle}{1 - \nu \langle \psi_E, Y \rangle} \phi_E \\ \Rightarrow \psi &= \phi_E + \frac{1}{\frac{1}{\nu} - \langle \psi_E, Y \rangle} \langle \phi_E, Y \rangle \psi_E = (E - H)^{-1}\phi + \frac{1}{\frac{1}{\nu} - \langle \psi_E, Y \rangle} \langle \phi, \psi_{\bar{E}} \rangle \psi_E. \end{aligned} \quad (\text{A.6})$$

Conversely, given some $\phi \in L^2(\mathcal{M})$, let

$$\psi = (E - H)^{-1}\phi + \frac{1}{\frac{1}{\nu} - \langle \psi_E, Y \rangle} \langle \phi, \psi_{\bar{E}} \rangle \psi_E, \quad (\text{A.7})$$

in which case $\psi \in \text{Dom}(H)$. Then

$$(E - H)\psi = \phi + \frac{1}{\frac{1}{\nu} - \langle \psi_E, Y \rangle} \langle \phi, \psi_{\bar{E}} \rangle Y, \quad (\text{A.8})$$

$$\begin{aligned} \nu \langle \psi, Y \rangle Y + \phi &= \nu \left(\langle \phi_E, Y \rangle + \frac{1}{\frac{1}{\nu} - \langle \psi_E, Y \rangle} \langle \phi, \psi_{\bar{E}} \rangle \langle \psi_E, Y \rangle \right) Y + \phi \\ &= \nu \left(\langle \phi, \psi_{\bar{E}} \rangle + \frac{1}{\frac{1}{\nu} - \langle \psi_E, Y \rangle} \langle \phi, \psi_{\bar{E}} \rangle \langle \psi_E, Y \rangle \right) Y + \phi \\ &= \nu \left(1 + \frac{\langle \psi_E, Y \rangle}{\frac{1}{\nu} - \langle \psi_E, Y \rangle} \right) \langle \phi, \psi_{\bar{E}} \rangle Y + \phi = \frac{1}{\frac{1}{\nu} - \langle \psi_E, Y \rangle} \langle \phi, \psi_{\bar{E}} \rangle Y + \phi, \end{aligned} \quad (\text{A.9})$$

so the equation $(E - H)\psi = \nu \langle \psi, Y \rangle Y + \phi$ is satisfied, and thus $(E - H')\psi = \phi$.

It is thus concluded that for each $E \in \mathbb{C} \setminus (\text{Spec}(H') \cup \text{Spec}(H))$,

$$(E - H')^{-1} = (E - H)^{-1} + \frac{1}{\frac{1}{\nu} - \langle \psi_E, Y \rangle} \langle \cdot, \psi_{\bar{E}} \rangle \psi_E. \quad (\text{A.10})$$

This formula for the resolvent operator $(E - H')^{-1}$ agrees with Theorem 1.1.1 in [AK00] for $E \in \mathbb{C} \setminus \mathbb{R}$.

Moving on to case (ii), although $(E - H)^{-1}$ is this time not a well-defined operator, we can nevertheless define the following operator:

$$(E - H)^{\widetilde{-1}} := \mathcal{P}_{\mathbb{R} \setminus \{E\}}^{(H)} \circ (E - H)^{-1} \circ \mathcal{P}_{\mathbb{R} \setminus \{E\}}^{(H)} : L^2(\mathcal{M}) \rightarrow \text{Dom}(H). \quad (\text{A.11})$$

This is a well-defined bounded linear operator – well-defined in that $\forall f \in L^2(\mathcal{M}) \exists g \in \text{Dom}(H)$ s.t. $(E - H)g = \mathcal{P}_{\mathbb{R} \setminus \{E\}}^{(H)} f$, and furthermore $\forall g, h \in \text{Dom}(H)$ satisfying $(E - H)g = (E - H)h = \mathcal{P}_{\mathbb{R} \setminus \{E\}}^{(H)} f$ it holds that $\mathcal{P}_{\mathbb{R} \setminus \{E\}}^{(H)} g = \mathcal{P}_{\mathbb{R} \setminus \{E\}}^{(H)} h =: (E - H)^{\widetilde{-1}} f$. Letting $E = \mathcal{E}_k$, for any $f = \sum_{j=1}^{\infty} c_j \Psi_j \in L^2(\mathcal{M})$,

$$(E - H)^{\widetilde{-1}} f = \sum_{j:j \neq k} \frac{c_j}{E - \mathcal{E}_j} \Psi_j. \quad (\text{A.12})$$

