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Discrete Spectrum of Non-selfadjoint Schrödinger Operators and An Application to Ocean Acoustics

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Discrete Spectrum of Non-selfadjoint Schrödinger Operators and An Application to Ocean Acoustics

Ph.D. thesis in the field of Functional Analysis & Operator Theory

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Certificate

Certified that the work presented in this thesis entitled "**Discrete Spectrum of Non-selfadjoint Schrödinger Operators and An Application to Ocean Acoustics**" is based on the authentic record of research work carried out by Mr. Satheesh Kumar S. under my guidance in the Department of Mathematics, Cochin University of Science and Technology, Kochi- 682 022 and has not been included in any other thesis submitted for the award of any degree. Also certified that all the relevant corrections and modifications suggested by the audience during the Pre-synopsis seminar and recommended by the Doctoral Committee of the candidate have been incorporated in the thesis and the work done is adequate and complete for the award of Ph. D. Degree.

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Declaration

I, Satheesh Kumar S., hereby declare that the work presented in this thesis entitled "**Discrete Spectrum of Non-selfadjoint Schrödinger Operators and An Application to Ocean Acoustics**" is based on the original research work carried out by me under the supervision and guidance of Dr. M. N. Narayanan Namboodiri, formerly Professor, Department of Mathematics, Cochin University of Science and Technology, Kochi- 682 022 and has not been included in any other thesis submitted previously for the award of any degree.

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"It is not true that people stop pursuing dreams because they grow old, they grow old because they stop pursuing dreams."

Gabriel García Márquez

Dedicated to my Wife

COCHIN UNIVERSITY OF SCIENCE AND TECHNOLOGY

Abstract

Doctor of Philosophy

Discrete Spectrum of Non-selfadjoint Schrödinger Operators and An Application to Ocean Acoustics

by SATHEESH KUMAR S.

Evolution of discrete spectrum of Schrödinger operator, $H(z) = -\frac{d^2}{dx^2}+V_0+zV_1$ where V_0 and V_1 are compactly supported and continuous on its support, is studied as z varies along a path in $\mathbb{C}$. It is found that the path traced by a discrete spectral element $\kappa(z)$ of $H(z)$ as z moves along a path terminates, if it, at the essential spectrum $[0,\infty)$. We have further extended this result and proved that any discrete spectral element of the nonself-adjoint operator $H(i) = -\frac{d^2}{dx^2}+V_0+iV_1$ is evolved from either a discrete spectral element or a resonance of the self-adjoint Schrödinger operator $H(0) = -\frac{d^2}{dx^2} + V_0$. Further, a more general case is discussed where the potential V_0 and V_1 satisfy $\int\limits_0^\infty xV_j dx < \infty$. Here it is proved that any discrete spectral element of $H(i)$ is evolved from either a discrete element of $H(0)$ or a spectral singularity of $H(it_0)$ for some $0 < t_0 < 1$. An estimate for lower bound of the number of discrete spectral elements of self-adjoint Schrödinger operator is derived based on this analysis. Also it is proved that the spectrum of a non-self adjoint Schrödinger operator $-\frac{d^2}{dx^2} + V_0 + iV_1$ with $V_1 > 0$ (or $V_1 < 0$) contains more discrete elements than that of the self-adjoint operator $-\frac{d^2}{dx^2} + V_0$. Finally, a new numerical scheme is devised for estimating eigenvalues of a Schrödinger operator based on the theoretical analysis. This scheme is implemented for underwater acoustic modelling.

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SATHEESH KUMAR *S.*

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A, B	Linear operators
$\mathscr{B}$	Banach space
$\mathbb{C}$	Field of complex numbers
Δ	Laplacian operator
Dom(A)	Domain of A
Ran(A)	Range of A
Ker(A)	Kernel of A
f, g	Elements of Banach spaces or Hilbert spaces
H	Operator on Hilbert spaces
$\mathscr{H}$	Hilbert space
M	Multiplication operator
m, n	Integers
$\mathbb{N}$	Set of natural numbers
$\mathbb{R}$	Field of real numbers
$\rho(H)$	Resolvent set of H
$\sigma(H)$	Spectrum of H
$\sigma_{\text{ess}}(H)$	Essential spectrum of H
$\sigma_{\text{d}}(H)$	Discrete spectrum of H
Ω	An open domain in $\mathbb{R}^n$
$C_c^\infty(\Omega)$	Space of smooth functions with compact support in Ω
$L^p(\Omega)$	Space of measurable functions f with $\int_\Omega f^p < \infty$
$L^p_{loc}(\Omega)$	Space of functions f with $\int_K f^p < \infty$ for K compact in Ω
$\mathbf{x}, \mathbf{y}, \mathbf{z}$	Elements in $\mathbb{R}^n$

Chapter 1

Preliminaries

The preliminary definitions and results are discussed in this chapter. Our work concentrates on the spectrum of non-selfadjoint Schrödinger operators which are compact perturbations of the free Schrödinger operator. This chapter provides basis for our work. The references for this chapter are mainly [Dav95] and [Kat80].

1.1 Introduction

Sonar (SOund Navigation And Ranging) is an equipment designed to use in underwater environments that uses acoustic waves to navigate, detect, communicate or image other objects. Underwater acoustic modelling plays a major role in sonar design and its performance prediction under given oceanic conditions. The mathematical model which describes acoustic propagation in underwater environments is the wave equation:

$$\rho \bigtriangledown \cdot \left(\frac{1}{\rho} \bigtriangledown P \right) = \frac{1}{c^2} \frac{\partial^2 P}{\partial t^2} \tag{1.1}$$

where P is the acoustic pressure field, $c = c(x, y, z, t)$ is the sound speed and $\rho = \rho(x, y, z)$ is the static density of the medium. Here the source is assumed to be away from the medium and boundary conditions are applied based on the environment.

Assuming that the acoustic parameters of the medium is not varying much during the acoustic transmission (*that is*, $c(x, y, z, t) =$

$c(x, y, z)$) and the source emits a harmonic signal of angular frequency ω, the pressure field is taken as:

$$P(x, y, z, t) = P(x, y, z) \exp(-i\omega t) \tag{1.2}$$

and substituting this into Equation 1.1, we have the model in frequency domain:

$$\rho \bigtriangledown \cdot \left(\frac{1}{\rho} \bigtriangledown P \right) + k^2 P = 0 \tag{1.3}$$

This equation is called Helmholtz equation. Here $k = \frac{\omega}{c}$ is the wave number of the medium.

Even though this transformation reduces the dimension of the domain by one, the equation is still not an efficient model for operational use. Further simplifications are done (details can be seen in [Boy84; Jen+11]) and the below operator,

$$\rho \frac{d}{dz} \left(\frac{1}{\rho} \frac{d}{dz} \right) + k^2(z),$$

defined in $L^2(0, \infty)$ with domain $\{f : f, f', (\frac{1}{\rho} f')' \in L^2(0, \infty), f(0) = 0\}$, and its spectrum play a major role in modelling the pressure field P. Spectral characteristics of this operator is same as that of the Schrödinger operator in $L^2(0, \infty)$ with potential $-k^2$.

Absorption in the ocean medium makes the potential $-k^2$ of the operator a complex function and hence the operator is a nonself-adjoint operator. Further the domain of the acoustic problem reduces this potential to a compactly supported potential. These operators are coming under the class of operators that are compact perturbations of self-adjoint operators. This work concentrates on the discrete spectrum of such class of operators.

This chapter of the doctoral thesis contains preliminary definitions and results that form the basic background for the study. Chapter 2 discusses and reviews the results regarding the compact perturbations of self-adjoint Schrödinger operator. Lieb-Thirring type inequalities and recent developments in estimate for number of bound states are discussed in this chapter. In chapter 3, the main results obtained in this study are detailed. The evolution of discrete spectrum as the potential moves analytically is discussed and demonstrated with an example. Chapter 4 contains application of the theoretical study in solving Ocean acoustic propagation numerically. Finally, the summary of work done and suggestions of future study are included in Chapter 5

1.2 Unbounded Linear Operators

Linear operators on a Banach space or Hilbert space are in general defined on the whole of the space. Continuous or bounded operators are such a class of operators that can be defined on the whole space. But to study unbounded operators like differential operators we may have to start with a more general definition for linear operator. One way to do this is to drop the requirement that the domain equals to the whole of the space. This in turn means that we are fixing the boundary condition on the differential equation which is to be studied. Thus the domain of definition is as important as the formula by which the operator is defined. The same formula defined on two different domains (boundary conditions) leads to entirely different spectrum for the operators.

Definition 1.2.1. A **linear operator** defined in a Banach space $\mathscr{B}$ is a pair (A, L) consisting of a dense subspace L of $\mathscr{B}$ and a linear map $A : L \to \mathscr{B}$. L is the domain of the operator A and we write $\mathrm{Dom}(A) := L$. If $\bar{L}$ is a linear subspace of $\mathscr{B}$ and $\bar{A} : \bar{L} \to \mathscr{B}$ is a linear map such that $L \subseteq \bar{L}$ and $\bar{A}(f) = A(f)$ for all $f \in \mathrm{Dom}(A)$ then $\bar{A}$ is called an **extension** of A.

Definition 1.2.2. A complex number λ is said to be an **eigenvalue** of an operator (A, L) in a Banach space $\mathscr{B}$ if there exists a non-zero $f \in L$ such that $Af = \lambda f$. We call the non-zero f, an **eigenfunction** of the operator A.

Definition 1.2.3. If A is a linear operator in $\mathscr{B}$ with domain L then a complex number z is said to be a member of the **resolvent** set of A, denoted by $\rho(A)$, if the operator $z - A$ maps L one-one onto $\mathscr{B}$, and its inverse (or resolvent) operator, denoted by $R(z, A)$ or $(z - A)^{-1}$, is bounded. The **spectrum** $\sigma(A)$ is defined as the complement of the resolvent set $\rho(A)$ in $\mathbb{C}$.

So $z \in \mathbb{C}$ belongs to $\sigma(A)$ if $z - A$ does not have a bounded inverse. *That is*, $z - A$ is not either one-one or onto, or the inverse $(z - A)^{-1}$ exists but is not bounded. In case if the operator $z - A$ is not one-one, then there exists a non-zero $f \in \mathrm{Dom}(A)$ such that $(z - A)f = 0$ and hence z is an eigenvalue of A. Thus the set of eigenvalues of A is contained in $\sigma(A)$. For finite dimensional Banach spaces both these sets are same but in other cases $\sigma(A)$ is often a much larger set.

The eigenvalue of an operator is determined by not just the formula by which the operator is defined; it is also dependent on the domain of its definition. The following examples demonstrate this fact.

Example 1.2.1. Consider an operator A defined by the formula $Af = -f''$ defined in the Banach space $\mathscr{B}$ of all continuous functions on $[a, b]$ with domain equal to the subspace of all smooth (infinitely differentiable) functions on $[a, b]$. Then each complex number $\lambda = -\kappa^2$ is an eigenvalue with corresponding eigenfunctions $f(x) = \exp(\pm i\kappa x)$.

Example 1.2.2. Define the same formula $Af = -f''$ in the Banach space $\mathscr{B}$ of all periodic continuous functions on the interval $[a, b]$ with domain, the subspace of all smooth continuous periodic functions on $[a, b]$ then the same formula defines a different operator with countable spectrum.

Example 1.2.3. (Dirichlet boundary conditions) Consider the operator H given by the formula $Hf = -f''$ in the Hilbert space $\mathscr{H} = L^2(a, b)$ with domain L_D consisting of all twice continuously differentiable functions f on $[a, b]$ for which $f(a) = f(b) = 0$. The eigenvalues of this operator can be estimated using elementary operations. The countable eigenvalues lie on the real line and its eigenfunctions form a Fourier orthonormal complete set in $L^2(a, b)$.

Example 1.2.4. (Neumann boundary conditions) Consider the operator H given by the formula $Hf = -f''$ in the Hilbert space $\mathscr{H} = L^2(a, b)$ with domain L_N consisting of all twice continuously differentiable functions f on $[a, b]$ for which $f'(a) = f'(b) = 0$. The eigenvalues of this operator too are countable real numbers and the eigenfunctions form a Fourier orthonormal complete set in $L^2(a, b)$. Note that the spectral properties are similar to the operator defined in previous example. But the spectral points are totally different. For example, 0 is an eigenvalue of this operator but it is not for the above operator.

Continuity or boundedness is a nice property we would like to have for operators. In case if an operator A defined in a Banach space $\mathscr{B}$ with dense subspace is bounded then it is possible to extend the domain to the whole space. Because if $f_n \to f$ in $\mathscr{B}$, the boundedness of the operator ensures the convergence of Af_n in $\mathscr{B}$. Unbounded operator does not have this property. At the same time differential operators have a property that is close to boundedness, *closedness*.

1.3 Closedness of an Operator

Definition 1.3.1. Let A be an operator in $\mathscr{B}$ with $\mathrm{Dom}(A) = L$. Then A is **closed** if whenever f_n is a sequence in L with $f_n \to f$ in $\mathscr{B}$ and there exists $g \in \mathscr{B}$ such that $\lim_{n\to\infty} Af_n = g$; it follows that $f \in L$ and $Af = g$.

There is an equivalent way of defining this. If A is an operator in $\mathscr{B}$ with domain L then the graph of $A = \{(f, Af) : f \in L\}$ is a subspace of the Banach space $\mathscr{B} \times \mathscr{B}$. It is evident that A is closed *if and only if* its graph is a closed subspace of $\mathscr{B} \times \mathscr{B}$. Note that the Banach space $\mathscr{B} \times \mathscr{B} = \{(f, g) : f, g \in \mathscr{B}\}$ is equipped with the norm defined by $\|(f, g)\|^2 = \|f\|^2 + \|g\|^2$.

The following lemma explains the importance of the notion of closedness and importance of knowing size of norm of an operator. The size of norm of the resolvent operator is important in locating the spectrum of the operator in $\mathbb{C}$.

Lemma 1.1. *[Dav95, p. 4] If the operator A does not have spectrum equal to the whole of the complex plane $\mathbb{C}$ then A must be closed. The spectrum $\sigma(A)$ of a linear operator is closed or resolvent set $\rho(A)$ is open. More specifically, let $z \notin \sigma(A)$ and let $c = \|R(z, A)\|$. Then the spectrum does not intersect the ball $\{w \in \mathbb{C} : |z - w| < c^{-1}\}$. The resolvent operator is a norm analytic function of z and for all $z, w \notin$ Spec(A).*

$$R(z, A) - R(w, A) = -(z - w)R(z, A)R(w, A)$$

$$R(z, A)R(w, A) = R(w, A)R(z, A), \quad \frac{d}{dz}R(z, A) = -R(z, A)^2.$$

Initially, differential operators may be defined on simple domains (like domain of smooth functions) where they are not closed. But most of the time these domains can be extended to make the operator closed.

Lemma 1.2. *[Dav95, p. 6] An operator A in $\mathscr{B}$ with domain L is said to be **closable** if it has a closed extension $\tilde{A}$. In this case there exists a closed* *extension $\overline{A}$ of A, called* ***closure*** *of A, whose domain is the smallest among all closed extensions.*

1.4 Self-adjoint Operators

Now we concentrate on operators defined in Hilbert spaces and the concept of **self-adjointness** is introduced, it is a bit different from the case of bounded operators where the domain is the whole space.

Definition 1.4.1. An operator H with dense domain L in a Hilbert space $\mathscr{H}$ is symmetric if

$$< Hf, g >=< f, Hg >, \text{ for all } f, g \in L.$$

The operators H_D and H_N in Examples 1.2.3, 1.2.4 are clearly symmetric because of the identity

$$\int_a^b (f''\overline{g} - f\overline{g''})dx = \left[f'\overline{g} - f\overline{g'}\right]_a^b.$$

Lemma 1.3. *[Dav95, p. 6] Every symmetric operator H is closable and its closure is also symmetric.*

Thus, without any loss of generality, symmetric operators are assumed to be closed.

Definition 1.4.2. If A is a linear operator in a Hilbert space $\mathscr{H}$ then the adjoint operator A^* is defined by the condition that

$$< Af, g >=< f, A^*g >$$

for all $f \in \mathrm{Dom}(A)$ and $g \in \mathrm{Dom}(A^*)$. The domain of A^* is defined to be the set $\mathscr{D}$ of all $g \in \mathscr{H}$ for which there exists unique $k \in \mathscr{H}$ such that

$$< Af, g >=< f, k >$$

for all $f \in \mathrm{Dom}(A)$.

Next result talks about the existence of adjoint operator.

Lemma 1.4. *[Dav95, p. 7] If A is a closed operator with dense domain then adjoint A^* is also a closed linear operator with dense domain.*

In fact, the closedness of the operator A makes the domain of A^* dense, and dense domain of A makes A^* a closed operator.

Definition 1.4.3. An operator H defined in a Hilbert space $\mathscr{H}$ is called **self-adjoint** if its adjoint H^* exist and $H^* = H$.

This means, operator H defined in Hilbert space $\mathscr{H}$ is self-adjoint if it is symmetric and $\text{Dom}(H^*) = \text{Dom}(H)$. For a bounded operator symmetry implies self-adjointness, but for unbounded operators symmetry need not imply that the operator is self-adjoint. But the condition of symmetry assures that the adjoint operator can be defined and its domain contains domain of the operator. That is to say that adjoint operator of a symmetric operator H is an extension of H.

Definition 1.4.4. An operator H defined in a Hilbert space $\mathscr{H}$ is said to be **essentially self-adjoint** if it is symmetric and its closure is self-adjoint.

The following lemma provides method for identifying essentially self-adjoint operators. This is useful for symmetric operators whose eigenvalues and eigenfunctions can be determined explicitly.

Lemma 1.5. *[Dav95, p. 8] Let H be a symmetric operator in a Hilbert space $\mathscr{H}$ with domain L, and let $\{f_n\}_{n=1}^{\infty}$ be a complete orthonormal set in $\mathscr{H}$. If each f_n lies in L and there exist $\lambda_n \in \mathbb{R}$ such that $Hf_n = \lambda_n f_n$ for every n, then H is essentially self-adjoint. Moreover, the spectrum of $\overline{H}$ is the closure in $\mathbb{R}$ of the set of all λ_n.*

Thus the operators defined in Examples 1.2.3, 1.2.4 are symmetric operators with self-adjoint closure. The classical Sturm-Liouville analysis brings out that the operator

$$H = -\frac{d}{dx}\left(p(x)\frac{d}{dx}\right) - q(x)$$

with $p(x), p'(x), q(x)$ real and continuous, $p(x) \neq 0$ defined in $L^2(a, b)$ (a, b are finite) with domain, the space of all smooth functions f satisfying either Dirichlet or Neumann boundary conditions belongs to the class of essentially self-adjoint operators. Later we bring out the fact that the Laplacian operator Δ defined in $L^2(\mathbb{R}^n)$ with domain $C_c^\infty(\mathbb{R}^n)$, the set of all smooth functions with compact support in $\mathbb{R}^n$ is essentially self-adjoint.

There are also operators that are symmetric but not essentially self-adjoint. The question of self-adjointness of any of their extension is addressed using the analysis with the **Cayley transform** and **deficiency indices**.