Observe furthermore that

$$(E - H)^{\widetilde{-1}} f = \sum_{j:j \neq k} \frac{c_j}{E - \mathcal{E}_j} \Psi_j \Rightarrow (E - H)(E - H)^{\widetilde{-1}} f = \sum_{j:j \neq k} c_j \Psi_j = \mathcal{P}_{\mathbb{R} \setminus \{E\}}^{(H)} f. \quad (\text{A.13})$$

Likewise with $g = \sum_{j=1}^{\infty} d_j \Psi_j \in \text{Dom}(H)$,

$$(E - H)g = \sum_{j=1}^{\infty} (E - \mathcal{E}_j) d_j \Psi_j \Rightarrow (E - H)^{\widetilde{-1}}(E - H)g = \sum_{j:j \neq k} d_j \Psi_j = \mathcal{P}_{\mathbb{R} \setminus \{E\}}^{(H)} g. \quad (\text{A.14})$$

Finally, $(E - H)^{-1}$ is self-adjoint, since for any $f = \sum_{j=1}^{\infty} c_j \Psi_j, g = \sum_{j=1}^{\infty} d_j \Psi_j \in L^2(\mathcal{M})$,

$$\left\langle (E - H)^{-1} f, g \right\rangle = \sum_{j:j \neq k} \frac{c_j \bar{d}_j}{E - \mathcal{E}_j} = \left\langle f, (E - H)^{-1} g \right\rangle. \quad (\text{A.15})$$

So now, given some $\psi = \sum_{j=1}^{\infty} a_j \Psi_j \in \text{Dom}(H)$ and $\phi = \sum_{j=1}^{\infty} b_j \Psi_j \in L^2(\mathcal{M})$, suppose $(E - H)\psi = \phi$. Then by (A.2),

$$\begin{aligned} \begin{cases} a_j = \frac{\nu \langle \psi, Y \rangle y_j + b_j}{E - \mathcal{E}_j} & \text{for } j \neq k \\ \nu \langle \psi, Y \rangle y_k + b_k = 0 \end{cases} & \Rightarrow \begin{cases} a_j = \frac{-\frac{b_k}{y_k} y_j + b_j}{E - \mathcal{E}_j} & \text{for } j \neq k \\ \langle \psi, Y \rangle = \sum_{l=1}^{\infty} a_l \bar{y}_l = -\frac{b_k}{\nu y_k} \end{cases} \\ & \Rightarrow \begin{cases} a_j = \frac{-\frac{b_k}{y_k} y_j + b_j}{E - \mathcal{E}_j} & \text{for } j \neq k \\ a_k = -\frac{b_k}{\nu |y_k|^2} - \frac{1}{y_k} \sum_{l:l \neq k} a_l \bar{y}_l. \end{cases} \end{aligned} \quad (\text{A.16})$$

Thus, letting $\psi_E := (E - H)^{-1} Y$, we have

$$\mathcal{P}_{\mathbb{R} \setminus \{E\}}^{(H)} \psi = -\frac{1}{y_k} \langle \phi, \Psi_k \rangle \psi_E + (E - H)^{-1} \phi, \quad (\text{A.17})$$

$$\begin{aligned} \mathcal{P}_{\{E\}}^{(H)} \psi &= \left(-\frac{1}{\nu |y_k|^2} \langle \phi, \Psi_k \rangle - \frac{1}{y_k} \left\langle \mathcal{P}_{\mathbb{R} \setminus \{E\}}^{(H)} \psi, Y \right\rangle \right) \Psi_k \\ &= \left(-\frac{1}{\nu |y_k|^2} \langle \phi, \Psi_k \rangle + \frac{1}{|y_k|^2} \langle \phi, \Psi_k \rangle \langle \psi_E, Y \rangle - \frac{1}{y_k} \langle \phi, \psi_E \rangle \right) \Psi_k \\ &= \left\langle \phi, \frac{\langle \psi_E, Y \rangle - \frac{1}{\nu}}{|y_k|^2} \Psi_k - \frac{1}{y_k} \psi_E \right\rangle \Psi_k. \end{aligned} \quad (\text{A.18})$$

Hence

$$\psi = (E - H)^{-1} \phi - \frac{1}{y_k} \langle \phi, \Psi_k \rangle \psi_E + \left\langle \phi, -\frac{1}{y_k} \psi_E + \frac{\langle \psi_E, Y \rangle - \frac{1}{\nu}}{|y_k|^2} \Psi_k \right\rangle \Psi_k. \quad (\text{A.19})$$

Conversely, given some $\phi \in L^2(\mathcal{M})$, let ψ be defined as given by (A.19), in which case $\psi \in \text{Dom}(H)$. Then

$$(E - H)\psi = \mathcal{P}_{\mathbb{R} \setminus \{E\}}^{(H)} \phi - \frac{1}{y_k} \langle \phi, \Psi_k \rangle \mathcal{P}_{\mathbb{R} \setminus \{E\}}^{(H)} Y, \quad (\text{A.20})$$

$$\begin{aligned} & \nu \langle \psi, Y \rangle Y + \phi \\ &= \nu \left(\langle \phi, \psi_E \rangle - \frac{1}{y_k} \langle \phi, \Psi_k \rangle \langle \psi_E, Y \rangle - \langle \phi, \psi_E \rangle + \frac{\langle \psi_E, Y \rangle - \frac{1}{\nu}}{y_k} \langle \phi, \Psi_k \rangle \right) Y + \phi \\ &= -\frac{1}{y_k} \langle \phi, \Psi_k \rangle Y + \phi = -\frac{1}{y_k} \langle \phi, \Psi_k \rangle \mathcal{P}_{\mathbb{R} \setminus \{E\}}^{(H)} Y + \mathcal{P}_{\mathbb{R} \setminus \{E\}}^{(H)} \phi - \frac{1}{y_k} \langle \phi, \Psi_k \rangle y_k \Psi_k + \langle \phi, \Psi_k \rangle \Psi_k \\ &= -\frac{1}{y_k} \langle \phi, \Psi_k \rangle \mathcal{P}_{\mathbb{R} \setminus \{E\}}^{(H)} Y + \mathcal{P}_{\mathbb{R} \setminus \{E\}}^{(H)} \phi, \end{aligned} \quad (\text{A.21})$$

so again the equation $(E - H)\psi = \nu \langle \psi, Y \rangle Y + \phi$ is satisfied, and thus $(E - H')\psi = \phi$.

It is thus concluded that for each $E \in \text{Spec}(H) \setminus \text{Spec}(H')$, writing $E = \mathcal{E}_k$, noting that E is a simple eigenvalue of H and that $y_k \neq 0$, we have

$$(E - H')^{-1} = (E - H)^{-1} - \frac{1}{y_k} \langle \cdot, \Psi_k \rangle \psi_E + \left\langle \cdot, -\frac{1}{y_k} \psi_E + \frac{\langle \psi_E, Y \rangle - \frac{1}{\nu} \Psi_k}{|y_k|^2} \Psi_k \right\rangle \Psi_k. \quad (\text{A.22})$$

In conclusion, we have now obtained explicit formulae for all resolvents $\{(E - H')^{-1} : E \in \mathbb{C} \setminus \text{Spec}(H')\}$ of H' .

A.2 Further Observation of the Analogy between the Delta Potential and Rank-One Perturbations

In §4.3.1 a construction is given for the eigenvalues and eigenfunctions of a rank-one perturbation of H . In §4.3.2 the construction for the eigenvalues and eigenfunctions of the delta-perturbed operator, originally stated in §2.2.5, is restated so as to enable comparison with the rank-one perturbation. On the basis of the similarities in these constructions, further observations can be drawn on the analogous features between the rank-one perturbations and the delta perturbations.