Definition 1.4.5. If H is a symmetric operator, then

$$\|(H+i)f\|^2 = \|Hf\|^2 + \|f\|^2 = \|(H-i)f\|^2$$

for all $f \in \mathrm{Dom}(H)$. Therefore there exists an isometric linear operator $U = (H-i)(H+i)^{-1}$ mapping $\mathrm{Ran}(H+i)$ one-one onto $\mathrm{Ran}(H-i)$. This operator is called **Cayley transformation** of H.

Lemma 1.6. *[Dav95, p. 11] There exists a one-one correspondence between symmetric extensions of H and its Cayley transform U.*

Definition 1.4.6. The **deficiency indices** of a symmetric operator H is defined to be the dimensions of the deficiency subspaces:

$$\begin{aligned} L^{\pm} &:= \{f \in \mathrm{Dom}(H^*) : H^* f = \pm i f\} \\ &= \{f \in \mathscr{H} :< Hh, f >= \mp i < h, f > \quad \text{for all } h \in \mathrm{Dom}(H)\}. \end{aligned}$$

Theorem 1.1. *[Dav95, p. 12] If H is a symmetric operator in $\mathscr{H}$ then there exist self-adjoint extensions of H if and only if the deficiency indices are equal. Moreover, the following conditions are equivalent:*

1. *H is essentially self-adjoint*

2. *The deficiency indices of H are both zero*

3. *H has exactly one self-adjoint extension*

Example 1.4.1. If an operator H is defined with same formula of H_D in Example 1.2.3 or H_N in Example 1.2.4 with domain

$$\begin{aligned} \mathrm{Dom}(H) &= \mathrm{Dom}(H_D) \cap \mathrm{Dom}(H_N) \\ &= \{f \in C^2[a,b] : f(a) = f'(a) = f(b) = f'(b) = 0\}. \end{aligned}$$

Then this opearator has at least two self-adjoint extensions namely $\overline{H_D}$ and $\overline{H_N}$.

Symmetric but cannot be extended to self-adjoint operator: Consider the operator in $L^2(0,\infty)$ defined by

$$Hf = if'$$

with domain the space $C_c^\infty(0,\infty)$ of smooth functions with compact support within $(0,\infty)$. To find the deficiency indices of this opeartor consider the equations

$$\begin{aligned} < Hh, f > &= \mp i < h, f > \text{ for all } h \in C_c^\infty(0,\infty) \\ < h', f > &= \mp < h, f > \text{ for all } h \in C_c^\infty(0,\infty). \end{aligned}$$

Now assume that the derivative (in the weak sense) of f exists in $L^2(0,\infty)$ then from the above equation

$$\int_0^\infty (f \mp f')h = 0 \text{ for all } h \in C_c^\infty(0,\infty).$$

This implies

$$f = \pm f' \Longrightarrow f = c\mathrm{e}^{\pm x}.$$

But $e^x \notin L^2(0,\infty)$. Hence the deficiency indices are respectively $\dim(L^+) = 0 \neq 1 = \dim(L^-)$. Therefore by the above theorem H does not have any self-adjoint extension. Whereas if the operator is defined in $L^2(0,1)$ with domain $C_c^\infty(0,1)$, then H has infinitely many self-adjoint extensions.

The next theorem is important in the spectral studies of self-adjoint operator. It allows to restrict our search for spectral elements of self-adjoint operator to real line.

Theorem 1.2. *[Dav95, p. 14] The spectrum of any self-adjoint operator H is real and non-empty. If $z \notin \mathbb{R}$ then*

$$\|(z-H)^{-1}\| \leq |Im(z)|^{-1}. \tag{1.4}$$

Moreover

$$(\overline{z}-H)^{-1} = ((z-H)^{-1})^*. \tag{1.5}$$

1.5 Spectral Theorem

Here the spectral analysis of a simple self-adjoint operator is done initially. This operator plays an important role in the spectral analysis of self-adjoint operator which is described in spectral theorem of self-adjoint operators.

Let E be a Borel subset of $\mathbb{R}^n$ and let μ be a non-negative countably additive Borel measure that is finite on every bounded Borel subset of $\mathbb{R}^n$. Define $\mathscr{H} := L^2(E, d\mu)$ to be the space of all measurable functions $f : E \to \mathbb{C}$ such that

$$\|f\| := \left[\int_E |f(x)|^2 d\mu\right]^{1/2} < \infty.$$

Then $\mathscr{H}$ is a Hilbert space subject to identifying two functions on $\mathscr{H}$ if they are equal almost everywhere.

Let $a : E \to \mathbb{R}$ be a measurable function such that the restriction of a to any bounded subset of E is a bounded function. Define an operator A using the formula

$$(Af)(x) := a(x)f(x)$$

in $\mathscr{H}$ with domain

$$\mathrm{Dom}(A) = \left\{ f \in \mathscr{H} : \int_E (1 + a(x)^2)|f(x)|^2 d\mu < \infty \right\}.$$

Theorem 1.3. *[Dav95, p. 16] The operator A defined above is self-adjoint. If L^2_c is the set of functions $f \in \mathscr{H}$ which vanish outside some bounded subset of E, then A is essentially self-adjoint on L^2_c. The spectrum of A equals the essential range of a, that is the set of all $\lambda \in \mathbb{R}$ such that*

$$\mu\{x : |a(x) - \lambda| < \epsilon\} > 0$$

for all $\epsilon > 0$. If $\lambda \notin \mathit{Spec}(A)$ then

$$\left((\lambda - A)^{-1} f \right)(x) = (\lambda - a(x))^{-1} f(x)$$

for all $x \in E$ and $f \in \mathscr{H}$, and

$$\|(\lambda - A)^{-1}\| = [\mathit{dist}(\lambda, \mathit{Spec}(A))]^{-1}.$$

The following form of spectral theorem unitarily identifies any self-adjoint operator with a multiplication operator in an L^2-space. Thus the estimation of spectrum of a self-adjoint operator reduces to finding the unitarily equivalent multiplication operator and its essential range.

Theorem 1.4. *[Dav95, p. 36] Let H be a self-adjoint operator in a Hilbert space $\mathscr{H}$ with spectrum S. Then there exists a finite measure μ on $S \times \mathbb{N}$*

and a unitary operator

$$U : \mathscr{H} \to L^2 := L^2(S \times \mathbb{N}, d\mu)$$

with the following properties. If $h : S \times \mathbb{N} \to \mathbb{R}$ is the function $h(s,n) = s$, then the element ξ of $\mathscr{H}$ lies in Dom(H) if and only if $h \cdot U(\xi) \in L^2$. We have

$$UHU^{-1}\psi = h\psi$$

for all $\psi \in U($Dom$(H))$.

1.6 Spectrum of Free Schrödinger Operator

The self-adjointness of the free Schrödinger operator $-\Delta$ in $L^2(\mathbb{R}^n)$ and its spectrum is explained with related results. Initially the operator is defined on the space of smooth functions, then using *Friedrichs* theorem it is shown that the operator can be extended to a self-adjoint operator. The domain of this self-adjoint operator is then explained and finally the spectrum is obtained using Fourier unitary transformation.

Definition 1.6.1. Let $\Omega \subset \mathbb{R}^n$, and $C_c^\infty(\Omega)$ be the space of all infinitely differentiable functions with compact support in Ω. Define the **Laplacian operator** $-\Delta$ in the Hilbert space $L^2(\Omega)$ with domain $C_c^\infty(\Omega)$ using the formula

$$-\Delta f := -\sum_{j=1}^{n} \frac{\partial^2 f}{\partial {x_j}^2}. \tag{1.6}$$

The identity

$$\int_\Omega (\Delta f \overline{g} - f \overline{\Delta g}) d^n\mathbf{x} = 0$$

which is followed from the theorem of Green, indicates that the above operator is symmetric. That is,

$$< f, -\Delta g >=< -\Delta f, g > \text{ for all } f, g \in C_c^\infty(\Omega)$$

.

This operator is not self-adjoint, in particular it is not closed. For example, if we consider a function $f \in L^2(\Omega)$ that is smooth up to its second derivative, with f and its derivatives up to the second order vanishing at the boundary of Ω, then it is easy to construct a sequence f_n in $C_c^\infty(\Omega)$ such that $f_n \to f$ and $\Delta f_n \to \Delta f$. We can prove that this operator has a self-adjoint extension.

Definition 1.6.2. A symmetric operator H in a Hilbert space $\mathscr{H}$ is said to be **bounded below** if there exists a real number m such that

$$< Hf, f > \quad \geq \quad m\|f\|^2$$

for all $f \in \mathrm{Dom}(H)$. In particular if $m = 0$, the operator H is called a **non-negative** operator.

It is also easy to prove that the operator $-\Delta$ is non-negative. That is

$$< f, -\Delta f >= \int_\Omega \sum_{j=1}^n \left| \frac{\partial f}{\partial x_j} \right|^2 d\mathbf{x} \geq 0$$

for all $f \in C_c^\infty(\Omega)$.

Theorem 1.5. *(Friedrichs) Let $\mathscr{H}$ be a Hilbert space and H be a symmetric non-negative operator in $\mathscr{H}$. then H has atleast one self-adjoint extension which is also non-negative.*

Thus the symmetric operator $-\Delta$ in $L^2(\Omega)$ with domain $C_c^\infty(\Omega)$ has a non-negative self-adjoint extension. Let H_0 be that extension. To obtain the domain of H_0, we note that any function in

$g \in \mathrm{Dom}(H_0)$ has the following property

$$< -\Delta f, g > = < f, H_0 g > \text{ for all } f \in C_c^\infty(\Omega).$$

Now it is helpful to introduce the idea of weak derivative and Sobolev spaces.

Definition 1.6.3. Let $\Omega \subset \mathbb{R}^n$, and let α be a multi-index. We say that $g \in L^1_{loc}(\Omega)$ (space of all functions which are integrable on any compact subset of Ω) is the α^{th} **weak derivative** $D^\alpha f$ of $f \in L^1_{loc}(\Omega)$ if

$$\int_\Omega f D^\alpha \varphi = (-1)^{|\alpha|} \int_\Omega g\varphi \qquad \text{for all } \varphi \in C_c^\infty(\Omega).$$

A function $f \in L^2(\Omega)$ is said to lie in the **Sobolev space** $\mathscr{H}^m = W^{m,2}(\Omega)$ if the weak partial derivatives $D^\alpha f$ lie in $L^2(\Omega)$ for all $|\alpha| \leq m$. The Sobolev norm of such functions are defined by

$$\|f\|^2_{\mathscr{H}^m} := \sum_{|\alpha| \leq m} \|D^\alpha f\|^2.$$

Thus if we consider

$$L_D := \{f \in L^2(\Omega) : Df, D^2 f \text{ exists in } L^2(\Omega), f = 0 \text{ on } \partial\Omega\}$$

or

$$L_N := \{f \in L^2(\Omega) : Df, D^2 f \text{ exists in } L^2(\Omega), Df = 0 \text{ on } \partial\Omega\}$$

then by the Green's identity $-\Delta$ is symmetric with domain L_D or L_N. Also it is clear that these are self-adjoint extensions of the symmetric operator $-\Delta$ with domain $C_c^\infty(\Omega)$. In case if $\Omega = \mathbb{R}^n$, then both extensions are the same and the operator $-\Delta$ with domain $C_c^\infty(\mathbb{R}^n)$ is essentially self-adjoint. Domain of the essentially self-adjoint operator is the Sobolev space $\mathscr{H}^2 = W^{2,2}(\mathbb{R}^n)$.

Spectrum of the free Schrödinger operator

The self-adjoint operator $-\Delta$ defined in $L^2(\mathbb{R}^n)$ is known as the free Schrödinger operator. The spectrum of this operator can be obtained easily if we can find the unitarily equivalent multiplication operator. Consider the Fourier transformation U defined on $L^2(\mathbb{R}^n)$ by

$$Uf(\mathbf{x}) = \int_{\mathbb{R}^n} f(\mathbf{t}) \mathrm{e}^{-2\pi i <\mathbf{x},\mathbf{t}>} d\mathbf{t}.$$

This Fourier transformation is a unitary operator on $L^2(\mathbb{R}^n)$ and it is easy to see that

$$U(-\Delta f)(\mathbf{x}) = (2\pi)^2 \|\mathbf{x}\|^2 Uf(\mathbf{x}) \quad \text{for all } f \in \mathrm{Dom}(-\Delta).$$

Or in other words $-\Delta$ on $L^2(\mathbb{R}^n)$ is unitarily equivalent to the multiplication operator M defined in $L^2(\mathbb{R}^n)$ by

$$Mf(\mathbf{x}) = m(\mathbf{x}) f(\mathbf{x}), \quad \text{where } m(\mathbf{x}) = (2\pi)^2 \|\mathbf{x}\|^2.$$

The domain of M is given by

$$\mathrm{Dom}(M) = \{f \in L^2(\mathbb{R}^n) : mf \in L^2(\mathbb{R}^n)\}.$$

Thus the spectrum of $-\Delta$ is equal to the spectrum of the multiplication operator M. That is

$$\sigma(-\Delta) = [0, \infty).$$

1.7 Discrete and Essential Spectrum

Based on the properties of the spectral elements, the spectrum is separated as discrete or essential spectrum. For a closed operator it is proven that this separation is disjoint and for self-adjoint operators this result in a disjoint decomposition of the spectrum.

Definition 1.7.1. Let H be an operator in the Hilbert space $\mathscr{H}$ and let $\lambda \in \sigma(H)$ be an isolated point of the spectrum, the Riesz projection of H with respect to λ is defined by

$$P(\lambda, H) := \frac{1}{2\pi i} \int_{\gamma} R(z, H) dz$$

where γ is a counterclockwise circle centered at λ such that there is no other point of $\sigma(H)$, except λ, on or inside γ.

Since $R(z, H)$ is an operator analytic function, Riesz projection is well-defined and γ can be any closed contour in the resolvent set of H enclosing λ and not containing any other spectral element of H other than λ. The projection $P(\lambda, H)$ is simply denoted by P_λ if the underlying operator is clear. Riesz projection is indeed a projection operator and has the following properties.

Proposition 1.1. *[GGK90, p. 326] The projection defined above satisfies the following:*

1. *P_λ is a projection, that is, $P_\lambda^2 = P_\lambda$.*
2. *Ran(P_λ) and Ker(P_λ) are H-invariant.*
3. *$\sigma(H|_{Ran(P_\lambda)}) = \{\lambda\}$ and $\sigma(H|_{Ker(P_\lambda)}) = \sigma(H) \backslash \{\lambda\}$.*

The above proposition reveals that the Riesz projection of H decomposes the spectrum of H. In fact this can be stated in a more general setting. Let $\sigma_0 \subset \sigma(H)$ be an isolated part of $\sigma(H)$, *that is*, both σ_0 and $\sigma_1 = \sigma(H) \backslash \sigma_0$ are closed and let γ be a closed contour in the resolvent set of H with σ_0 in its interior and separating σ_0 from σ_1, then the Riesz projection P_{σ_0} decomposes the spectrum of H in the sense that $\sigma(H|_{\mathrm{Ran}(P_{\sigma_0})}) = \sigma_0$ and $\sigma(H|_{\mathrm{Ker}(P_{\sigma_0})}) = \sigma_1$.

Definition 1.7.2. $\lambda \in \sigma(H)$ is said to be a **discrete** eigenvalue if λ is an isolated point of $\sigma(H)$ and the Riesz projection P_λ is of finite rank. In this case the positive integer $m_\lambda = \mathrm{Rank}(P_\lambda)$ is called the **algebraic multiplicity** of λ with respect to H.

The set of all discrete eigenvalues of an operator H is called its discrete spectrum denoted by $\sigma_{\mathrm{d}}(H)$. It is clear from the properties of the Riesz projection that the eigenspace of λ, $\mathrm{Ker}(\lambda - H)$, is a subspace of $\mathrm{Ran}(P_\lambda)$. Thus the geometric multiplicity, *that is* the dimension of eigenspace, of an isolated spectral element λ is always less than or equal to its algebraic multiplicity.

Definition 1.7.3. A closed operator H in Hilbert space $\mathscr{H}$ is called a **Fredholm operator** if it has a closed range and both its kernel and co-kernel are finite dimensional.

If H is an operator in the Hilbert space $\mathscr{H}$ then its kernel $\mathrm{Ker}(H)$ contains solutions of the homogeneous equation $Hf = 0$. Or in other words dimension of $\mathrm{Ker}(H)$ represents the number of degrees of freedom of the system represented by the model $Hf = g$. Co-kernel of the operator H is the quotient space $\mathscr{H}/\mathrm{Ran}(H)$. So if the dimension of co-kernel increases, it means that the range of H *decreases* or the number of constraints in the system increases. Thus a system represented by Fredholm operator has finite number of degrees of freedom and finite number of constraints.

Definition 1.7.4. The **essential spectrum**, $\sigma_{\mathrm{ess}}(H)$, of H is defined as

$$\sigma_{\mathrm{ess}}(H) = \{\lambda \in \mathbf{C} : \lambda - H \text{ is not a Fredholm operator}\}.$$

There is an important result known as **Weyl's criterion** that characterizes or identifies the spectral elements and essential spectral elements of a self-adjoint operator. Before stating that result, it is required to introduce one more concept.

Definition 1.7.5. A sequence $\{f_n\}_{n\in\mathbb{N}}$ in a Hilbert space $\mathscr{H}$ is said to be **weakly converging** to $f \in \mathscr{H}$ ($f_n \to f$ weakly) if

$$< f_n, g > \to < f, g > \quad \text{for all } g \in \mathscr{H}.$$

See that if $f_n \to f$ then $f_n \to f$ weakly, but the converse is not true.

Theorem 1.6. *(**Weyl's criterion**) Let H be a self-adjoint operator in $\mathscr{H}$. A point λ belongs to $\sigma(H)$ if and only if there exists a sequence $\{f_n\}_{n\in\mathbb{N}} \subset$ Dom(H) such that*

1. $\|f_n\| = 1$ *for all* $n \in \mathbb{N}$.

2. $Hf_n - \lambda f_n \to 0$ *in* $\mathscr{H}$ *as* $n \to \infty$.

Moreover $\lambda \in \sigma_{ess}(H)$ *if and only if in addition to the above properties*

3. $f_n \to 0$ *weakly in* $\mathscr{H}$.

The result stated next gives the direct connection between the spectrum of an operator and that of its resolvent. It also helps to change the focus, if necessary, from the spectrum of an unbounded operator to that of a bounded resolvent operator.

Proposition 1.2. *([EN00, p.243, 247] and [Dav07, p. 331]) Let H be a closed operator and let its resolvent, $\rho(H)$, be non-empty. If $a \in \rho(H)$ then,*

$$\sigma(R(a, H))\backslash\{0\} = \{(a-\lambda)^{-1} : \lambda \in \sigma(H)\}.$$

The same is true for the essential spectrum and discrete spectrum. That is,

$$\sigma_{ess}(R(a, H))\backslash\{0\} = \{(a-\lambda)^{-1} : \lambda \in \sigma_{ess}(H)\}$$

and

$$\sigma_d(R(a, H)) = \{(a-\lambda)^{-1} : \lambda \in \sigma_d(H)\}.$$

More precisely, λ is an isolated point of $\sigma(H)$ if and only if $(a-\lambda)^{-1}$ is an isolated point of $\sigma(R(a, H))$ and in this case the projection operators

$$P_\lambda := P(\lambda, H) = P\left((a-\lambda)^{-1}, R(a, H)\right) := P_{(a-\lambda)^{-1}}.$$

In particular the algebraic multiplicity of $\lambda \in \sigma_d(H)$ and $(a-\lambda)^{-1} \in \sigma_d(R(a, H))$ are equal.