Observe that for fixed $Y \in L^2(\mathcal{M}) \setminus \{0\}$, the family of operators $\{H + \nu \langle \cdot, Y \rangle Y : \nu \in \mathbb{R} \setminus \{0\}\}$ can be constructed as follows:

Partition $\mathbb{R} \setminus \{\mathcal{E} \in \text{Spec}(H) : \mathcal{P}_{\{\mathcal{E}\}}^{(H)} Y \neq 0\}$ into equivalence classes, defined by the equivalence relation \sim_Y , where $\lambda \sim_Y \mu$ if and only if

$$\lim_{L \rightarrow \infty} \left(\left\langle \mathcal{P}_{(-\infty, L] \setminus \{\lambda\}}^{(H)} (\lambda - H)^{-1} Y, Y \right\rangle - \left\langle \mathcal{P}_{(-\infty, L] \setminus \{\mu\}}^{(H)} (\mu - H)^{-1} Y, Y \right\rangle \right) = 0. \quad (\text{A.23})$$

This is a particular way of formulating the equation $\text{LHS}(4.83)_{E=\lambda} = \text{LHS}(4.83)_{E=\mu}$ which will be useful here when comparing with the delta potential. For all but one of these equivalence classes (or all if Y coincides with an eigenfunction of H) there is a corresponding self-adjoint operator satisfying the following:

- (a) Performing steps (i) and (ii) of the earlier described construction of the orthonormal eigenbasis of H' , each function remaining after step (ii) is an eigenfunction of this self-adjoint operator, with the same corresponding eigenvalue as for H .
- (b) For each value E in the specified equivalence class under \sim_Y , $\mathcal{P}_{\mathbb{R} \setminus \{E\}}^{(H)} (E - H)^{-1} Y$ is an eigenfunction of this self-adjoint operator with corresponding eigenvalue E .
- (c) The eigenfunctions stated in point (a) here, together with the normalisation of those stated in (b), form an orthonormal basis of the Hilbert space $L^2(\mathcal{M})$.

This eigenbasis of the self-adjoint operator is countable, and can be arranged into a sequence for which the corresponding eigenvalue is non-decreasing and tending to infinity. Lemma 2.1.1 then applies to this self-adjoint operator with its eigenbasis and corresponding eigenvalues, just as it applies to the unperturbed operator H , and thus (a), (b) and (c) above are sufficient to determine fully this self-adjoint operator.

Note that this construction fails for the equivalence class corresponding to $\text{LHS}(4.83)=0$ (i.e. $\nu = \pm\infty$), because all eigenfunctions produced under this construction would in this case be orthogonal to Y , and thus could not form an orthonormal basis of the Hilbert space. If however, Y coincides with an eigenfunction of H , the equation $\text{LHS}(4.83)=0$ will then have no solution.

We now have a family of self-adjoint operators associated with the family of equivalence classes under \sim_Y . This family of self-adjoint operators is the family $\{H + \nu \langle \cdot, Y \rangle Y : \nu \in \mathbb{R} \setminus \{0\}\}$.

The family of operators $\{H_\Theta : \Theta \in (0, 2\pi)\}$ corresponding to the delta potential can then be constructed with precisely the same construction, replacing Y with δ_p (where $\langle f, \delta_p \rangle := f(p) \forall f \in C(\mathcal{M}^\circ)$), and noting that just as we have:

$$\left\langle f, \mathcal{P}_{\{\mathcal{E}\}}^{(H)} Y \right\rangle = \left\langle \mathcal{P}_{\{\mathcal{E}\}}^{(H)} f, Y \right\rangle \quad \forall f \in L^2(\mathcal{M}) \quad \forall \mathcal{E} \in \text{Spec}(H), \quad (\text{A.24})$$

$$\begin{aligned} \left\langle f, \mathcal{P}_{S \setminus \{E\}}^{(H)} (E - H)^{-1} Y \right\rangle &= \left\langle \mathcal{P}_{S \setminus \{E\}}^{(H)} (E - H)^{-1} \mathcal{P}_{\mathbb{R} \setminus \{E\}}^{(H)} f, Y \right\rangle \\ \forall f \in L^2(\mathcal{M}) \quad \forall E \in \mathbb{R} \setminus \{E \in \text{Spec}(H) : \mathcal{P}_{\{E\}}^{(H)} Y \neq 0\} \quad \forall S \subset \mathbb{R}, \end{aligned} \quad (\text{A.25})$$

$\mathcal{P}_{\{\mathcal{E}\}}^{(H)} \delta_p, \mathcal{P}_{S \setminus \{E\}}^{(H)} (E - H)^{-1} \delta_p \in L^2(\mathcal{M})$ can be defined through the following equations:

$$\left\langle f, \mathcal{P}_{\{\mathcal{E}\}}^{(H)} \delta_p \right\rangle = \left\langle \mathcal{P}_{\{\mathcal{E}\}}^{(H)} f, \delta_p \right\rangle \quad \forall f \in L^2(\mathcal{M}) \quad \forall \mathcal{E} \in \text{Spec}(H), \quad (\text{A.26})$$

$$\begin{aligned} \left\langle f, \mathcal{P}_{S \setminus \{E\}}^{(H)} (E - H)^{-1} \delta_p \right\rangle &= \left\langle \mathcal{P}_{S \setminus \{E\}}^{(H)} (E - H)^{-1} \mathcal{P}_{\mathbb{R} \setminus \{E\}}^{(H)} f, \delta_p \right\rangle \\ \forall f \in L^2(\mathcal{M}) \quad \forall E \in \mathbb{R} \setminus \{E \in \text{Spec}(H) : \mathcal{P}_{\{E\}}^{(H)} \delta_p \neq 0\} \quad \forall S \subset \mathbb{R}. \end{aligned} \quad (\text{A.27})$$

All equivalence classes in the partition of $\mathbb{R} \setminus \{E \in \text{Spec}(H) : \mathcal{P}_{\{E\}}^{(H)} \delta_p \neq 0\}$ under \sim_δ give a well-defined self-adjoint operator under this construction. The relation \sim_δ here is defined by (A.23) but replacing Y with δ_p - now a reformulation of $\text{LHS}(4.95)_{E=\lambda} = \text{LHS}(4.95)_{E=\mu}$, making use also of (4.101).

A significant difference now between the rank-one perturbations and the delta potential operators is as follows:

For each $\nu \in \mathbb{R} \setminus \{0\}$, define

$$X_\nu := \left\{ E \in \mathbb{R} : \mathcal{P}_{\{E\}}^{(H)} Y = 0, \left\langle \mathcal{P}_{\mathbb{R} \setminus \{E\}}^{(H)} (E - H)^{-1} Y, Y \right\rangle = \frac{1}{\nu} \right\}. \quad (\text{A.28})$$

Likewise define $X_{\pm\infty}$ similarly to X_ν but replacing $\frac{1}{\nu}$ with 0. The family $\{X_\nu : \nu \in (\mathbb{R} \setminus \{0\}) \cup \{\pm\infty\}\}$ is then the family of equivalence classes under \sim_Y , with a corresponding self-adjoint operator being well-defined for each X_ν with ν finite. On the other hand, with the delta potential we have

$$\left\langle \mathcal{P}_{(-\infty, L] \setminus \{E\}}^{(H)} (E - H)^{-1} \delta_p, \delta_p \right\rangle \xrightarrow{L \rightarrow \infty} -\infty \quad (\text{A.29})$$

$\forall E \in \mathbb{R} \setminus \{\mathcal{E} \in \text{Spec}(H) : \mathcal{P}_{\{\mathcal{E}\}}^{(H)} \delta_p \neq 0\}$. This further hints at the claim (along with discussion in §2.2.4) that the 2D delta potential, as constructed by means of the self-adjoint extension theory, is intuitively speaking a negative “delta” potential of infinitesimal strength.

Bibliography

- [AGHHE88] S. Albeverio, F. Gesztesy, R. Høegh-Krohn, H. Holden and P. Exner (Appendix): *Solvable Models in Quantum Mechanics* (Second Edition). American Mathematical Society (1988).
- [AK00] S. Albeverio and P. Kurasov: *Singular Perturbations of Differential Operators*. London Math. Soc. Lecture Note Ser. **271**. Cambridge University Press (2000).
- [AKKN07] V. I. Arnold, E. Khukhro, V. V. Kozlov and A. I. Neishtadt: *Mathematical Aspects of Classical and Celestial Mechanics*. Springer (2007).
- [AKN09] N. Anantharaman, H. Koch and S. Nonnenmacher: *Entropy of Eigenfunctions*. New Trends in Mathematical Physics: Selected contributions of the XVth International Congress on Mathematical Physics (Editor: V. Sidoravicius), p.1, Springer (2009).
- [BB96] A. Bouzouina and S. De Bièvre: *Equipartition of the eigenfunctions of quantized ergodic maps on the torus*. Commun. Math. Phys. **178**, 83 (1996).
- [Ber85] M. V. Berry: *Semiclassical theory of spectral rigidity*. Proc. R. Soc. Lond. A **400**, 229 (1985).
- [Ber87] M. V. Berry: *Quantum chaology*. Proc. R. Soc. Lond. A **413**, 183 (1987).
- [BF61] F. A. Berezin and L. D. Faddeev: *A Remark on Schrödinger's Equation with a Singular Potential*. Russian: Dokl. Akad. Nauk SSSR **137**, 1011 (1961). English translation (by Z. Rubinstein): Sov. Math. Dokl. **2**, 372 (1961).
- [BGS84a] O. Bohigas, M. J. Giannoni and C. Schmit: *Spectral properties of the Laplacian and random matrix theories*. J. Phys. Lett. **45**, 1015 (1984).
- [BGS84b] O. Bohigas, M. J. Giannoni and C. Schmit: *Characterization of Chaotic Quantum Spectra and Universality of Level Fluctuation Laws*. Phys. Rev. Lett. **52**, 1 (1984).