Note that $0 \in \sigma(R(a,H))$ if and only if H is not a bounded operator. Moreover if H is closed and defined on a dense subspace of $\mathscr{H}$, then

$$0 \in \sigma(R(a,H)) \Longleftrightarrow 0 \in \sigma_{\text{ess}}(R(a,H)).$$

Now we have the following few results that talk about the disjointedness of discrete spectrum and essential spectrum and also about the disjoint decomposition of spectrum into discrete and essential spectrum.

Proposition 1.3. *[Dav07, p. 122] If H is a closed operator and λ is an isolated point of $\sigma(H)$, then $\lambda \in \sigma_{ess}(H)$ if and only if Rank$(P_\lambda) = \infty$. In particular $\sigma_{ess}(H) \cap \sigma_d(H) = \emptyset$.*

If we consider the left shift operator on the sequence space $\mathscr{H} = l^2(\mathbb{N})$ defined by

$$H(e_j) = e_{j-1}.$$

It is easy to see that $\|H\| = 1$ and hence $\sigma(H)$ is contained in the closed unit disk. One can also verify easily that $\lambda \in \mathbb{C}$ with $|\lambda| < 1$ is an eigenvalue of the operator. Since spectrum is a closed set, it follows that $\sigma(H) = \{\lambda \in \mathbb{C} : |\lambda| \leq 1\}$. It can be proven using Weyl's criterion that the essential spectrum of this operator, $\sigma_{\text{ess}}(H)$ is the unit circle $\{\lambda \in \mathbb{C} : |\lambda| = 1\}$ and the discrete spectrum of this operator is empty as the eigenvalues are not isolated. Thus the spectrum of the left shift operator cannot be represented as a disjoint union of discrete and essential spectrum.

Proposition 1.4. *[GGK90, p. 373] Let H be a closed operator and let $\Omega \subset \mathbb{C} \backslash \sigma_{ess}(H)$ be open and connected. If Ω contains at least one resolvent point of H, that is $\Omega \cap \rho(H) \neq \emptyset$, then $\sigma(H) \cap \Omega \subset \sigma_d(H)$.*

This result states that if Ω is a component (maximal open connected subset) of $\mathbb{C} \backslash \sigma_{\text{ess}}(H)$ then either of the two happens:

1. Ω contains resolvent points of H and hence the spectral elements of H, if any, contained in Ω are discrete.

2. Ω does not contain any resolvent point of H, that is $\Omega \subset \sigma(H)$.

The next result is a direct consequence of the previous one.

Corollary 1.6.1. *Let H be a closed operator and let $\sigma_{ess}(H) \subset \mathbb{R}$. If the upper and lower half planes of $\mathbb{C}$ contain resolvent points of H, then $\sigma(H) = \sigma_{ess}(H)\dot{\cup}\sigma_d(H)$, where $\dot{\cup}$ indicates the disjoint union. In particular, the spectrum of a self-adjoint operator H can be decomposed as $\sigma(H) = \sigma_{ess}(H)\dot{\cup}\sigma_d(H)$.*

Definition 1.7.6. Let H be closed linear operator in the Hilbert space $\mathscr{H}$. The **numerical range** of H is defined as

$$\mathrm{Num}(H) = \{< Hf, f >: f \in \mathrm{Dom}(H), \|f\| = 1\}.$$

$\mathrm{Num}(H)$ is a convex subset $\mathbb{C}$ containing all the eigenvalues of H. Furthermore, if the complement of the closure of $\mathrm{Num}(H)$ contains at least one resolvent point of H then $\sigma(H) \subset \overline{\mathrm{Num}}(H)$ and

$$\|R(z, H)\| \leq 1/\mathrm{dist}(z, \overline{\mathrm{Num}}(H)) \quad \text{for all } z \in \mathbb{C}\backslash\overline{\mathrm{Num}}(H).$$

If H is a **normal operator** (operator that commutes with its adjoint) then $\overline{\mathrm{Num}}(H)$ is the **complex hull** of $\sigma(H)$, that is the smallest convex set containing $\sigma(H)$.

1.8 Perturbation of a Linear Operator

Definition 1.8.1. Let H_0 be an operator with dense domain $\mathscr{D}$ in a Hilbert space $\mathscr{H}$. Let A be an operator whose domain contains $\mathscr{D}$. We say that A is **relatively bounded** with respect to H_0 (Or simply A is H_0-bounded), with **relative bound** $\alpha \geq 0$, if there exists $c < \infty$ such that

$$\|Af\| \leq \alpha\|H_0 f\| + c\|f\| \quad \text{for all } f \in \mathscr{D}.$$

The operator defined by $H := H_0 + A$ in $\mathscr{H}$ with domain $\mathscr{D}$ is called a **relative bounded perturbation** of H_0.

If A is a bounded operator then it is clearly a relative bounded operator with relative bound 0 and hence $H_0 + A$ is a relative bounded perturbation of H_0.

Theorem 1.7. *[Dav95, p. 18] Let H_0 be a self-adjoint operator and let A be symmetric and is H_0-bounded with relative bound less than 1. Then the relative bounded perturbation $H := H_0 + A$ is self-adjoint with Dom$(H) =$ Dom(H_0).*

Let H_0 be an operator with dense domain and A be an operator whose domain contains the domain of H_0. Let $f \in \text{Dom}(H_0)$, $z \in \rho(H_0)$ and let $g := (z - H_0)f$ then $R(z, H_0)g = f$. If $AR(z, H_0)$ is bounded then there exists $c < \infty$ such that

$$\|AR(z, H_0)g\| \leq c\|g\| \;\Leftrightarrow\; \|Af\| \leq c\|H_0 f\| + \alpha\|f\| \text{ where } \alpha = c|z|.$$

Thus A is relative bounded with respect to H_0 if and only if $AR(z, H_0)$ is bounded for some (in fact, for all) $z \in \rho(H_0)$. Using this idea, relative compact perturbation can be defined.

Definition 1.8.2. Let $\mathscr{B}$ be a Banach space and let K be a bounded operator which satisfies any of the following equivalent conditions

1. The image of any bounded subset of $\mathscr{B}$ under K is relatively compact.
2. $\{Kf_n\}$ contains a Cauchy sequence for any bounded sequence $\{f_n\}$ in $\mathscr{B}$.

Then K is called a **compact** operator.

If K_1, K_2 are compact operators then $\alpha_1 K_1 + \alpha_2 K_2$ is compact for any $\alpha_1, \alpha_2 \in \mathbb{C}$. If $\{K_n\}$ is a sequence of compact operators and if $K_n \to K$, then K is compact. Thus the space of all compact operators on $\mathscr{B}$ is a Banach subspace of the space of all bounded operators and is denoted by $\mathcal{S}_\infty(\mathscr{B})$.

A compact operator on a Hilbert space $\mathscr{H}$ can be thought of as the norm limit of finite rank operators. Or the Banach space $\mathcal{S}_\infty(\mathscr{H})$ as the completion (or closure) of the space of all finite rank operators in the Banach space of all bounded operators. The spectrum of a compact operator consists of non-zero discrete eigenvalues with a possible accumulation point 0. If the Hilbert space is not finite dimensional then for any compact operator K on $\mathscr{H}$, $\sigma_{\text{ess}}(K) = \{0\}$.

For any $K \in \mathcal{S}_\infty(\mathscr{H})$, we can find orthonormal sets (not necessarily complete) $\{f_n\}$ and $\{g_n\}$ and a set of positive numbers $\{\lambda_n\}$ with $\lambda_1 \geq \lambda_2 \geq \ldots > 0$ such that

$$Kf = \sum_n \lambda_n < f, f_n > g_n, \quad \text{for all } f \in \mathscr{H}.$$

The positive numbers λ_n's are called singular values of K and they are precisely the eigenvalues of the square root of the positive operator K^*K.

Definition 1.8.3. Let H_0 be an operator with dense domain in the Hilbert space $\mathscr{H}$ and K be a compact operator on $\mathscr{H}$. Then the operator $H := H_0 + K$ is called a **compact perturbation** of H_0.

Any compact perturbation of a Fredholm operator is Fredholm, that is, if H_0 is Fredholm and K is compact then $H := H_0 + K$ is Fredholm. This property leads to the fact that essential spectrum of an operator cannot be changed by any compact perturbation, that is $\sigma_{\text{ess}}(H_0) = \sigma_{\text{ess}}(H_0 + K)$.

Definition 1.8.4. Let H_0 be an operator with dense domain in $\mathscr{H}$ and the resolvent of H_0, $\rho(H_0)$ be non-empty. An operator A is called H_0-compact or **relatively compact** with respect to H_0 if $\text{Dom}(H_0) \subset \text{Dom}(A)$ and $AR(z, H_0) \in \mathcal{S}_\infty(\mathscr{H})$ for some $z \in \rho(H_0)$. The operator $H := H_0 + A$ is called a **relative compact perturbation** of H_0.

Every H_0-compact operator is H_0-bounded with relative bound 0. Moreover if A is H_0-compact and H_0 is Fredholm then $H := H_0 + A$ is Fredholm. This leads to Weyl's theorem:

Theorem 1.8. *(Weyl's theorem)Let $H = H_0 + A$ where H_0 is a closed operator in $\mathscr{H}$ and A is H_0-compact. Then $\sigma_{ess}(H) = \sigma_{ess}(H_0)$.*

If H_0, H are closed operators in $\mathscr{H}$ and suppose that $\rho(H) \cap \rho(H_0) \neq \emptyset$. Let $z \in \rho(H) \cap \rho(H_0)$, then it is easy to see the identity

$$R(z, H) - R(z, H_0) = R(z, H)(H - H_0)R(z, H_0)$$

Thus H is a relative compact perturbation of H_0 if and only if their resolvent difference is compact and hence $\sigma_{\text{ess}}(R(z, H)) = \sigma_{\text{ess}}(R(z, H_0))$. Now using Proposition 1.2 we have the following:

Proposition 1.5. *Let H_0, H be closed operators in $\mathscr{H}$ and let $z \in \rho(H_0) \cap \rho(H)$. If the resolvent difference $R(z, H) - R(z, H_0)$ is compact then $\sigma_{ess}(H) = \sigma_{ess}(H_0)$.*

If H_0 is self-adjoint and H is a relative compact perturbation of H_0 then it is shown that the resolvent, $\rho(H)$ contains points from upper and lower half planes of $\mathbb{C}$. Using the previous theorem $\sigma_{\text{ess}}(H) = \sigma_{\text{ess}}(H_0) \subset \mathbb{R}$. Now using corollory of Proposition 1.4 we have

Theorem 1.9. *If H is a relative compact perturbation of a self-adjoint operator H_0 then*

$$\sigma(H) = \sigma_{ess}(H) \dot{\cup} \sigma_d(H).$$

1.9 Schrödinger Operator

In this section we consider operators defined in $L^2(\mathbb{R}^n)$ by the expression

$$Hf = -\Delta f + Vf.$$

Here V is a multiplication operator with a real or complex function $v(\mathbf{x}), \mathbf{x} \in \mathbb{R}^n$ which is appropriately chosen to make the operator a perturbation of the free Schrödinger operator discussed in Section 1.6.

This operator and its spectral analysis have special importance in quantum mechanics. The Schrödinger equation given by

$$\frac{\partial f}{\partial t} = -iHf$$

plays a role in quantum mechanics equivalent to Newton's second law of motion in classical mechanics. This Schrödinger equation controls the evolution of a quantum system with solution $f(\mathbf{x}, t) = e^{-iHt} f(\mathbf{x}, 0)$. Here f represents the state of the system and the operator H, the Hamiltonian of the system. The total energy of the system, which is equal to $< Hf, f >$, is divided between the kinetic energy $< -\Delta f, f >$ and the potential energy $< Vf, f >$. The different eigenvalues, if exist, correspond to different discrete excitations of the system. The smallest of these eigenvalues represents the ground state energy and the corresponding eigenfunction is the ground state of the system.

The above detailing is an over-simplified description of quantum system and quantum theory. Our interest is to study the Schrödinger operator rather as a mathematical tool. But here it is intended to indicate the importance of differential operators and their spectrum in the study of quantum theory, one of the most important scientific theories of this century.

In this section the conditions on real potential V to make the Schrödinger operator a self-adjoint operator are discussed. For the case of complex potential, conditions on V so that it becomes a relatively compact perturbation of the free Schrödinger operators are discussed.

If V is a real potential such that Hf exists in $L^2(\mathbb{R}^n)$ for f in a subspace of $L^2(\mathbb{R}^n)$, then Green's theorem ensures the symmetry of the operator. But the self-adjointness or the denseness of the domain is not ensured without setting conditions on the potential. If the multiplication function is locally integrable, a term defined below, then one can ensure the denseness of the domain. Whereas the self-adjointness (or essential self-adjointness) is proven if the potential considered is $-\Delta$-bounded with relative bound zero.

Definition 1.9.1. A function $V : \mathbb{R}^n \to \mathbb{C}$ is said to be **locally p-integrable** or said to be a member of $L^p_{\text{loc}}(\mathbb{R}^n)$ if it is p-integrable on every bounded subset of $\mathbb{R}^n$.

A function V is said to be in $L^p + L^\infty$ ($L^p(\mathbb{R}^n) + L^\infty(\mathbb{R}^n)$) if we can express V as $V = V_p + V_\infty$ where $V_p \in L^p(\mathbb{R}^n)$ and $V_\infty \in L^\infty(\mathbb{R}^n)$ (or equivalently V_∞ is measurable and bounded).

If the potential V is in L^2_{loc}, then it is easy to see that the operator $H := -\Delta + V$ can be defined on $C_c^\infty(\mathbb{R}^n)$, the space of smooth or infinitely differentiable functions with compact support in $\mathbb{R}^n$, a dense subspace of $L^2(\mathbb{R}^n)$. In fact it can be defined on $C_c^2(\mathbb{R}^n)$, the space of functions which have derivative (in the weak sense) up to second order and have compact support. Thus H can be defined on a dense domain.

If the real potential V is in $L^\infty(\mathbb{R}^n)$ then we can make it a positive operator by adding a sufficiently large positive number, if required, to $-\Delta + V$. Hence by an application of Friedrichs theorem (Theorem 1.5) there exists self-adjoint extension for the operator $-\Delta + V$. Or otherwise, if the real V is in $L^\infty(\mathbb{R}^n)$, then the multiplication operator is bounded with norm $\|V\|_{L^\infty}$ and hence it is $-\Delta$-bounded with relative bound 0. So using Theorem 1.7, $-\Delta + V$ is essentially self-adjoint with domain equal to $\text{Dom}(-\Delta) = \mathscr{H}^2 = W^{2,2}(\mathbb{R}^n)$.

The following few theorems talk about the essential self-adjointness of the Schrödinger operator $-\Delta + V$ defined in $\mathscr{H} =$

$L^2(\mathbb{R}^n)$ with domain $C_c^\infty(\mathbb{R}^n)$ for the case of potentials with singularity.

Theorem 1.10. *[Dav95, p. 157] If $0 \leq V \in L^1_{loc}$, then the non-negative Schrödinger operator defined in $L^2(\mathbb{R}^n)$ with domain $C_c^\infty(\mathbb{R}^n)$ is essentially self-adjoint).*

The next theorem is about Schrödinger operator in $L^2(\mathbb{R}^3)$

Theorem 1.11. *([Dav95, p. 159] and [Kat80, p. 304]) If H is defined in $L^2(\mathbb{R}^3)$ by $Hf := -\Delta f + Vf$, where the real potential V is in $L^2 + L^\infty$, then H is self-adjoint and bounded below with the same domain as the free Schrödinger operator $H_0 := -\Delta$. In addition if $V(\mathbf{x}) \to 0$ as $|\mathbf{x}| \to \infty$, then the spectrum of H consists of $\sigma_{ess}(H) = [0, \infty)$ and discrete spectrum equals to a countable set of negative real numbers which accumulate at 0, if it is infinite.*

The second part of the theorem is proved by showing that V is H_0-compact if $V(\mathbf{x}) \to 0$ as $|\mathbf{x}| \to \infty$. This is true even if V is complex valued, but then H is not symmetric and self-adjointness is out of question. Even though using Theorem 1.9, it can be shown that spectrum of H consists of $\sigma_{\text{ess}}(H) = [0, \infty)$ and $\sigma_{\text{d}}(H)$ equals to a countable set of non-positive points in $\mathbb{C}$ which accumulate, if $\sigma_{\text{d}}(H)$ is infinite, to a point in $[0, \infty)$.

Even though the above theorem is of great importance its applicability is limited to a smaller class of potentials compared to the following theorem.

Theorem 1.12. *[Dav95, p. 160] Let $n \geq 3$, let the real potential $V \in L^p + L^\infty$ for some $p > n/2$ and let the operator $H := -\Delta + V$ be defined on a dense subspace of $L^2(\mathbb{R}^n)$. Then H can be extended to a self-adjoint operator which is bounded below.*

Now we turn to the case of complex valued potential V. Then the operator $H := -\Delta + V$ is a nonself-adjoint operator. Much of the discussion on the topic is postponed to the next chapter, where we review the results regarding relative compact perturbations of free Schrödinger operators in detail. Theorem 1.11 gives the condition to make complex potential V a relative compact perturbation of $-\Delta$ on $L^2(\mathbb{R}^3)$. We end this section by noting a result that provides conditions on complex potential V to make it a relative compact perturbation of $-\Delta$ on $L^2(\mathbb{R}^n)$.

Theorem 1.13. *[DHK13a] If the complex potential $V \in L^p(\mathbb{R}^n)$ with $p \geq 2$ if $n \leq 3$ and $p > n/2$ if $n \geq 4$, then V is relatively compact with respect to $-\Delta$, the operator $H := -\Delta + V$ has domain equal to Dom$(-\Delta) = W^{2,2}(\mathbb{R}^n)$ and its spectrum is a disjoint union of $\sigma_{ess}(H) = [0, \infty)$ and $\sigma_d(H)$ equals to a countable set of discrete eigenvalues which can accumulate only at $[0, \infty)$.*

1.10 Operator Valued Analytic Functions

In this section we refer few results from [Kat80] regarding operator valued analytic functions. We start with defining analytic vector valued functions and operator valued functions.

Definition 1.10.1. Let $\mathscr{B}$ be a Banach space, $\Omega \subset \mathbb{C}$ an open subset in $\mathbb{C}$. A vector valued function $F : \Omega \to \mathscr{B}$ is said to be analytic or holomorphic in Ω if it is differentiable at each point of Ω. *That is*, for each $z \in \Omega$ there exists $G(z)$ such that

$$\left\| \frac{F(z + \Delta z) - F(z)}{\Delta z} - G(z) \right\| \to 0 \text{ as } \Delta z \to 0.$$

In a Hilbert space $\mathscr{H}$, a function $F : \Omega \to \mathscr{H}$ is analytic *if and only if* $z \in \Omega$ has a neighborhood in which $\|F(z)\|$ is bounded and the complex valued function $< F(z), f >$ is analytic for each $f \in \mathscr{H}$. This last statement is equivalent to saying that the function F is analytic in Ω in the weak sense.

Now we turn to the case of operator valued functions, and first we consider bounded operator valued functions.