- [BKS07] G. Berkolaiko, J. P. Keating, and U. Smilansky: *Quantum ergodicity for graphs related to interval maps*. Commun. Math. Phys. **273**, 137 (2007).
- [BKW03] G. Berkolaiko, J. P. Keating, and B. Winn: *Intermediate Wave Function Statistics*. Phys. Rev. Lett. **91**(13), 134103 (2003).
- [BKW04] G. Berkolaiko, J. P. Keating, and B. Winn: *No Quantum Ergodicity for Star Graphs*. Commun. Math. Phys. **250**, 259 (2004).
- [Bog00] E. B. Bogomolny: *Spectral statistics and periodic orbits*. New Directions in Quantum Chaos, p.333. Società Italiana di Fisica (2000).
- [BR86] M. V. Berry and M. Robnik: *Statistics of energy levels without time-reversal symmetry: Aharonov-Bohm chaotic billiards*. J. Phys. A **19**, 649 (1986).
- [BT77] M. V. Berry and M. Tabor: *Level Clustering in the Regular Spectrum*. Proc. R. Soc. Lond. A **356**, 375 (1977).
- [CCG85] G. Casati, B. V. Chirikov and I. Guarneri: *Energy-Level Statistics of Integrable Quantum Systems*. Phys. Rev. Lett. **54**, 1350 (1985).
- [CLM94] Z. Cheng, J. L. Lebowitz and P. Major: *On the number of lattice points between two enlarged and randomly shifted copies of an oval*. Probab. Theory Related Fields **100**, 253 (1994).
- [CVG80] G. Casati, F. Valz-Griz, and I. Guarneri: *On the Connection between Quantization of Nonintegrable Systems and Statistical Theory of Spectra*. Lett. Nuovo Cimento Soc. Ital. Fis. **28**, 279 (1980).
- [Dav95] E. B. Davies: *Spectral Theory and Differential Operators*. Cambridge University Press (1995).
- [Dei96] P. Deift: *Integrable Hamiltonian systems*. Lectures in Appl. Math. **31**, 103 (1996).
- [Del15] G. Dell'Antonio: *Lectures on the Mathematics of Quantum Mechanics I*. Atlantis Press (2015).
- [DF90] H. Donnelly and C. Fefferman: *Nodal sets for eigenfunctions of the Laplacian on surfaces*. J. Amer. Math. Soc. **3**, 333 (1990).
- [DT09] D. Dürr and S. Teufel: *Bohmian Mechanics: The Physics and Mathematics of Quantum Theory*. Springer (2009).

- [EMM05] A. Eskin, G. Margulis and S. Mozes: *Quadratic forms of signature (2,2) and eigenvalue spacings on rectangular 2-tori*. Ann. of Math. **161**, 679 (2005).
- [ENW06] M. Degli Esposti, S. Nonnenmacher and B. Winn: *Quantum variance and ergodicity for the baker's map*. Commun. Math. Phys. **263**, 325 (2006).
- [Far81] M. Farris: *Egorov's theorem on a manifold with diffractive boundary*. Comm. P.D.E. **6**(6), 651 (1981).
- [FJ98] F. G. Friedlander and M. Joshi: *Introduction to the Theory of Distributions*, 2nd edition. Cambridge University Press (1998).
- [GL93] P. Gérard and E. Leichtnam: *Ergodic Properties of Eigenfunctions for the Dirichlet Problem*. Duke Math. J. **71**, 559 (1993).
- [GN12] P. G. Grinevich and R. G. Novikov: *Faddeev eigenfunctions for point potentials in two dimensions*. Phys. Lett. A **376**, 1102 (2012).
- [HB80] J. H. Hannay and M. V. Berry: *Quantization of linear maps on a torus - Fresnel diffraction by a periodic grating*. Physica **1D**, 267 (1980).
- [HMR87] B. Helffer, A. Martinez and D. Robert: *Ergodicité et limite semi-classique*. Commun. Math. Phys. **109**, 313 (1987).
- [Hör85a] L. Hörmander: *The Analysis of Linear Partial Differential Operators III: Pseudo-Differential Operators*. Springer (1985).
- [Hör85b] L. Hörmander: *The Analysis of Linear Partial Differential Operators IV: Fourier Integral Operators*. Springer (1985).
- [Jak97] D. Jakobson: *Quantum limits on flat tori*. Ann. of Math. (2) **145**, 235 (1997).
- [JSSV15] D. Jakobson, Y. Safarov, A. Strohmaier and Y. Colin de Verdière (Appendix): *The semiclassical theory of discontinuous systems and ray-splitting billiards*. Amer. J. Math. **137**(4), 859 (2015).
- [KMS86] S. Kerckhoff, H. Masur, and J. Smillie: *Ergodicity of billiard flows and quadratic differentials*. Ann. of Math. (2) **124**, 293 (1986).
- [KMW10] J. P. Keating, J. Marklof and B. Winn: *Localized eigenfunctions in Šeba billiards*. J. Math. Phys. **51**, 062101 (2010).

- [KU14] P. Kurlberg and H. Ueberschär: *Quantum Ergodicity for Point Scatterers on Arithmetic Tori*. *Geom. Funct. Anal.* **24**, 1565 (2014).
- [KU(Pr15)] P. Kurlberg and H. Ueberschär: *Superscars in the Šeba billiard*. Preprint arXiv:1409.6878v3 (2015).
- [LSS05] M. de Llano, A. Salazar and M. A. Solís: *Two-dimensional delta potential wells and condensed-matter physics*. *Rev. Mex. Fis.* **51**(6), 626 (2005).
- [LZS06] W. T. Lu, W. Zeng and S. Sridhar: *Duality between quantum and classical dynamics for integrable billiards*. *Phys. Rev. E* **73**, 046201 (2006).
- [Mao88] H. Maoan: *Unique Ergodicity of Flows on the Torus and the Rotation Number*. *Acta Math. Sin. (New Series)* **4**, 338 (1988).
- [Mar01] J. Marklof: *The Berry-Tabor Conjecture*. *Progr. Math.* **202**, 421 (2001).
- [Mar03] J. Marklof: *Pair correlation densities of inhomogeneous quadratic forms*. *Ann. of Math.* **158**, 419 (2003).
- [Meg98] R. E. Megginson: *An Introduction to Banach Space Theory*. *Grad. Texts in Math.* **183**. Springer (1998).
- [Meh67] M. L. Mehta: *Random Matrices and the Statistical Theory of Energy Levels*. Academic Press (1967).
- [MK79] S. W. McDonald and A. N. Kaufman: *Spectrum and Eigenfunctions for a Hamiltonian with Stochastic Trajectories*. *Phys. Rev. Lett.* **42**, 1189 (1979).
- [MR12] J. Marklof and Z. Rudnick: *Almost all eigenfunctions of a rational polygon are uniformly distributed*. *J. Spectr. Theory* **2**, 107 (2012).
- [Non13] S. Nonnenmacher: *Anatomy of Quantum Chaotic Eigenstates*. *Prog. Math. Phys.* **66**, 193 (2013).
- [Per77] I. C. Percival: *Semiclassical Theory of Bound States*. *Adv. chem. Phys.* **36**, 1 (1977).
- [Poh13] J. Pohlmann: *Interacting Ultracold Atoms in External Potentials*. Master thesis, Institute for Theoretical Physics, Goethe University Frankfurt (2013).
- [Por65] C. E. Porter (editor): *Statistical Theories of Spectra: Fluctuations*. Academic Press (1965).