Definition 1.10.2. Let Ω be a complex domain, and let A be a bounded-operator valued function. *That is*, for each z in Ω, $A(z)$ be a bounded or continuous operator from Banach space $\mathscr{B}_1$ to Banach space $\mathscr{B}_2$. We say A to be analytic in Ω if it is differentiable at each $z \in \Omega$. *That is*, there exists a $B(z)$ for each z such that

$$\left\| \frac{A(z+\Delta z) - A(z)}{\Delta z} - B(z) \right\| \to 0 \text{ as } \Delta z \to 0.$$

Here $\|\cdot\|$ indicate the norm in the Banach space of all bounded operators from $\mathscr{B}_1$ to $\mathscr{B}_2$.

If the underlying Banach spaces are Hilbert, say $\mathscr{H}_1$ and $\mathscr{H}_2$, then the bounded-operator valued function $A(z)$ is analytic in Ω *if and only if* each z in Ω has a neighborhood in which $A(z)$ is bounded and $< A(z)f, g >$ is analytic for each $f \in \mathscr{H}_1$ and $g \in \mathscr{H}_2$.

Analyticity of Unbounded Operators

Definition 1.10.3. Let $A(z)$ be a closed operator from $\mathscr{B}_1$ to $\mathscr{B}_2$ for each z in a complex domain. Then $A(z)$ is said to be analytic at z_0 if there exist a Banach space $\mathscr{B}$ and two operator valued functions $B(z)$ and $C(z)$ which are bounded-holomorphic at z_0, where each $B(z)$ is a bounded operator from $\mathscr{B}$ to $\mathscr{B}_1$ and each $C(z)$ is a bounded operator from $\mathscr{B}$ to $\mathscr{B}_2$, such that $B(z)$ maps $\mathscr{B}$ one-one onto $\text{Dom}(A(z))$ and

$$A(z)B(z) = C(z).$$

$A(z)$ is analytic in a complex domain Ω if it is analytic at each $z \in \Omega$.

An important result which connects the analyticity of unbounded operator valued function to that of bounded operator valued function is given below.

Theorem 1.14. *[Kat80, p. 367] Let $A(z)$ be defined on a neighborhood of z_0 and let $\zeta \in \rho(A(z_0))$, the resolvent set of $A(z_0)$. Then A is holomorphic at z_0 if and only if $\zeta \in \rho(A(z))$ and the resolvent $R(\zeta, z) := R(\zeta, A(z)) = (\zeta - A(z))^{-1}$ is bounded-holomorphic for sufficiently small $|z - z_0|$. $R(\zeta, z)$ is even bounded-holomorphic in the two variables on the set of all ζ, z such that $\zeta \in \rho(A(z_0))$ and $|z - z_0|$ is sufficiently small (depending on ζ).*

If we have any result regarding the spectrum (for example continuity, analyticity) of a bounded-analytic operator valued function, using the above theorem and Proposition 1.2 it can be transferred to the case of unbounded operator valued analytic functions.

One of the important results which we make use of in our analysis is the following.

Theorem 1.15. *[Kat80, p. 370] If $A(z)$ is holomorphic in z near $z = z_0$, then any finite system of eigenvalues $\{\lambda_j(z)\}_{j=1}^{m}$ of $A(z)$ consists of branches of one or several analytic functions which have at most algebraic singularities near $z = z_0$.*

Example 1.10.1. Consider the operator valued function $A(z)$ defined on the extended complex plane where each $A(z)$ is the operator on $L^2(0,1)$ defined by $A(z) := -i\frac{d}{dx}$ with the domain, $\mathrm{Dom}(A(z)) = \{f \in L^2(0,1) : f' \in L^2(0,1) \text{ and } (1+iz)f(0) = (1-iz)f(1)\}$. The eigenvalues can be found out using the equations

$$-i\frac{df}{dx} = \lambda f \text{ and } (1+iz)f(0) = (1-iz)f(1)$$

and the eigenvalues are

$$\lambda_n(z) = 2\arctan z + 2n\pi, \quad n = 0, \pm 1, \pm 2, \ldots.$$

Thus all these eigenvalues $\lambda_n(z)$ form a single analytic function $2\arctan z$, which has a logarithmic singularity at $\pm i$. Also we can directly verify that at $z = \pm i$, the operators $A(\pm i)$ do not have any eigenvalues.

There is an important special case of holomorphic family of operators $A(z)$ which is referred as analytic family of type (A) and is defined as follows.

Definition 1.10.4. A function $A(z)$ defined on a complex domain Ω, whose values are closed operators from a Banach space $\mathscr{B}_1$ to Banach space $\mathscr{B}_2$, is said to be **analytic of type (A)** if (i) Dom$(A(z))$=$\mathscr{D}$ is independent of z and (ii) $A(z)f$ is analytic for each $z \in \Omega$ and for every $f \in \mathscr{D}$.

It is easy to see that if $A(z)$ is analytic of type (A) then it is indeed an analytic function in the sense of Definition 1.10.3. To see this, convert the common domain $\mathscr{D}$ to a Banach space $\mathscr{B}$ by defining a norm by $\|f\|_{\mathscr{B}} = \|f\|_{\mathscr{B}_1} + \|A(z_0)f\|_{\mathscr{B}_2}$ where $z_0 \in \Omega$. This is possible because $A(z)$ is closed for each z in particular $A(z_0)$ is closed. Now consider the operator B which sends $f \in \mathscr{B}$ to $f \in \mathscr{B}_1$; B clearly maps $\mathscr{B}$ one-one onto $\mathscr{D}$ and is bounded since $\|f\|_{\mathscr{B}_1} \leq \|f\|_{\mathscr{B}}$. Also each $A(z)$ can be regarded as an operator from $\mathscr{B}$ to $\mathscr{B}_2$ and is denoted by $C(z)$. The closedness of $A(z)$ implies the closedness of $C(z)$ and since $C(z)$ is defined on the entire Banach space $\mathscr{B}$, $C(z)$ is bounded. Since $C(z)f = A(z)f$ is analytic for every $f \in \mathscr{B}$, it follows that $C(z)$ is bounded-analytic. Finally, from the construction it is obvious that $A(z)B = C(z)$ and hence $A(z)$ is analytic in the sense of Definition 1.10.3.

Chapter 2

Literature Survey

Spectral analysis of nonself-adjoint operators is very much an active topic. In particular, both Mathematicians and Physicists have shown interest in the nonself-adjoint Schrödinger operators because of their physical significance. Most of the research articles generated in this area are concerned with the discrete spectrum, its finiteness, accumulation (if infinite), rate of convergence and its boundedness. This chapter contains survey of some important literature which we have come across during this study. Most of these are related to Schrödinger operators with relative compact perturbations. This survey will be covered in two sections. Section 2.1 covers results specific to self-adjiont Schrödinger operators. The last section is devoted for the discussion of articles pertaining to nonself-adjoint Schrödinger operators with relative compact potentials. This section is categorized into three, discussing the results related to (i) boundedness of discrete spectrum, (ii) Lieb-Thirring type inequalities and (iii) estimate for number of eigenvalues or bound states.

2.1 Self-adjoint Schrödinger operators

Documentation of our survey starst with results given in [Bar52] for a self-adjoint Schrödinger operator acting in $L^2(\mathbb{R}^3)$. This brief note contains estimate for number of bound states (discrete spectrum) of radial wave equation

$$\frac{d^2 f}{dr^2} - l(l+1)\frac{1}{r^2}f + \lambda f = V(r)f$$

which is obtained from the Schrödinger equation

$$-\Delta f(\mathbf{x}) + V(\mathbf{x})f(\mathbf{x}) = \lambda f(\mathbf{x}) \text{ for } \mathbf{x} \in \mathbb{R}^3.$$

The above Schrödinger equation is first converted to spherical coordinate system (r, θ, ϕ), then a solution of the form $f(r)g(\theta, \phi)$ is assumed and the equation is separated into two. The radial wave equation is one of the two resulting equations that corresponds to radial r. The separation constant is taken as $l(l+1)$ and l is called the angular momentum for physical considerations. In [Bar52], an estimate of the number of bound states n_l of the radial wave equation with potential which satisfies the condition

$$I = \int_0^\infty rV(r)dr < \infty$$

is sought and this article tries to extend an earlier study which concluded that $n_l = 0$ if $I < 1$. The extended general result derived in this article is

$$(2l+1)n_l < I.$$

The operator valued function

$$H(\lambda) = -\Delta + \lambda V, \quad \lambda \in \mathbb{R},$$

where $-\Delta$ is the free Laplacian defined on $L^2(\mathbb{R}^3)$ and V is a real valued function which belongs to the Rollnik class of functions (V is a Rollnik function *if and only if* $\int_{\mathbb{R}^6} |V(\mathbf{x})||V(\mathbf{y})||\mathbf{x}-\mathbf{y}|^{-2}d\mathbf{x}\, d\mathbf{y} < \infty$) has been studied in [KS80] using perturbation theory. In this article, the nature of the negative eigenvalues is studied as λ approaches a coupling threshold constant, say λ_0. Here, λ_0 is a coupling threshold constant, means that if $\lambda \to \lambda_0$ then a negative eigenvalue of $H(\lambda)$ goes to 0 and gets absorbed in the essential spectrum. It has been noted that the threshold behavior is very much dependent on the dimension of the underlying configuration space $\mathbb{R}^n$. For the case of $n = 3$ it is proved that, if $E(\lambda)$ denotes the negative eigenvalue that get absorbed in the essential spectrum as $\lambda \to \lambda_0$, then $E(\lambda)$ behaves as

$$E(\lambda) = O((\lambda - \lambda_0)^2)$$

or

$$E(\lambda) = O(\lambda - \lambda_0)$$

as $\lambda \to \lambda_0$ and $E(\lambda)$ is analytic in the first case and has a square root branch point in the second case. Several authors have studied this threshold behavior and in [GH87] the above results have been improved by finding out the coefficients of the first term in the expansion of $E(\lambda)$ in terms of $(\lambda - \lambda_0)$.

Resonances and antibound states (negative resonance) of self-adjoint operator in one-dimension is studied in [Sim00]. A simple definition similar to the definition of eigenvalues is derived for resonances. Here the function (similar to eigenfunction) corresponding to the resonance does not belong to $L^2(\mathbb{R})$ or $L^2(0, \infty)$. This definition of resonance is used in our study. A result regarding the number of antibound state is proved in this article, the same is illustrated in our analysis.

As we have seen earlier, if the potential V is a relative compact perturbation (see Section 1.9 for more details) then its spectrum contains the essential spectrum $[0, \infty)$ and a countable set of discrete eigenvalues that can only accumulate at $[0, \infty)$. Several authors have studied the rate of convergence of such a discrete spectrum. If $\{\lambda_j\}$ is the set of discrete eigenvalues then the sum $\sum\limits_j (\text{dist}(\lambda_j, [0, \infty)))^\gamma$ represents a measure for the convergence of discrete spectrum. The convergence of the sum for smaller values of γ indicates faster convergence of λ_j to the essential spectrum. In the self-adjoint case, all the discrete eigenvalues are negative real numbers and their accumulation, if it happens, is towards 0. The above mentioned sum, in this case, reduces to $\sum\limits_j |\lambda_j|^\gamma$. Providing an estimate to this sum and improving this estimate are important research topics in this field. The estimate to this sum is in general referred to as the Lieb-Thirring type inequalities as it was first derived in [LT76]. The results from [LT76], [Lie76], [Roz76], [Cwi77] and [Wei96] suggest the existence of a constant $L(p,n)$ that depends only on p and n such that for potentials $V \in L^p(\mathbb{R}^n)$ with $p \geq 1$ if $n = 1$, $p > 1$ if $n = 2$ and $p \geq \frac{n}{2}$ if $n \geq 3$,

$$\sum_j |\lambda_j|^{p-\frac{n}{2}} \leq L(p,n) \int_{\mathbb{R}^n} V_-(\mathbf{x})^p d\mathbf{x}$$

where $V_-(\mathbf{x}) = \max\{-V(\mathbf{x}), 0\}$ is the negative part of V. Estimating sharp constant $L(p,n)$ has also attracted several authors. There exists a classical constant derived from Weyl's asymptotic formula denoted by $L^{\mathrm{cl}}(p,n)$ given by

$$L^{\mathrm{cl}}(p,n) = \frac{\Gamma(p - \frac{n}{2} + 1)}{2^n \pi^{n/2} \Gamma(p+1)} \text{ for } p \geq \frac{n}{2}$$

such that

$$L^{\mathrm{cl}}(p,n) \leq L(p,n).$$

In [LW00], it is proven that the sharp constant for $p \geq 2$ and for $n \in \mathbb{N}$ is equal to this classical constant $L^{\mathrm{cl}}(p,n)$. For the case of $1 \leq p < 2$, improved estimate of the constant $L(p,n)$ has been established in [HLW00].

2.2 Nonself-adjoint Schrödinger operators with compact perturbation

2.2.1 Boundedness of Discrete Spectrum

In [Pav67], the spectral properties of the nonself-adjoint Schrödinger operator on the half-line with nonself-adjoint boundary condition has been studied. *That is*, a one-dimensional differential operator H_h on $L^2(0,\infty)$ is considered which is defined by the expression

$$H_h f = -f'' + V(x)f$$

with boundary condition

$$f(0) - hf'(0) = 0$$

where h is a complex number, $V(x)$ is a complex valued measurable function that satisfies

$$\int_0^\infty x|V(x)|dx < \infty.$$

If $V(x)$ is real valued then the above condition assures that $\sigma_{\mathrm{d}}(H_h)$ is finite and for a complex potential the finiteness of $\sigma_{\mathrm{d}}(H_h)$ is proved in [Nai52] assuming

$$\sup_{x>0}\{|V(x)|\exp(\epsilon x)\} < \infty \quad \text{for any } \epsilon > 0.$$

Several researchers have addressed this large disparity between the above two conditions for self-adjoint and nonself-adjoint cases. In [Pav67], the condition for finiteness of $\sigma_{\mathrm{d}}(H_h)$ for the case of complex valued $V(x)$ has been improved to

$$\sup_{x>0}\{|V(x)|\exp(\epsilon\sqrt{x})\} < \infty \quad \text{for any } \epsilon > 0.$$

It further asserts that the condition is optimal in the sense that there exist complex potentials satisfying

$$\sup_{x>0}\{|V(x)|\exp(\epsilon x^{\beta})\} < \infty \quad \text{for any } \epsilon > 0 \text{ and for } \beta \in (0, 1/2)$$

such that operator H_h has an infinite number of discrete eigenvalues. Also in the same article, a similar improvement is proved for Schrödinger operators in $L^2(\mathbb{R}^3)$ with complex potential.

The research work by [AAD01] is one of most referred articles in the field of nonself-adjoint Schrödinger operators. The authors have found bounds for complex eigenvalues of nonself-adjoint Schrödinger operator and resonances of self-adjoint Schrödinger operator. This also slightly improved the results given in [Pav67] about the conditions on the complex potential V to have a finite discrete spectrum. The two important results in this regard applicable for nonself-adjoint Schrödinger operators in $L^2(\mathbb{R})$ are the following

Theorem 2.1. *If the complex potential $V \in L^1(\mathbb{R}) \cap L^2(\mathbb{R})$, then every eigenvalue λ of $H := -\Delta + V$ which does not lie on the positive real line satisfies*

$$|\lambda| \leq \|V\|_1^2/4.$$

Theorem 2.2. *Let the potential V satisfies*

$$\|V(x)e^{\gamma x}\|_1 < \infty$$

for all $\gamma \in \mathbb{R}$. Then the number of eigenvalues of $H := -\Delta + V$ is finite and all the eigenvalues satisfy

$$|\lambda| \leq \frac{9}{4}\|V\|_1^2.$$

This article also describes and illustrates two numerical techniques for finding complex resonances of self-adjoint Schrödinger operators with exponentially decaying potential.

The case of potentials which are slowly decaying has been analysed in [DN02]. The authors have considered potentials of the form $V = W + X$ where $W \in L^1(\mathbb{R})$ and $X \in L_0^\infty(\mathbb{R})$ (A function $X \in L_0^\infty(\mathbb{R})$ *if and only if* X is bounded, measurable and $\lim_{|x|\to\infty} X(x) = 0$) and found useful bounds for the discrete spectrum of the operator $H := -\Delta + V$ defined on $L^2(\mathbb{R})$. They improved Theorem 2.1 and proved the same result for the complex potential $V \in L^1(\mathbb{R})$. Another important result proved in this article is about bounds of eigenvalues of Schrödinger operator with potentials $V \in L^p(\mathbb{R})$.

Theorem 2.3. *If $V \in L^p(\mathbb{R}), p > 1$ and $z = -\lambda^2$ is an eigenvalue of $H := -\Delta + V$, where $\lambda = \lambda_1 + \mathrm{i}\lambda_2$ and $\lambda_1 > 0$ then*

$$\lambda_1 \leq \mu = k^{q/2(q+1)}$$

and

$$|\lambda_2| \leq \sqrt{\frac{k^2}{4}\lambda_1^{-2/q} - \lambda_1^2}$$

where $k = \|V\|_p(2/q)^{1/q}$ and $1/p + 1/q = 1$.

2.2.2 Lieb-Thirring type Inequalities

Lieb-Thirring type inequalities for the case of complex valued potential are first appeared in [Fra+06]. In this article, an estimate is derived for the set of eigenvalues which are lying outside a cone about the positive real axis on the right half-plane.

Theorem 2.4. *Let $n \geq 1, p \geq \frac{n}{2} + 1$ and let the complex potential $V \in L^p(\mathbb{R}^n)$ and $\{\lambda_j\}$ be the eigenvalues of the operator $H := -\Delta + V$. If $\varkappa > 0$, then for eigenvalues outside the cone $\{z \in \mathbb{C} : Im(z) < \varkappa Re(z)\}$*

$$\sum_{Im(\lambda_j) \geq \varkappa Re(\lambda_j)} |\lambda_j|^{p-\frac{n}{2}} \leq C(p,n)\left(1 + \frac{2}{\varkappa}\right)^p \int_{\mathbb{R}^n} |V(\mathbf{x})|^p d\mathbf{x}.$$

This estimate is useful for discrete spectral elements which are converging to 0. Compared to the self-adjoint case (see Section 2.1) this result is weaker and it is evident from the conditions on γ.

The case of eigenvalues which are lying inside the cone $\{z \in \mathbb{C} : \mathrm{Im}(z) < \varkappa \mathrm{Re}(z), \varkappa > 0\}$ is analyzed in [LS09]. Their result provides information about the accumulation of eigenvalues to the positive real axis. This also contains bounds for the discrete spectrum of nonself-adjoint Schrödinger operator on $L^2(\mathbb{R}^n)$. Their main result is

Theorem 2.5. *Let $Re(V) \geq 0$ be a bounded function. Assume that $Im(V) \in L^p(\mathbb{R}^n)$, where $p > n/2$ if $d \geq 2$ and $p \geq 1$ if $n = 1$. Then the eigenvalues λ_j of the operator $H := -\Delta + V$ satisfy the estimate*

$$\sum_j \left(\frac{Im(\lambda_j)}{|\lambda_j + 1|^2 + 1} \right)_+^p \leq C(p, n) \int_{\mathbb{R}^n} (ImV(\mathbf{x}))_+^p d\mathbf{x}.$$

A more general result, in the sense that is involving all eigenvalues of Schrödinger operator is proved in [DHK09]. This result can also be compared directly with the results of the self-adjoint case.