- [Raj82] C. K. Raju: *Products and compositions with the Dirac delta function*. J. Phys. A: Math. Gen. **15**, 381 (1982).
- [RS75] M. Reed and B. Simon: *Methods of Modern Mathematical Physics II - Fourier Analysis, Self-Adjointness*. Academic Press (1975).
- [RS78] M. Reed and B. Simon: *Methods of Modern Mathematical Physics IV - Analysis of Operators*. Academic Press (1978).
- [RS80] M. Reed and B. Simon: *Methods of Modern Mathematical Physics I - Functional Analysis*. Academic Press (1980).
- [RU12] Z. Rudnick and H. Ueberschär: *Statistics of Wave Functions for a Point Scatterer on the Torus*. Commun. Math. Phys. **316**, 763 (2012).
- [Sai91] X. Saint Raymond: *Elementary Introduction to the Theory of Pseudodifferential Operators*. CRC Press (1991).
- [Sar97] P. Sarnak: *Values at Integers of Binary Quadratic Forms*. Harmonic Analysis and Number Theory, CMS Conf. Proc. **21**, p.181, Amer. Math. Soc. (1997).
- [Sch01] R. Schubert: *Semiclassical localization in phase space*. Ph.D. thesis, University of Ulm (2001).
- [Sch11] R. E. Schwartz: *Mostly Surfaces*. American Mathematical Society (2011).
- [Shu01] M. A. Shubin: *Pseudodifferential Operators and Spectral Theory* (Second Edition). Springer (2001).
- [Sni74] A. I. Šnirel'man: *Ergodic properties of eigenfunctions*. Usp. Mat. Nauk **29**, 181 (1974).
- [Tay96a] M. E. Taylor: *Partial Differential Equations I - Basic Theory*. Springer (1996).
- [Tay96b] M. E. Taylor: *Partial Differential Equations II - Qualitative Studies of Linear Equations*. Springer (1996).
- [TK05] T. N. Trí and T. H. Koornwinder: *The Colombeau Theory of Generalized Functions*. Master's thesis, KdV Institute, University of Amsterdam (2005).
- [Ueb14] H. Ueberschär: *Quantum chaos for point scatterers on flat tori*. Phil. Trans. R. Soc. A **372**, 20120509 (2014).

- [Ver85] Y. Colin de Verdière: *Ergodicité et fonctions propres du laplacien*. Commun. Math. Phys. **102**, 497 (1985).
- [Wal82] P. Walters: *An Introduction to Ergodic Theory*. Grad. Texts in Math. **79**. Springer (1982).
- [Wim14] S. Wimberger: *Nonlinear Dynamics and Quantum Chaos: An Introduction*. Springer (2014).
- [Win03] B. Winn: *The Laplacian on a Graph and Quantum Chaology*. Ph.D. thesis, University of Bristol (2003).
- [Yes13] N. Yesha: *Eigenfunction statistics for a point-scatterer on a three-dimensional torus*. Ann. Henri Poincaré **14**(7), 1801 (2013).
- [Yes15] N. Yesha: *Quantum Ergodicity for a Point Scatterer on the Three-Dimensional Torus*. Ann. Henri Poincaré **16**(1), 1 (2015).
- [Zas77] G. M. Zaslavskii: *Statistics of energy levels when the integrals of motion are violated*. Sov. Phys. JETP **46**, 1094 (1977).
- [Zel86] S. Zelditch: *Pseudo-differential analysis on hyperbolic surfaces*. J. Funct. Anal. **68**, 72 (1986).
- [Zel87] S. Zelditch: *Uniform distribution of eigenfunctions on compact hyperbolic surfaces*. Duke Math. J. **55**, 919 (1987).
- [Zel92] S. Zelditch: *Quantum Ergodicity on the Sphere*. Commun. Math. Phys. **146**, 61 (1992).
- [ZF74] G. M. Zaslavskii and N. N. Filonenko: *Statistical properties of the energy spectrum of "gliding" electrons with mixed classical trajectories*. Sov. Phys. JETP **38**, 317 (1974).
- [ZFC05] C. K. Zachos, D. B. Fairlie and T. L. Curtright: *Quantum Mechanics in Phase Space*. World Scientific (2005).
- [Zor80] J. Zorbas: *Perturbation of self-adjoint operators by Dirac distributions*. J. Math. Phys. **21**(4), 840 (1980).
- [ZZ96] S. Zelditch and M. Zworski: *Ergodicity of eigenfunctions for ergodic billiards*. Comm. Math. Phys. **175**, 673, (1996).