Theorem 2.6. *Let $H := -\Delta + V$ acting on $L^2(\mathbb{R}^n)$, where $n \geq 1$. Suppose that $V \in L^p(\mathbb{R}^n)$ with $p \geq n/2 + 1$. Then for any $0 < \tau < 1$,*

$$\sum_{\lambda \in \sigma_d(H)} \frac{dist(\lambda, [0, \infty))^{p+\tau}}{|\lambda|^{\frac{n}{2}+\tau}} \leq C(p, n, \tau) \int_{\mathbb{R}^n} |V(\mathbf{x})|^p d\mathbf{x}.$$

This result too falls short of the corresponding result in the self-adjoint case in two counts (1) the presence of τ which can not be set to 0 as the constant C depends on τ and is not known to be bounded as $\tau \to 0$ (2) the restriction on p compared to the self-ajoint case.

Further in [DHK13b], the Lieb-Thirring type inequalities are derived for relative compact perturbation of self-adjoint operators using two different approaches. The approach based on complex analysis initially defines an analytic function whose zeros are exactly matching with the discrete spectral elements of the operator and derives the result. This approach applied to Schrödinger operators with relative compact perturbation yields the following results.

Theorem 2.7. *Let $H := -\Delta + V$ defined on $L^2(\mathbb{R}^n)$ with $V \in L^p(\mathbb{R}^n)$, where $p \geq 2$ if $n \leq 3$ and $p > n/2$ if $n > 4$. Then for $\tau \in (0,1)$ the following holds:*

1. *If $p \geq n - \tau$ then*

$$\sum_{\lambda \in \sigma_d(H)} \frac{dist(\lambda, [0,\infty))^{p+\tau}}{|\lambda|^{\frac{n}{2}}(|\lambda|+a)^{2\tau}} \leq C(p,n,\tau)a^{-\tau} \int_{\mathbb{R}^n} |V(\mathbf{x})|^p d\mathbf{x}$$

2. *If $p < n - \tau$ then*

$$\sum_{\lambda \in \sigma_d(H)} \frac{dist(\lambda, [0,\infty))^{p+\tau}}{|\lambda|^{\frac{p+\tau}{2}}(|\lambda|+a)^{\frac{n-p+3\tau}{2}}} \leq C(p,n,\tau)a^{-\tau} \int_{\mathbb{R}^n} |V(\mathbf{x})|^p d\mathbf{x}$$

Here $a > 0$ is such that

$$Re(\lambda) < -a \Rightarrow \|(\lambda - H)^{-1}\| \leq |Re(\lambda) + a|^{-1}.$$

Note that compared to the restrictions on p in [DHK09] this is an improved result.

2.2.3 Number of Eigenvalues

For a self-adjoint Schrödinger operator on the half-line, it is given that ([Bar52]) the number of eigenvalues is bounded by $\int |x||V(x)|dx$. But for non-self-adjoint case it is proved that ([Pav61; Pav62; Pav67]) there exists a potential which is decaying at the rate of $e^{-cx^{\alpha}}$, $c > 0$, $0 < \alpha < 1/2$ but has countably infinite numebr of eigenvalues. It is also proven that if $|V(x)| \leq Ce^{-cx^{1/2}}$ for some $C, c > 0$ then the operator has only finite number of eigenvalues. Estimate for number of eigenvalues for the case of nonself-adjoint Schrödinger with finite descrete spectrum were analyzed by several authors and is a very active topic even today (see [Ste14; FLS16; Ste17]). The estimate for the number of eigenvalues $|\sigma_{\mathrm{d}}(-\Delta+V)|$ of Schrodinger operator in $L^2(\mathbb{R}^3)$ with compactly supported or exponentially decaying complex potential V has been discussed in [Ste14]. In [FLS16], the authors have considered nonself-adjoint Schrödinger operator in $L^2(\mathbb{R}^n)$ with exponentially decaying potential in odd dimension (n is odd) and proved the following estimate.

Theorem 2.8. *The number of eigenvalues of $H := -\frac{d}{dx^2} + V$ in $L^2(\mathbb{R}_+)$ with a Dirichlet boundary condition, counting algebraic multiplicities, satisfies, for any $\epsilon > 0$,*

$$|\sigma_d(H)| \leq \frac{1}{\epsilon^2}\left(\int\limits_0^\infty e^{\epsilon x}|V(x)|dx\right)^2 .$$

Theorem 2.9. *Let $n \geq 3$ and be odd. Then the number of eigenvalues of $H := -\Delta + V$ in $L^2(\mathbb{R}^n)$, counting algebraic multiplicities, satisfies, for any $\epsilon > 0$,*

$$|\sigma_d(H)| \leq \frac{C_n}{\epsilon^2}\left(\int_{\mathbb{R}^n} e^{\epsilon|\mathbf{x}|}|V(\mathbf{x})|^{\frac{n+1}{2}}d\mathbf{x}\right)^2$$

where C_n depends only on n.

Chapter 3

Discrete Spectrum of One-Dimensional Schrödinger Operators

This chapter contains our analysis on the discrete spectrum of nonself-adjoint Schrödinger operator in $L^2(0,\infty)$ which satisfies Dirichlet condition at 0. Our analysis considers a holomorphic function $H(z)$ defined on the complex plane $\mathbb{C}$ whose values are Schrödinger operators, then finds the movement of the discrete spectrum of $H(z)$ as z varies in $\mathbb{C}$. If $H(z_0)$ is self-adjoint for some z_0, then the existence of min-max principles and spectral theorem make it relatively easy to find the discrete spectrum which lies on the negative real axis. In this work, our idea is to obtain the discrete spectrum of a nonself-adjoint Schrödinger operator, say $H(z_1)$, from the discrete spectrum of a self-adjoint Schrödinger operator, say $H(z_0)$, as it evolves analytically or continuously. Section 3.1 introduces the topic and Section 3.2 discusses the preliminary results required for our analysis. The evolution of discrete spectrum of Schrödinger operator with compactly supported complex potential is studied in Section 3.3. The result is further extended to the case of potentials V with $\int_0^\infty x|V(x)|dx < \infty$ in Section 3.4. Though our result about potentials with compact support can be deduced from Section 3.4, we keep the analysis separate and prove the result in a different way in

Section 3.3. Finally a simple example is provided in Section 3.5 to illustrate the evolution of discrete spectrum.

3.1 Introduction

We consider the operator valued analytic function

$$H(z) = -\frac{d^2}{dx^2} + V_0 + zV_1 \tag{3.1}$$

defined on the complex plane $\mathbb{C}$, where V_0, V_1 are real valued bounded measurable functions vanishing sufficiently rapidly as $|x| \to \infty$. $H(z)$ is a Schrödinger operator in $L^2(0, \infty)$ with domain $\text{Dom}(H(z)) = \{f \in L^2(0, \infty) : f', f'' \in L^2(0, \infty), f(0) = 0\}$. In this work, continuous evolution of the discrete spectrum of $H(z)$ is studied as z varies along a continuous path in $\mathbb{C}$. In particular, as z varies along the imaginary line from 0 to i, the evolution of the discrete spectrum of the self-adjoint operator $H(0) = -\frac{d^2}{dx^2} + V_0$ is of special interest to us.

The distribution of the discrete spectrum of selfadjoint Schrödinger operator has been studied extensively, the same is not the case with non-selfadjoint Schrödinger operator. The spectral theorem and min-max principles for the selfadjoint case play major role in its theoretical development, whereas such tools are not available for non-selfadjoint operators. Each non-selfadjoint problem needs to be studied separately. Our effort to extract some information on the discrete spectrum of the non-selfadjoint Schrödinger operator

$$H(i) = -\frac{d^2}{dx^2} + V_0 + iV_1 \tag{3.2}$$

using the discrete spectrum of corresponding self-adjoint Schrödinger operator

$$H(0) = -\frac{d^2}{dx^2} + V_0 \tag{3.3}$$

is quite a different approach and we intend to prove the following result.

Theorem 3.2. *If V_0 and V_1 are such that $\int_0^\infty x|V_j(x)|dx < \infty$, $j = 0, 1$ and let κ_1 be in the discrete spectrum of $H(i)$ then there exist (1) t_0 ($0 \leq t_0 < 1$), (2) a real number κ_0, a member in the discrete spectrum or a spectral singularity of the operator $H(it_0)$ and (3) a continuous path $\kappa(t)$ such that $\kappa(0) = \kappa_0$, $\kappa(1) = \kappa_1$ and each $\kappa(t)$, $0 < t \leq 1$, is a discrete eigenvalue of the operator $H(i(t_0 + t))$.*

3.2 Potentials with Compact Support

We assume initially, that V_0 and V_1 are bounded, continuous (except for finite number of jump discontinuity) and compactly supported real functions, then it follows from [AAD01] that the spectrum of the operator $H(z)$ consists of the essential spectrum $\sigma_{ess}(H) = [0, \infty)$ and a finite number of discrete eigenvalues. Further $H(z)$ is an operator valued analytic function (in fact an analytic function of type (A), see Section 1.10) and hence from [Kat80, p. 370], the finite system of eigenvalues of $H(z_0)$ are branches of one or several analytic functions that have at most algebraic singularities near $z = z_0$. Also it follows from [Kat80] that if $\kappa(z) = -\lambda^2(z)$, with $\mathrm{Re}(\lambda(z)) > 0$, is a member of the discrete spectrum of $H(z)$ and is analytic at z, then its derivative

$$\kappa'(z) = \frac{\langle V_1\phi(z,\cdot), \bar{\phi}(z,\cdot)\rangle}{\langle \phi(z,\cdot), \bar{\phi}(z,\cdot)\rangle} = \frac{\int_0^\infty V_1(x)\phi^2(z,x)dx}{\int_0^\infty \phi^2(z,x)dx} \tag{3.4}$$

where $\phi(z,\cdot)$ is the normalized eigenfunction of $H(z)$ corresponding to $\kappa(z)$.

Before proceeding, it is desirable to state few results which are useful in our discussion.

Lemma 3.1. *[San79, p. 136] Let the differential equation $\mathbf{x}' = f(t, \mathbf{x}, \lambda)$, t a scalar variable, $\mathbf{x} = (x_1, x_2, \ldots, x_n)$ and $\lambda = (\lambda_1, \lambda_2, \ldots, \lambda_\nu)$ be given,* *where $f(t, \mathbf{x}, \lambda)$ and $\partial f / \partial x_i$ are defined and continuous in some domain B contained in $\mathbb{R}^{n+\nu+1}$. If $(t_0, \mathbf{x}_0, \lambda_0)$ belongs to B, then there exist positive numbers r and p such that*

1. *Given any λ such that $\|\lambda - \lambda_0\| \leq p$, there exists a unique solution $\mathbf{x} = \mathbf{x}(t, \lambda)$ of the given differential equation, defined for $|t - t_0| \leq r$ and satisfying $\mathbf{x}(t_0, \lambda) = \mathbf{x}_0$.*

2. *The solution $\mathbf{x} = \mathbf{x}(t, \lambda)$ is a continuous function of t and λ.*

Lemma 3.2. *[HS74, p. 169] Let $W \subset E$ be open in $\mathbb{R}^n$ and suppose $f : W \to E$ has Lipschitz constant K. Let $\mathbf{y}(t)$, $\mathbf{z}(t)$ be solutions to*

$$\mathbf{x}' = f(\mathbf{x}) \tag{3.5}$$

on the closed interval $[t_0, t_1]$. Then for all $t \in [t_0, t_1]$:

$$|\mathbf{y}(t) - \mathbf{z}(t)| \leq |\mathbf{y}(t_0) - \mathbf{z}(t_0)| \exp(K(t - t_0)).$$

Lemma 3.1 talks about the continuity of the solution of differential equation with respect to the coefficient parameters, and Lemma 3.2 is about the continuity with respect to the initial conditions. Combining both we will have the following result for a second order linear differential equation.

Lemma 3.3. *Let the second order linear differential equation $x'' + p_n(t)x' + q_n(t)x = r_n(t)$ be given. $p_n(t)$, $q_n(t)$, and $r_n(t)$ be continuous on $[a, b]$ and $p_n \to p$, $q_n \to q$, and $r_n \to r$ uniformly on $[a, b]$. Let $x_n(t)$ be the solution of the differential equation on $[a, b]$ satisfying the initial conditions: $x_n(a) = \alpha_n$, $x_n'(a) = \beta_n$. Also assume that $\alpha_n \to \alpha$ and $\beta_n \to \beta$. Then $x_n \to x$ uniformly on $[a, b]$, where $x(t)$ is the solution of the differential equation satisfying $x(a) = \alpha$, $x'(a) = \beta$.*

3.3 Evolution of the Discrete Spectrum

Consider any path in the complex plane $\mathbb{C}$ traced by z starting from 0, then each of the discrete spectral element of $H(z)$ moves in the complex plane until it ceases to exist as a discrete spectrum member. And it follows from [Kat80] that this movement is analytic except for isolated points of algebraic singularities. If z varies along the real line, then $H(z)$ is a family of self-adjoint operators and the discrete eigenvalues, if exist, move on the negative real axis and all are simple (see Lemma 3.4). Let κ_0 be an eigenvalue of $H(0)$ and as z varies from 0 to ∞ over the positive real line, the eigenvalue $\kappa(z)$ starts moving continuously (analytically) from κ_0 and if we further assume V_1 is positive on its support then at some $\zeta > 0$ the path traced by $\kappa(z)$ terminates (if we choose a large $\zeta > 0$ for which $V_0+\zeta V_1 \geq 0$, then the entire discrete spectrum of $H(z)$ disappears). On the other hand as z varies along the negative real axis, $\kappa(z)$ moves further to negative side and remains as analytic function since its derivative $\int_0^\infty V_1\phi^2(z,x)dx > 0$, $\phi(z,x)$ is the normalized real eigenfunction corresponding to $\kappa(z)$.

As z varies along the imaginary axis starting from 0, then the discrete eigenvalues start moving along/opposite to the imaginary axis direction as analytic functions are conformal wherever derivative is non-zero. More precisely, if $V_1 \geq 0$, then as z moves in the positive imaginary axis, $\kappa(z)$ also moves with tangent along the positive imaginary axis. For small values of imaginary $z = it$, the eigenvalue can be approximated as $\kappa(z) = \kappa(0) + it\int_0^a V_1\phi^2(z,x)dx$, where $[0,a]$ is the support of $V_j, j = 0, 1$.

In general, as z varies over a continuous path in the complex plane, the eigenvalue $\kappa(z)$ also moves continuously until it ceases to be an eigenvalue. The function $\kappa(z)$ is analytic except at those points where it meets one or more such functions determined by the discrete spectrum of $H(z)$ or in other words the algebraic multiplicity of $\kappa(z)$ exceeds one. The following lemma characterizes this situation and it is an elementary result.

Lemma 3.4. *All the discrete eigenvalues of $H(z)$ are of geometric multiplicity one. And an eigenvalue $\kappa(z) = -\lambda^2(z)$ with eigenfunction $\phi(z,x)$ is not simple* if and only if

$$\int_0^\infty \phi^2(z,x)dx = 0.$$

Proof. First it is observed that if $\kappa(z) = -\lambda^2(z)$, with $\mathrm{Re}(\lambda(z)) > 0$, is an eigenvalue of $H(z)$ and the support of $V(z) = V_0 + zV_1$ is $[0,a]$, then the corresponding eigenfunction $\phi(z,x)$ satisfies:

$$\phi(z,x) = b\,\mathrm{e}^{-\lambda(z)x}, \quad \text{for } \; x \geq a \tag{3.6}$$

for some non-zero b.

Let $\phi_1(z,x)$, $\phi_2(z,x)$ be two eigenfunctions corresponding to $\kappa(z)$, then there exist non-zero b_1 and b_2 such that, $\phi_1(z,x) = b_1\mathrm{e}^{-\lambda(z)x}$ and $\phi_2(z,x) = b_2\mathrm{e}^{-\lambda(z)x}$ for $x \geq a$. Thus $\phi(z,x) = b_2\phi_1(z,x) - b_1\phi_2(z,x)$ is the unique solution of the differential equation

$$-\frac{d^2\phi(z,x)}{dx^2} + V(z)\phi(z,x) = -\lambda^2(z)\phi(z,x)$$

on $[0,a]$ satisfying the condition $\phi(z,a) = 0$ and $\phi'(z,a) = 0$, prime denotes derivative with respect to x. Thus $\phi(z,x) = 0$ or the geometric multiplicity of $\kappa(z)$ is one.

Now suppose $\kappa(z) = -\lambda^2(z)$ is not simple. Then $(H(z) + \lambda^2(z))^2\psi(z,x) = 0$ and $(H(z) + \lambda^2(z))\psi(z,x) \neq 0$ for some $\psi(z,x) \neq 0$ in $\mathrm{Dom}(H(z))$. Since the geometric multiplicity of $-\lambda^2(z)$ is one,

$$(H(z) + \lambda^2(z))\psi(z,x) = c\phi(z,x) \tag{3.7}$$

for some $c \neq 0$, where $\phi(z,x)$ is the normalized eigenfunction of $H(z)$ corresponding to $\kappa(z) = -\lambda^2(z)$. So we also have

$$(H(z) + \lambda^2(z))\phi(z,x) = 0. \tag{3.8}$$

From (3.7) and (3.8),

$$c\int_0^\infty \phi^2(z,x)dx = \int_0^\infty \frac{d}{dx}(\psi(z,x)\phi'(z,x) - \phi(z,x)\psi'(z,x))dx = 0.$$

Conversely assume that

$$\int_0^\infty \phi^2(z,x) = 0.$$

Since $\phi(z,x) = b\mathrm{e}^{-\lambda(z)x}$ is on $[a,\infty)$, the function $\psi(z,x) = \frac{1}{2\lambda(z)}bx\mathrm{e}^{-\lambda(z)x}$ is a solution of $(H(z) + \lambda^2(z))\psi(z,x) = \phi(z,x)$ on $[a,\infty)$. Extend the function $\psi(z,x)$ as a unique solution of $(H(z) + \lambda^2(z))\psi(z,x) = \phi(z,x)$ on $[0,a]$ satisfying the conditions, which makes ψ and ψ' continuous at $x = a$. Thus we have a function $\psi(z,x)$ on $[0,\infty)$ such that $\psi'(z,x)$, $\psi''(z,x)$ are in $L^2(0,\infty)$ and it satisfies Equation 3.7. Repeating the same process as before we arrive at

$$\int_0^\infty \frac{d}{dx}(\psi(z,x)\phi'(z,x) - \phi(z,x)\psi'(z,x))dx = \int_0^\infty \phi^2(z,x)dx = 0.$$

$$\implies \psi(z,a)\phi'(z,a) = 0 \implies \psi(z,a) = 0$$

This proves the existence of a function ψ in the domain of $H(z)$, such that $(H(z) + \lambda^2(z))\psi(z,x) \neq 0$ and $(H(z) + \lambda^2(z))^2\psi(z,x) = 0.$ $\square$

Next it is shown that if the curve traced by the discrete eigenvalue $\kappa(z)$ of $H(z)$ as z traces a curve in the complex plane terminates, then it terminates at the essential spectrum $[0,\infty)$ of $H(z)$.

Theorem 3.1. *Let $z = \gamma(t)$ be a path in $\mathbb{C}$ and let κ_0 be an eigenvalue of $H(\gamma(0))$. As z moves along the path $\gamma(t)$ starting from $\gamma(0)$, the eigenvalue* *traces a continuous path in $\mathbb{C}$, say $\kappa(\gamma(t))$ starting from κ_0. Assume that this path terminates at t_1 and let $\gamma(t_1) = \zeta$. Then $\kappa(\zeta) = \lim_{t \to t_1 -} \kappa(\gamma(t)) \geq 0$.*

Proof. Let us take $\kappa(z) = -\lambda^2(z)$. Since $z \to \zeta$, through a path in $\mathbb{C}$, we can find a sequence z_n in the path with $z_n \to \zeta$ and hence $-\lambda^2(z_n) \to -\lambda^2(\zeta)$. Since $-\lambda^2(z_n)$ is an eigenvalue of $H(z_n)$, we have $\mathrm{Re}(\lambda_n(z)) > 0 \ \Rightarrow \mathrm{Re}(\lambda(\zeta)) \geq 0$. Assume that $\mathrm{Re}(\lambda(\zeta)) > 0$, we will derive a contradiction.
For $x \geq a$, $H(z_n) + \lambda^2(z_n) = -\frac{d^2}{dx^2} + \lambda^2(z_n)$ and hence the corresponding eigenfunction is $\phi(z_n, x) = b(z_n)\mathrm{e}^{-\lambda(z_n)x}$. Without loss of generality we choose $b(z_n) = 1$. Thus for $x \geq a$, $\phi(z_n, x) = \mathrm{e}^{-\lambda(z_n)x} \to \mathrm{e}^{-\lambda(\zeta)x}$ uniformly.

On $[0, a]$, $\phi(z_n, x)$ is the solution of the differential equation

$$-\frac{d^2\phi(z_n, x)}{dx^2} + (V_0 + z_n V_1 + \lambda^2(z_n))\phi(z_n, x) = 0$$

satisfying the conditions

$$\phi(z_n, a) = \mathrm{e}^{-\lambda(z_n)a} \ \text{ and } \ \phi'(z_n, a) = -\lambda(z_n)\mathrm{e}^{-\lambda(z_n)a}.$$

Therefore using Lemma 3.3, $\phi(z_n, x) \to \phi(\zeta, x)$ uniformly on $[0, a]$, where $\phi(\zeta, x)$ satisfies the differential equation

$$\frac{-d^2\phi(\zeta, x)}{dx^2} + (V_0 + \zeta V_1)\phi(\zeta, x) = -\lambda^2(\zeta)\phi(\zeta, x) \tag{3.9}$$

on $[0, a]$ and $\phi(\zeta, a) = \mathrm{e}^{-\lambda(\zeta)a}$, $\phi'(\zeta, a) = -\lambda(\zeta)\mathrm{e}^{-\lambda(\zeta)a}$. Since $\phi(z_n, 0) = 0$ for all n, $\phi(\zeta, 0) = 0$. Thus we have proved that $\phi(z_n, x) \to \phi(\zeta, x)$ in $L^2(0, \infty)$, $\phi(\zeta, 0) = 0$ and satisfy the differential Equation 3.9. And hence $-\lambda^2(\zeta)$ is an eigenvalue of $H(\zeta)$, a contradiction. □

If κ_1 is a discrete spectrum member of $H(i) = -\frac{d^2}{dx^2} + V_0 + iV_1$. As $z := it$ moves from i to 0 (that is, t from 1 to 0) along the imaginary axis, κ_1 evolves continuously (analytically except for those points mentioned in Lemma 3.4) to trace a path $\kappa(t)$ in $\mathbb{C}$ and the above result ensures that either of the two possibilities occur:

1. $\kappa(t)$ reaches the negative real line at $\kappa(0) = \kappa_0$, a discrete eigenvalue of the self-adjoint operator $H(0) = -\frac{d^2}{dx^2} + V_0$.
2. $\kappa(t)$ reaches $[0, \infty)$ at κ_0, a spectral singularity of $H(it_0)$, $0 \leq t_0 < 1$.

This proves the statement of Theorem 3.2 for compact potentials. But for compactly supported potentials a more general result is possible.

We have the following definitions ([AAD01]):

Definition 3.3.1. Let $\kappa = -\lambda^2$ be a complex number and there exists a function $\phi(x)$ which satisfies the following conditions:

$$-\phi''(x) + V(x)\phi(x) = -\lambda^2\phi(x), \text{ on } [0, \infty)$$

$$\phi(0) = 0$$

$$\phi(x) = e^{-\lambda x} + o(|e^{\lambda x}|), \text{ as } x \to \infty.$$

Then if $\mathrm{Re}(\lambda) < 0$, κ is a **resonance** of the operator $H = -\frac{d^2}{dx^2} + V$ defined on the domain $\{f \in L^2(0, \infty) : f', f'', Vf \in L^2(0, \infty)$ and $f(0) = 0\}$. If $\mathrm{Re}(\lambda) = 0$, then κ is a **spectral singularity**.

For compactly supported potentials, a perturbation of the potential gives rise to a same order of variation in the resonances of the Schrödinger operator ([Agm98]). That is to say that the resonances of $H(z)$ move continuously with respect to z, provided $H(z)$ is not the free Schrödinger operator for any z (see Section 3.5). Thus we have the following:

Corollary 3.1.1. *Let $V_0 \neq 0$, then for any discrete eigenvalue κ_1 of $H(i)$, there exists a discrete eigenvalue, or a spectral singularity or a resonance κ_0 of the self-adjoint operator $H(0)$ such that κ_1 is continuously evolved from κ_0 as z varies along the imaginary line from 0 to i. That is, there exists a* *continuous path $\kappa(t)$ such that $\kappa(0) = \kappa_0$, $\kappa(1) = \kappa_1$ and each $\kappa(t)$ is a discrete eigenvalue, or a spectral singularity or a resonance of the operator $H(it)$.*

In fact, if $U \neq 0$, $V \neq 0$ are two compactly supported, complex continuous (except for jump discontinuity) functions on $[0, \infty)$, then any discrete eigenvalue of $H_V = -\frac{d^2}{dx^2} + V$ is evolved from a discrete eigenvalue, spectral singularity, or a resonance of $H_U = -\frac{d^2}{dx^2} + U$. This follows immediately from a similar analysis on the operator valued analytic function $H(z) = -\frac{d^2}{dx^2} + U + z(V - U)$. If V is a multiple of U, then it can happen that $U + z(V - U) = 0$ for some $0 \leq z \leq 1$. In this situation consider a different path so that the potential changes from U to V without taking 0 on that path (see Section 3.5).

Corollary 3.1.2. *Let $M = \max\{|V_1(x)| : x \in [0, a]\}$, κ_0 be a discrete eigenvalue of the self-adjoint operator $H(0) = -\frac{d^2}{dx^2} + V_0$. Let γ be a path in $\mathbb{R}$, say $\gamma(t) = t$, and $\kappa(t)$ be the path traced by discrete eigenvalue or spectral singularity or resonance of $H(t)$ with $\kappa(0) = \kappa_0$ as t varies over the real line starting from 0. Then for $|t| < |\kappa_0|/M$, $\kappa(t)$ remains to be a discrete eigenvalue of $H(t)$. In particular, if κ_0 is the discrete eigenvalue of $H(0)$ nearest to 0 then*

$$|\sigma_d(H(t))| \geq |\sigma_d(H(0))|$$

for real t with $|t| < |\kappa_0|/M$.

Proof. As t varies from 0 through the real line, the discrete eigenvalue $\kappa(t)$ starts from the negative real number κ_0 and moves analytically as a discrete eigenvalue of $H(t)$ until it reaches 0. Assume that at $t = t_0$ it reaches 0. Then

$$0 = \kappa_0 + \lim_{t \to t_0} \int_0^t \int_0^a V_1(x)\phi^2(s, x) dx\, ds$$

$$\Rightarrow |\kappa_0| \leq M|t_0|$$

here $\phi(s, \cdot)$ represents the normalized eigenfunction of $H(s)$ corresponding to $\kappa(s)$.

Hence $\kappa(t)$ remains to be an eigenvalue of $H(t)$, if $t \in \mathbb{R}$ is such that $|t| < |\kappa_0|/M$.

It immediately follows that if κ_0 is the discrete eigenvalue of $H(0)$ nearest to 0, then for real t with $|t| < |\kappa_0|/M$,

$$|\sigma_{\mathrm{d}}(H(t))| \geq |\sigma_{\mathrm{d}}(H(0))|.$$

$\square$

It is been observed in the beginning of this section that as z moves along the imaginary line starting from 0, each of the discrete eigenvalues of $H(z)$ starts moving in or opposite to the direction of imaginary axis. So one would expect, in general, a better estimate than the previous result.

Conjecture. If $V_1 > 0$ (or $V_1 < 0$) on $[0, a]$, the support of V_0 and V_1, then each of the discrete eigenvalue of the self-adjoint operator $H(0)$ continuously evolves to a discrete eigenvalue of $H(it)$ for any $t \in \mathbb{R}$. In particular

$$\left|\sigma_{\mathrm{d}}\left(-\frac{d^2}{dx^2} + V_0 + iV_1\right)\right| \geq \left|\sigma_{\mathrm{d}}\left(-\frac{d^2}{dx^2} + V_0\right)\right|$$

where the discrete eigenvalues are counted according to multiplicity.

3.4 A More General Case

In this section we assume that V_0, V_1 are bounded real measurable functions satisfying

$$\int_0^\infty x|V_j(x)|dx < \infty, \quad j = 0, 1. \tag{3.10}$$

Here the operator $H(z) = -\frac{d^2}{dx^2} + V_0 + zV_1$ is a compact perturbation of the free Schrödinger operator and hence its spectrum consists of essential spectrum $\sigma_{ess} = [0, \infty)$ and a countable number of discrete eigenvalues which can only accumulate to a point in the essential spectrum $[0, \infty)$. The spectral analysis of Schrödinger operator on the half-line with potential satisfying condition (3.10) has been carried out by several authors (see [Pav67] and references therein). Our approach is similar to the one in the previous section.

We start with presenting information required for our analysis. It is known that if a complex potential $V(x)$ has the property stated in (3.10), then the equation

$$-y'' + V(x)y = -\lambda^2 y, \quad \mathrm{Re}(\lambda) \geq 0 \tag{3.11}$$

has a unique solution $\phi(\lambda, x)$ satisfying the condition $\phi(\lambda, x)\,\mathrm{e}^{\lambda x} \to 1$ as $x \to \infty$. The function $\phi(\lambda, x)$ also satisfies ([AM59; Pav67]) the following estimates

$$|\phi(\lambda, x) - \mathrm{e}^{-\lambda x}| \leq K\,\mathrm{e}^{-\mathrm{Re}(\lambda)x} \int_x^\infty t|V(t)|dt, \quad \mathrm{Re}(\lambda) \geq 0, \tag{3.12}$$

$$|\phi_x(\lambda, x) + \lambda\,\mathrm{e}^{-\lambda x}| \leq K\,\mathrm{e}^{-\mathrm{Re}(\lambda)x} \int_x^\infty |V(t)|dt, \quad \mathrm{Re}(\lambda) \geq 0. \tag{3.13}$$

The famous Arzelà-Ascoli theorem (see [Rud76]) which is used in the proof of Theorem 3.2 is stated below.

Arzelà-Ascoli theorem *Consider a sequence of continuous functions $\{f_n\}_{n\in\mathbb{N}}$ defined on a compact subset of $\mathbb{R}^N$. If this sequence is uniformly bounded and equicontinuous, then there exists a subsequence $\{f_{n_k}\}_{k\in\mathbb{N}}$ that converges.*

Now we prove Theorem 3.2.

Proof. It is sufficient to prove the statement of Theorem 3.1 in this more general case of potentials. That is, if a sequence $z_n \to \zeta$ in $\mathbb{C}$ and discrete eigenvalue $\kappa(z_n) = -\lambda^2(z_n)$ of $H(z_n)$ converges to $\kappa(\zeta) = -\lambda^2(\zeta)$, then $\kappa(\zeta)$ is either a discrete eigenvalue or a spectral singularity of the operator $H(\zeta)$.

Suppose $\phi(z_n, x)$ be the corresponding unique eigenfunction that satisfies Equations 3.12, 3.13 and $\phi(z_n, x)\mathrm{e}^{\lambda(z_n)x} \to 1$. Since $|\phi(z_n, x)| \leq |\phi(z_n, x) - \mathrm{e}^{-\lambda(z_n)x}| + \mathrm{e}^{-\mathrm{Re}(\lambda(z_n))x}$ and $\mathrm{Re}(\lambda(z_n)) > 0$, it follows from the estimate (3.12) that $\{\phi(z_n, x)\}$ is a uniformly bounded sequence. In similar lines estimate (3.13) ensures that $\{\phi_x(z_n, x)\}$ is uniformly bounded or the sequence $\{\phi(z_n, x)\}$ is equicontinuous. Therefore by Arzelà-Ascoli theorem $\phi(z_n, x) \to \phi(\zeta, x)$ uniformly on any compact subset of $[0, \infty)$ and we will have $\phi(\zeta, x)\mathrm{e}^{\lambda(\zeta)x} \to 1$, $-\phi''(\zeta, x) + (V_0(x) + \zeta V_1(x))\phi(\zeta, x) = -\lambda^2(\zeta)\phi(\zeta, x)$, $\phi(\zeta, 0) = 0$. Thus if $\mathrm{Re}(\lambda(\zeta)) > 0$ then $\kappa(\zeta)$ is an eigenvalue otherwise (that is, if $\mathrm{Re}(\lambda(\zeta)) = 0$) it is a spectral singularity. $\square$

The following result can be proved the same way as it is done in the previous section.

Corollary 3.1.3. *Let* $M = \sup\{|V_1(x)| : x \in [0, \infty)\}$, κ_0 *be a discrete eigenvalue of the self-adjoint operator* $H(0) = -\frac{d^2}{dx^2} + V_0$. *Let* γ *be a path in* $\mathbb{R}$, *say* $\gamma(t) = t$, *and* $\kappa(t)$ *be the path starting at* κ_0 *traced by discrete eigenvalues, or spectral singularities or resonances of* $H(t)$ *as* t *varies over the real line starting from* 0. *Then for* $|t| < |\kappa_0|/M$, $\kappa(t)$ *remains to be a discrete eigenvalue of* $H(t)$. *In particular, if* κ_0 *is the discrete eigenvalue of* $H(0)$ *nearest to* 0 *then*

$$|\sigma_d(H(t))| \geq |\sigma_d(H(0))|$$

for real t *with* $t < |\kappa_0|/M$.

3.5 An Example

In this section we demonstrate the continuous movement of resonances and discrete spectrum of Schrödinger operators with potentials that are constant on their support. Consider the potential V defined on $[0, \infty)$ by

$$V = \begin{cases} -k^2 & \text{on } [0,1] \\ 0 & \text{elsewhere.} \end{cases} \tag{3.14}$$

Let $\kappa = -\lambda^2$ be an eigenvalue of the Schrödinger operator $H = -\frac{d^2}{dx^2} + V$ with domain $\mathrm{Dom}(H) = \{f : f, f', f'' \in L^2(0,\infty), f(0) = 0\}$, then there exists ϕ such that $H\phi = -\lambda^2\phi$, $\phi(0) = 0$, and $\phi,\ \phi',\ \phi'' \in L^2(0,\infty)$. All these conditions imply that $\mathrm{Re}(\lambda) > 0$ and

$$f(\lambda) = \lambda \sin(\sqrt{k^2 - \lambda^2}) + \sqrt{k^2 - \lambda^2} cos(\sqrt{k^2 - \lambda^2}) = 0 \tag{3.15}$$

which is the characteristic equation for the eigenvalue problem of the given operator. Also note that the spectral singularities and resonances of the given Schrödinger operator are also obtained from the above equation. They are $\kappa = -\lambda^2$ where λ satisfies the characteristic equation (other than $\pm k$) with $\mathrm{Re}(\lambda) = 0$ (spectral singularity)and $\mathrm{Re}(\lambda) < 0$ (resonance).

If the value of V on $[0, 1]$ is real, then the operator is a self-adjoint operator and all its eigenvalues are real and complex resonances exist in symmetric pairs. Consider a complex value $-k^2 + \zeta(t)$ on $[0, 1]$ for the potential V, where $\zeta(t)$ is a continuous path in $\mathbb{C}$. By Theorem 3.1, as t moves over the real line the eigenvalues or resonances of the operator move continuously in the complex plane and an eigenvalue moves to the resonance set through the positive real axis $[0, \infty)$ (which is the essential spectrum of the operator) and vice versa.

In particular, if we assume the value $-k^2 + t$ (k^2 is real) for V on $[0, 1]$, as t varies over the real line the eigenvalues analytically move over the negative real axis until they touch 0 and move to the resonance set. A complex pair of symmetric resonances traces a pair of symmetric curves until they meet at the real axis and at this meeting point $f'(\lambda) = 0$. That is

$$(\lambda + 1)\left[\sin(\sqrt{k^2 - \lambda^2}) - \frac{\lambda}{\sqrt{k^2 - \lambda^2}}\cos(\sqrt{k^2 - \lambda^2})\right] = 0. \qquad (3.16)$$

This gives either $\lambda = -1$ or

$$\sqrt{k^2 - \lambda^2}\sin(\sqrt{k^2 - \lambda^2}) - \lambda\cos(\sqrt{k^2 - \lambda^2}) = 0.$$

The above expression along with the characteristic equation $f(\lambda) = 0$ implies that $k = 0$ and $\exp(\lambda) = 0$. Thus the symmetric complex resonances meet in $\mathbb{R}$ at $-\lambda^2 = -1$ and at this point characteristic equation becomes

$$\tan(\sqrt{k^2 - 1}) = \sqrt{k^2 - 1}. \qquad (3.17)$$

That is, a pair of complex resonances meet at -1 as t varies over real line and at this meeting point the potential takes the value $-k^2 + t = -(\theta^2 + 1)$ on $[0, 1]$, where θ is a solution of the equation $\tan\theta = \theta$. Each interval $[n\pi, (2n + 1)\pi/2]$ for $n = 0, 1, 2, \ldots$ contains a solution θ_n of $\tan\theta = \theta$. But as $-k^2 + t \to -1 = -(\theta_0^2 + 1)$ it can be seen that the only real resonance (antibound state) of the operator reaches -1. As t moves further to the negative side, different complex symmetric pairs of resonances move symmetrically with respect to the real axis and meet at -1 as the value of the potential on $[0, 1]$ becomes $-k^2 + t = -(\theta_n^2 + 1), n = 1, 2, \ldots$. This is shown in Figure 3.1. This figure is zoomed about -1 and is shown in Figure 3.2. These figures show the movement of few symmetric pairs of resonances as the potential takes the value $-0.5 + t$ on $[0, 1]$, t varies from 0 to the negative side of the real line. The movement of the symmetric curve is restricted in these figures and is shown up to their meeting point -1

on the real line. As t moves further to the negative side, this symmetric pair of resonances once met at -1 keep moving in real line, one towards the negative side and the other towards the positive side. The resonance moving towards the positive side meets the positive real axis at 0 and re-bounces back as an eigenvalue. This is illustrated in Figure 3.3. The potential at which it meets the real axis is obtained from the characteristic equation by substituting $\lambda = 0$ in it and the corresponding potential is $-[(2n+1)\pi/2]^2$, for $n = 0, 1, 2, \ldots$. Thus we have the following:

Proposition 3.1. *Let $n \in \mathbb{N}$. If the potential V is a real constant, say $-k^2$, on its support $[0,1]$ and $[(2n-1)\pi/2]^2 < k^2 \leq [(2n+1)\pi/2]^2$ then the above Schrödinger operator has exactly n eigenvalues. If $K_n = \theta_n^2 + 1$ where θ_n is the root of $\tan\theta = \theta$ in the interval $[n\pi, (2n+1)\pi/2]$ then the above Schrödinger operator has exactly $n-1$ antibound states if $[(2n-1)\pi/2]^2 < k^2 < K_n$ and $n+1$ antibound states if $K_n \leq k^2 \leq [(2n+1)\pi/2]^2$.*

Theorem 3.2. *Let V be a real potential with compact support $[0,1]$. Suppose that there exists $m < n$ such that $-[(2n-1)\pi/2]^2 < V < -[(2m-1)\pi/2]^2$ on $[0,1]$. Then*

$$m < |\sigma_d(H)| < n$$

where $H = -\frac{d^2}{dx^2} + V$ is the self-adjoint Schrödinger operator.

Proof. This is an immediate consequence of Theorem 3.1 and Proposition 3.1. □

If the potential is constant on the support $[0,1]$, then Theorem 2.8 provides the following estimate

$$|\sigma_{\mathrm{d}}(H)| < \frac{|V|^2}{\epsilon^2}\left(\frac{\mathrm{e}^{\epsilon}-1}{\epsilon}\right)^2$$

where V is the constant value on the support. The minimum value of

$$\frac{1}{\epsilon^2}\left(\frac{\mathrm{e}^{\epsilon}-1}{\epsilon}\right)^2$$

can be found out numerically, ≈ 2.38436418. Thus the estimate reduces to

$$|\sigma_{\mathrm{d}}(H)| < 2.38436418\,|V|^2.$$

But if V is real and constant, we can use the result for a self-adjoint operator and obtain a better estimate

$$|\sigma_{\mathrm{d}}(H)| < \int_0^\infty xV_-(x)dx = \frac{|V|}{2}.$$

Whereas Theorem 3.2 gives us

$$|\sigma_{\mathrm{d}}(H)| = \text{integer part of}\left(\frac{1}{\pi}\sqrt{|V|} + \frac{1}{2}\right).$$

Or for a potential V which is continuous and bounded on its support $[0,1]$,

$$\frac{1}{\pi}\sqrt{\min(V_-)} + \frac{1}{2} < |\sigma_{\mathrm{d}}(H)| < \frac{1}{\pi}\sqrt{\max(V_-)} + \frac{1}{2}$$

where $\min(V_-), \max(V_-)$ are minimum and maximum of the negative part of V on its support $[0,1]$. Thus it is easy to see that if the variation of potentials on its support is minimal then Theorem 3.2 provides better estimate.

Now we go back to the example and demonstrate the evolution of eigenvalues or resonances as the imaginary part of $-k^2$ continuously moves and traces vertical lines in the complex plane. For an example, the value of the potential on $[0,1]$ is initially taken as -22. By Proposition 3.1, the corresponding self-adjoint Schrödinger operator has one eigenvalue and two antibound states on the real line. Consider these bound and antibound states and the symmetric pair of complex resonances that are close to the origin. The evolution of these eigenvalues and resonances of this operator as $-k^2$ varies from -22 to $-22+250i$ or $-22-250i$ are shown in Figure 3.4. It is observed that the eigenvalue of the self-adjoint operator remains to be

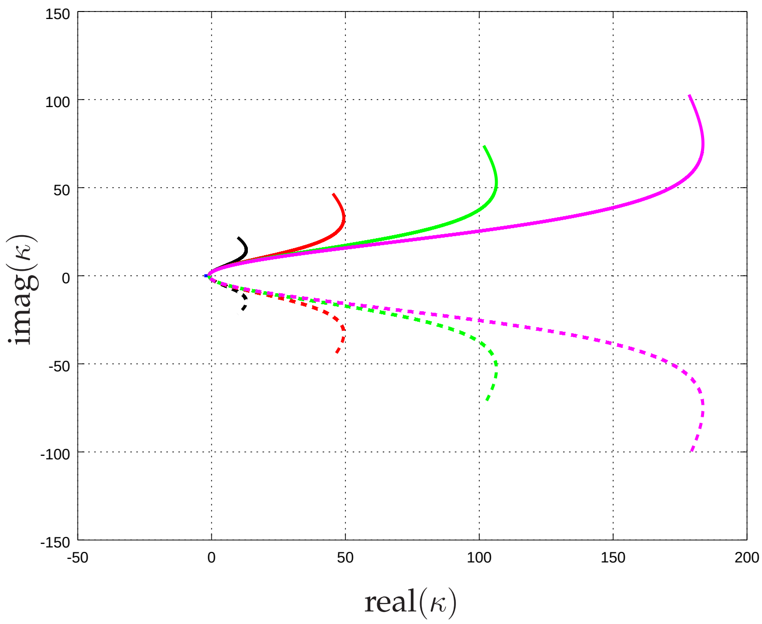


FIGURE 3.1: Evolution of resonances of the given Schrödinger operator as the value of $-k^2$ starts at -0.5 and decreases further. The blue curve represents the real resonance which moves right and becomes -1 at $-k^2 = -1 = -(\theta_0^2 + 1)$, $\theta_0 = 0$ is the first non-negative solution of $\tan\theta = \theta$. The black, red, green and magenta curves are the evolution of the four sets of symmetric resonances close to the origin. Each of these meet the real axis at -1 as $-k^2$ takes $-(\theta_1^2+1), -(\theta_2^2+1), -(\theta_3^2+1)$ and $-(\theta_4^2+1)$ respectively where θ_n is the solution of $\tan\theta = \theta$ in the interval $[n\pi, (2n+1)\pi/2]$, $n = 1, 2, 3, 4$

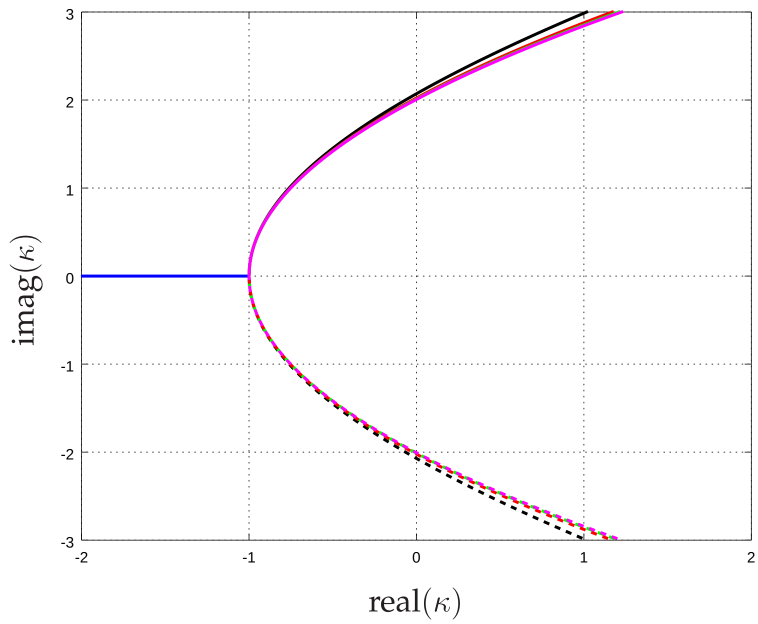


FIGURE 3.2: A zoomed version of the Figure 3.1 about the origin.

an eigenvalue as the imaginary part of $-k^2$ varies from 0 to the positive or negative side. The same thing happens to one of the real resonances (which is less than -1). Whereas the other resonance (on the right side of -1) traces a curve which crosses $[0, \infty)$ and changes to an eigenvalue as the imaginary part varies from 0 to 250 or -250 (see Figure 3.5 which is a zoomed version of Figure 3.4 about the origin). One of the complex resonances changes its status to eigenvalue and the other remains to be a resonance as the imaginary part of $-k^2$ changes from 0 to the positive or negative side.

Finding resonance for positive potential. It is evident from Equation 3.15 that if the value of k is zero or for the free Schrödinger operator, there is no eigenvalue or resonance in the complex plane. As the value of $-k^2$ varies from nonzero to zero, all the eigenvalues and resonances of the operator diverge to ∞. Thus to find evolution of resonances or eigenvalues of Schrödinger operators as the potential changes from $U \neq 0$ to another $V \neq 0$, one should choose a path so that for any z in the path, $H(z)$ does not become the free Schrödinger

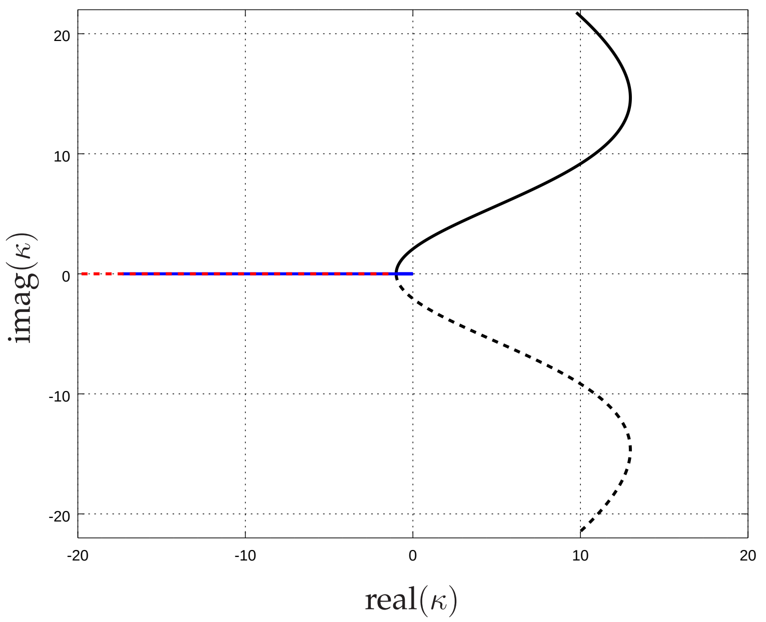


FIGURE 3.3: Evolution of resonance into eigenvalue of the Schrödinger operator. The black curves (solid and dashed) indicate the evolution of two complex symmetric resonances that meet at -1 as the real potential decreases to $-(\theta^2+1)$, where θ satisfies $\tan\theta = \theta$. Then they separate out and move in opposite directions along the real axis. The one (blue curve) moving to the positive direction meets the positive real axis at 0, as potential takes the value $-[(2n+1)\pi/2]^2$ and bounces back as an eigenvalue which moves further to the negative side as potential decreases further. The other (red dashed line) that moves to the negative direction continues as a real resonance (antibound state).

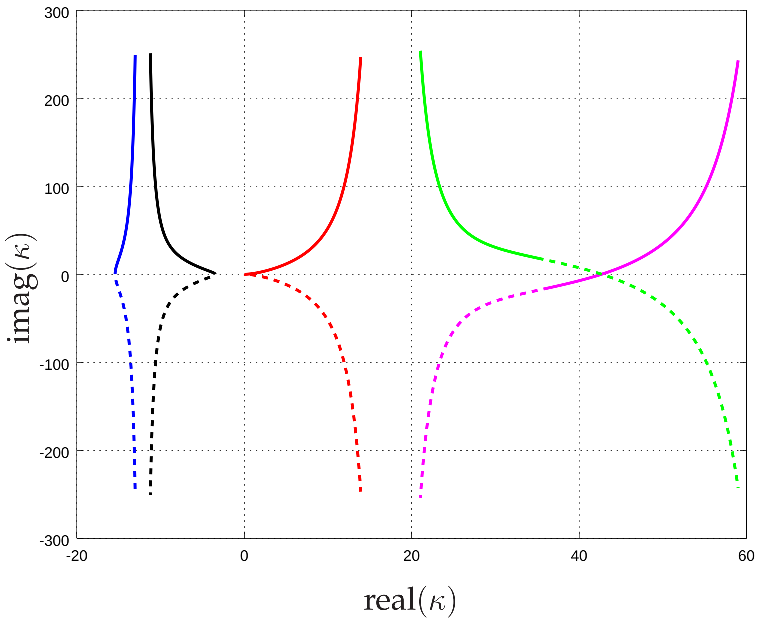


FIGURE 3.4: The evolution of the negative eigenvalue (≈ -15.42901680), two antibound states ($\approx -0.01187978, -3.48239885$) and a pair of complex resonances ($\approx 35.73924059 + 16.82276560i, 35.73924059 - 16.82276560i$) of the self-adjoint operator with potential equals to -22 on its support $[0, 1]$ as the imaginary part of the potential varies from 0 to 250 and to -250 on the support $[0, 1]$. The dashed curve corresponds to the variation from 0 to -250. The eigenvalue (blue curve) remains to be an eigenvalue, one of the negative resonance (black curve) remains as a resonance while the other resonance (red curve) crosses $[0, \infty)$ and moves to discrete spectrum. One resonance in the pair of complex resonances crosses $[0, \infty)$ and moves to the discrete spectrum while the other remains to be a resonance as the imaginary part varies from 0 to the positive side or to the negative side.

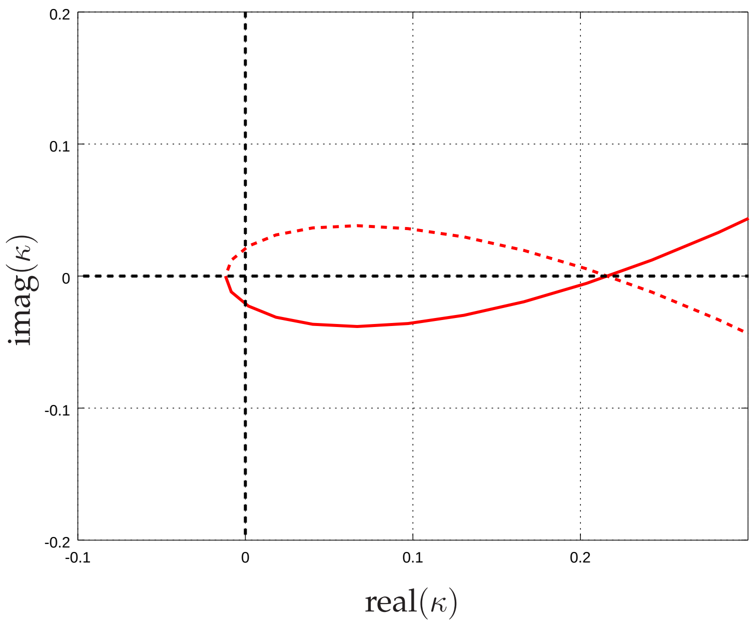


FIGURE 3.5: A zoomed version of Figure 3.4 about the origin. The evolution of the negative resonance on the right side of -1 as the imaginary part varies from 0 to positive or negative values. The resonance crosses $[0, \infty)$ and moves to the discrete spectrum of the corresponding Schrödinger operator.

operator. For example, consider the variation of $-k^2$ in Equation 3.14 from -0.5 to 1. If we choose the path along the real line, then at 0 the corresponding operator reduces to free Schrödinger operator. Thus it is required to consider a different path to get the evolution of the resonances. For example, if we consider the polygonal path $-0.5 \to -0.5 + i \to 1 + i \to 1$, then it may be possible to find the evolution of the resonances. The evolution of the antibound state of the operator with $-k^2 = -0.5$ to a resonance of the operator with $-k^2 = 1$ along this path is shown in Figure 3.6.

Finding eigenvalue for potential with non-negative real part. There does not exist any eigenvalue for self-adjoint Schrödinger operator with non-negative potential. But if an imaginary part is added to the potential then the corresponding nonself-adjoint Schrödinger operator can have discrete eigenvalues. If we want to find out these eigenvalues as an evolution of some negative eigenvalues of some self-adjoint Schrödinger operator, a similar idea explained in the above paragraph can be employed. Here first a sufficiently negative potential is considered and its eigenvalues are estimated. Then imaginary part is introduced continuously to the potential and finally the real part of the potential is increased to the required value. For example, consider the potential in Equation 3.14 and suppose we want to find out one eigenvalue when $-k^2$ takes the value $10 + 5i$. Initially $-k^2$ is assumed a negative value of -10 then it is changed along the polygonal path $-10 \rightarrow -10 + 5i \rightarrow 10 + 5i$. The evolution of the single discrete eigenvalue of the self-adjoint operator is shown in Figure 3.7. This method is employed in Chapter 4 for finding eigenvalues of depth dependent wave equation. A new numerical scheme is formulated based on this eigenvalue estimation method and is used for acoustic modelling (see Chapter 4 for more details).

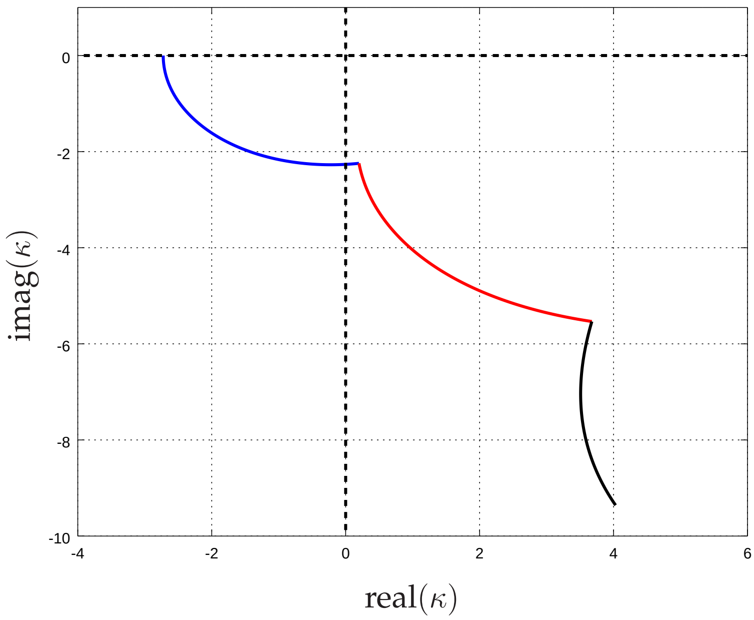


FIGURE 3.6: Evolution of a resonance as the value of $-k^2$ varies along straight lines from -0.5 to $-0.5+i$ (blue curve) then to $1+i$ (red curve) and finally to 1. The antibound state (≈ -1.65056781) of the Schrodinger operator with potential equal to -0.5 on its support $[0,1]$ becomes a resonance ($\approx 4.02995187 - 9.35784001i$) of the the operator with potential equal to 1 on its support.

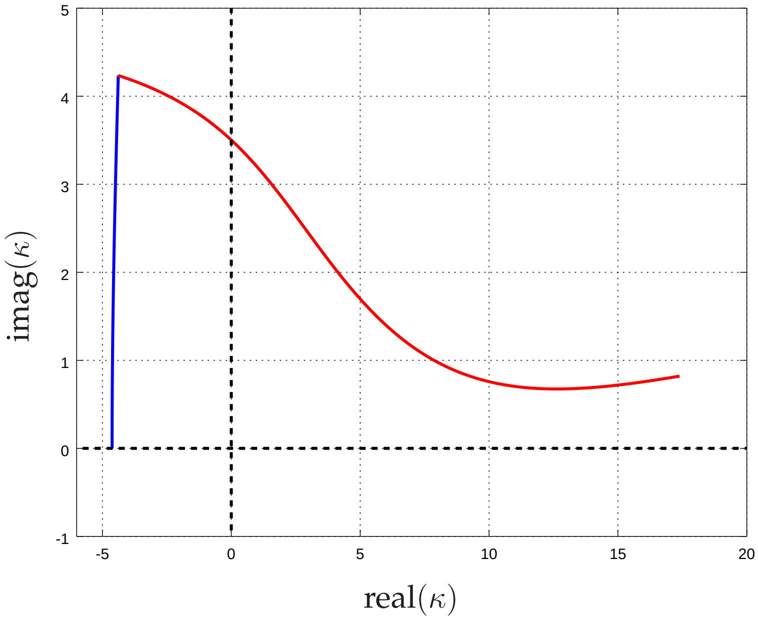


FIGURE 3.7: Evolution of the negative eigenvalue of the self-adjoint Schrödinger operator as the value of $-k^2$ in Equation 3.14 varies from -10 to $-10+5i$ and then to $10+5i$. Initially the discrete eigenvalue was ≈ -4.62419409, it gets evolved and becomes $\approx 17.39128151 + 0.82067130i$ as $-k^2$ reaches the value of $10+5i$.

Chapter 4

Applications - Underwater Acoustic Modeling

Acoustic signals undergo various physical processes such as refraction, reflection, diffraction and scattering as they propagate in the ocean medium. Modelling this propagation is important for designing and performance prediction of sonars. The analysis carried out in Chapter 3 is applied in this chapter for modelling underwater acoustic propagation. Here we concentrate on a numerical scheme for estimating the discrete spectral elements of nonself-adjoint Schrödinger operator. Section 4.1 gives a brief of acoustic modelling using normal mode method and the importance of finding discrete spectrum of Schrödinger operator. Different types of normal modes and their propagation characteristics are explained in Section 4.2. This section also contains discussion about the existing numerical schemes and their limitations to handle certain situations. A numerical scheme based on our analysis on the discrete spectrum of Schrödinger operator is detailed in Section 4.3. The method is illustrated with few examples in Section 4.4 and advantages over existing methods are brought out.

4.1 Normal Mode Modelling

The normal mode method is a wave theory approach for modelling acoustic field in a stratified medium where the pressure field is modelled as sum of contributions from individual components called normal modes (details can be found in [Boy84; Jen+11]). *That is*, consider a horizontally stratified (acoustic parameters are same in each horizontal plane or varies only in z) acoustic environment consisting of L layers with top layer being the water column. Let the layer interfaces be at depths $z_1 < z_2 < \ldots < z_{L-1}$ and $z_0 = 0, z_L = D$ be the surface and bottom boundaries, respectively. The surface boundary is modelled as pressure release and the bottom is modelled as a rigid boundary. Within each layer, the density ρ_l $(l = 0, 1, \ldots, L-1)$ is assumed to be constant and compressional sound speed $c_l(z)$ is continuous. The sound speed $c_l(z)$ is a complex quantity, the small imaginary part of which corresponds to the absorption loss of the medium. The pressure field generated by a harmonic point source of angular frequency ω located at $(0, z_s)$ in this medium is given by the sum of normal mode contributions as,

$$p(r, z) = \frac{i}{4}\frac{1}{\rho(z_s)}\sum_{n=1}^{\infty}\phi_n(z_s)\phi_n(z)H_0^1(\kappa_n r). \tag{4.1}$$

Here $\rho(z_s) = \rho_l(z_s)$ if $z_l < z_s < z_{l+1}$, $H_0^1(r)$ is the Hankel function of zeroth order and first kind, and $(\kappa_n^2, \phi_n(z))$'s are the eigen pairs of the depth separated wave equation

$$\frac{d^2\phi(z)}{dz^2} + [k^2(z) - \kappa^2]\phi(z) = 0. \tag{4.2}$$

The pressure-release surface and rigid-bottom boundary conditions are used to obtain $\phi(0) = 0, \phi'(D) = 0$. Here $k(z)$ is the local wave number $\omega/c(z)$ where $c(z) = c_l(z)$ for $z_l < z < z_{l+1}$, $l = 0, 1, \ldots, L-1$. At each layer interface, the pressure and particle velocity are continuous. Therefore, $\phi(z)$ and $\frac{1}{\rho(z)}\phi'(z)$ are continuous.

A more realistic approach in ocean acoustics is to treat the bottom as homogeneous acoustic half-space. That is for $z > D$ acoustic properties are constant and the medium is extending to infinity. Then Equation 4.2 is for $z \in [0, \infty)$ or in rigorous mathematical terms, κ^2 is the discrete spectral element of the operator $H = \frac{d^2}{dz^2} + k^2(z)$ defined on the Hilbert space $L^2(0, \infty)$ with domain given by

$$\mathrm{Dom}(H) = \left\{ f \in L^2(0, \infty) : f', \left(\frac{1}{\rho} f' \right)' \in L^2(0, \infty) \right\}. \tag{4.3}$$

If we take k_L^2 as the constant value of $k^2(z)$ for the homogeneous half-space and subtract H from this constant operator to get the new operator $-\frac{d^2}{dz^2} + V(z), V(z) = k_L^2 - k^2(z)$ defined on the same domain. It is easy to see that this operator is equivalent to the Schrödinger operator with compact support potential. In this case spectrum consists of $[0, \infty)$ and a finite number of discrete eigenvalues. Thus the summation in Equation 4.1 becomes a finite sum over this discrete spectrum and is an approximate expression for pressure field as we are neglecting the effect of continuous spectrum. In practice, this is a good approximation as we are interested in long ranges and the continuous spectrum effects are limited to short ranges.

4.2 Classification of Modes

In Equation 4.1, each component has a term that depends on the depth and another term that depends on the horizontal range, and is associated with a wave number κ. Depending on the wave number the mode is categorised as water trapped or leaky. If the real part of the wave number of the mode is greater than the real part of wave number corresponding to the compressional sound speed of the sediment bottom, the mode is called a water trapped mode. Or equivalently, a mode is water trapped if its phase speed, $2\pi f/\mathrm{Re}(\kappa)$, is less than the compressional sound speed of the sediment bottom.

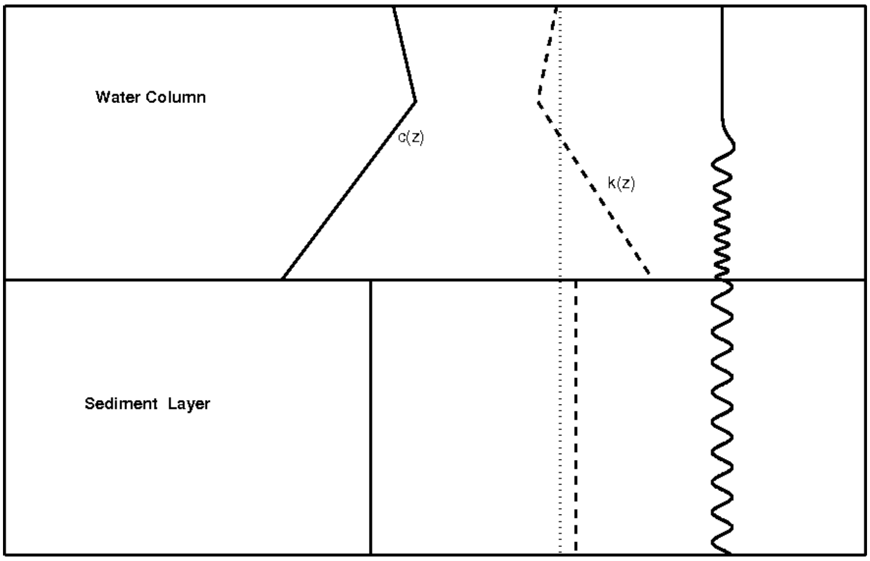


FIGURE 4.1: Mode function corresponding to a leaky mode is shown. The sound speed and corresponding $k(z)$ are schematically shown. The position of the wave number is indicated using a dotted line. Since the wave number is less than $k(z)$ of the sediment, it is categorized as a leaky mode.

Otherwise the mode is termed as a leaky mode ([Jen+11]). In general, leaky modes leak down to the sediment bottom and their contribution is limited to short ranges. The general behavior of a leaky mode is demonstarted in Figure 4.1.

In some environments, the long-range surface duct propagation is due to the modes that are leaky by the above definition. For example, consider the sound speed profile (Figure 4.2) computed using World Ocean Atlas data ([Loc+10; Ant+10]), corresponding to the geographical location $(10^o N, 75^o E)$ in the Indian Ocean for the month of January. The sound speed at the bottom is approximately 40 m/s less than that at the surface. Hence if the immediate sediment layer is soft (compressional sound speed ratio is near to 1), the mode that propagates in the surface duct (if it exists) comes under the category of leaky modes. But this mode does not leak into the sediment as its energy is confined to the surface duct. This mode behaves like a water trapped mode and propagates to longer ranges. A method is presented here to accurately estimate all modes including the leaky modes and its relevance in these environments is illustrated.

The numerical scheme based on Airy function solutions described in [WTC96] and its implementation ORCA is one of the efficient normal mode schemes. The numerical scheme described in [PR84; PR85] is attractive because it can be used for general sound speed profiles and its real wavenumber search algorithm is robust especially at low frequencies. Its FORTRAN implementation KRAKEN and KRAKENC ([Por10]) are very popular and they are used extensively in underwater acoustic applications. The method employs Richardson extrapolation to determine the wave numbers accurately. In absorptive media, either the linear perturbation theory (KRAKEN) or a direct complex eigenvalue search algorithm (KRAKENC) is utilised. In Appendix A.1, perturbation approximation is explained for a general operator. Linear perturbation theory fails to give accurate estimate of leaky modes and, at times, the complex eigenvalue search fails to converge ([WTC96]). Therefore, a new numerical scheme is proposed to estimate all the dominant modes (modes that are propagating to longer ranges with less attenuation) accurately and to use them to find the pressure field.

4.3 A New Numerical Approach

Our new approach is based on the analysis done in the previous chapter on the evolution of discrete spectrum of Schrödinger operators as the potential changes analytically. Initially we find out the discrete spectrum of the operator $-\frac{d^2}{dz^2} + V(z)$, where $V(z) = k_L^2 - k^2(z)$ for $z \leq D$ and 0 otherwise, the domain is given in Equation 4.3. This operator is equivalent to a Shrödinger operator with a compactly supported potential. Then wave numbers are obtained as $\kappa_j = \sqrt{k_L^2 - \nu_j}$, ν_j's are the discrete spectral elements of the Schrödinger operator. If we assume that the acoustic half-space is the sediment bottom for the medium, then from definition, trapped modes are

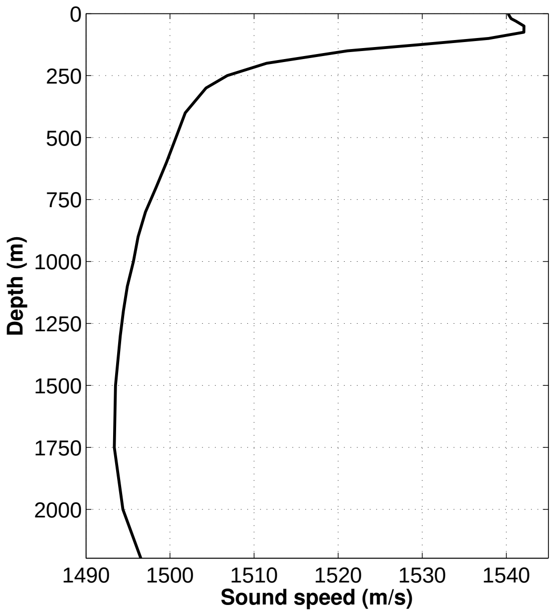


FIGURE 4.2: The sound speed profile computed using temperature, salinity data taken from the World Ocean Atlas corresponding to the location $(10^o N, 75^o E)$, for the month of January

obtained from discrete eigenvalues that are lying on the left half (real part less than 0) and leaky modes from the right half (real part greater 0) of the complex plane. This implies that leaky modes are mostly evolved from the resonance of the corresponding self-adjoint Schrödinger operator. Thus we use a method that is demonstrated in the last part of Section 3.5. *That is*, the value of the potential on the support $[0, D]$ is shifted to the negative side and all the eigenvalues of the corresponding self-adjoint Schrödinger operator are estimated. Shifting the potential means considering a sediment with more compressional speed. Thus how much the potential needs to be shifted depends on the practical problem at hand. For example, for finding the modes which are propagating in the surface duct we need to consider a compressional speed of more than the maximum of the sound speed in the surface duct. Then introduce the imaginary part of the potential continuously and find the evolved eigenvalues. Finally the real part of the potential is brought back to the original value by increasing it continuously and the evolved eigenvalues are estimated. In this process, any eigenvalue crossing the positive real axis is omitted.

A modified numerical scheme - KRAKENRQ The numerical approach followed in [PR84; PR85] (KRAKEN) initially consider the real part of $k(z)$ and uses Sturm sequence for isolating real eigenvalues of the resulting self-adjoint operator. A combination of bisection, Newton's and Brent's methods are used to estimate eigenvalues of Equation 4.2 for various discretisations. Richardson extrapolation is used to obtain the eigenvalues that correspond to infinitesimally small discretisation. Inverse iteration is done to estimate eigenfunctions. Finally linear perturbation approximation is used to estimate eigenvalues of the operator with complex $k(z)$. In this approach the leaky modes are not found as they are not evolved from these eigenvalues. To overcome this, in our modified approach, first the sound speed of the sediment half-space is increased sufficiently (*that is*, decrease the real part of k_L^2) and obtain $k_+^2(z)$. Find out the real eigenvalues and eigenfunctions of the operator with potential as real part of $k_+^2(z)$, as is done in KRAKEN. Then change the coefficient from Re$(k_+^2(z))$ to $k^2(z)$ using small increment and get the evolved eigenpair using Rayleigh Quotient iteration. Since the imaginary part of $k^2(z)$ or the attenuation factor is very small, we require only one incremental change (*that is*, directly change Re$(k_+^2(z))$ to $k^2(z)$) to get the required eigenvalues.

The procedure is as follows: Let A be the matrix operator obtained by discretising Equation 4.2 and applying the boundary conditions. Let B be the real matrix obtained from the same equation but $k^2(z)$ replaced with Re$(k_+^2(z))$, $k_+^2(z)$ is obtained by decreasing the real part of $k^2(z)$ sufficiently. In underwater environments and at sonar frequencies, A is considered to be a small complex perturbation of the real matrix B. Initially B is used to find its normalised eigenfunctions, as is done in [PR84]. Let the eigenfunctions be $\phi_{0,j}(z)$

for $j = 1, 2, \ldots, m$. Using these eigenfunctions as the initial estimate, Rayleigh quotient iteration is started to find the eigenvalues and eigenfunctions of A. *That is*, for each j,

1. $\lambda_{k,j} = \langle A\phi_{k,j}, \phi_{k,j} \rangle$
2. $\phi_{k+1,j} = (A - \lambda_{k,j} I)^{-1} \phi_{k,j}$
3. $\phi_{k+1,j} = \phi_{k+1,j} / < \phi_{k+1,j}, \bar{\phi}_{k+1,j} > .$

Iterate the above steps for $k = 0, 1, 2, \ldots$. Here the inner product is defined as,

$$\langle \phi, \psi \rangle = \sum_{l=0}^{L-1} \frac{h_l}{\rho_l} \left\{ \frac{1}{2}\phi(z_l)\overline{\psi(z_l)} \right. \\ \left. + \sum_{j=1}^{N_l - 1} \phi(z_l + jh_l)\overline{\psi(z_l + jh_l)} + \frac{1}{2}\phi(z_{l+1})\overline{\psi(z_{l+1})} \right\},$$

a trapezoidal quadrature approximation to $\int_0^D \frac{1}{\rho(z)}\phi(z)\overline{\psi(z)}dz$, h_l is the discretisation thickness and N_l is the number of discretised points in l^{th} layer.

If some of the layers support shear waves, the coupling between compressional and shear waves are handled in the same way as is done in [PR85]. Here too, wavenumbers and mode functions corresponding to pressure waves are estimated. The method described above is started with a modified matrix A corresponding to the compressional waves, that incorporates coupling with the shear waves. The rest of the procedure is the same as that described in [PR84; PR85]. The eigenvalues are estimated for finer discretisation of Equation 4.2. For each of the successive finer discretisations, the eigenvalues obtained in the previous step are used as an initial guess for the complex root finding algorithm. Finally, Richardson extrapolation is employed to accurately estimate the wave numbers. This method is implemented in FORTRAN modifying KRAKEN and is named as KRAKENRQ ([SK17]).

4.4 Illustration

An example is presented to demonstrate the robustness of the modified approach. The environment consists of a 2197 m deep water column. The sound speed profile is shown in Figure 4.2 and the surface layer is 50 m thick. The bottom is a soft sediment half-space having density 1.577 g/cm^3, compressional sound speed ratio 1.001 and compressional attenuation 0.38 dB/λ. The source is at 10 m depth. At 250 Hz, KRAKENC and KRAKENRQ yield the same results, and KRAKEN does not yield the correct results. As frequency increases KRAKENC becomes more and more inefficient and, at 10 kHz, only KRAKENRQ yields the correct results. This is demonstrated below.

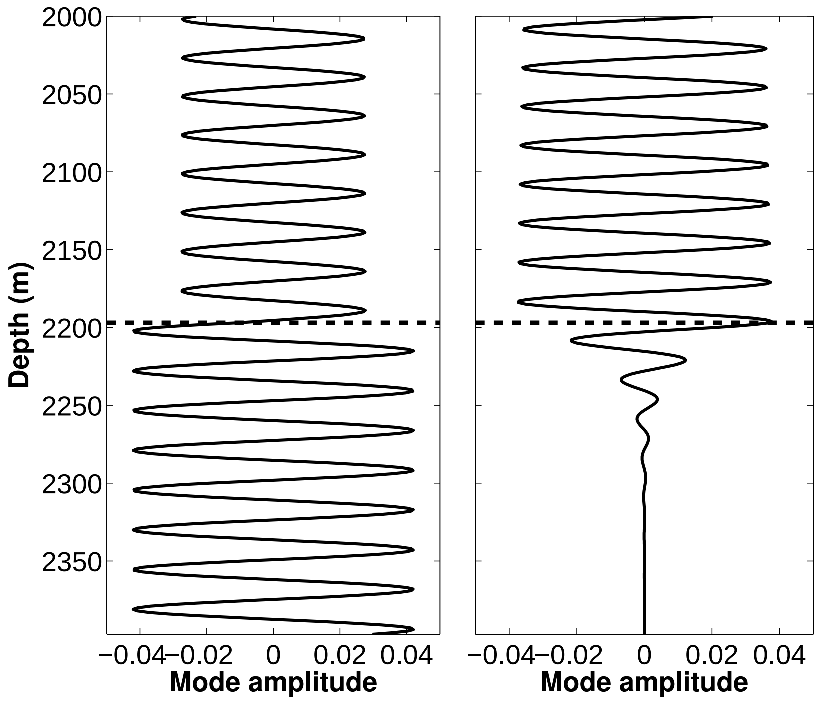
For comparison, wave numbers and mode functions are estimated using KRAKEN, KRAKENC and KRAKENRQ. The half-space is replaced with a 200 m sediment layer with a rigid bottom. The layer has the same acoustic parameters as that of the half-space. This approximation is used so that KRAKEN can be used to estimate leaky modes. The wavenumbers are estimated using KRAKEN and KRAKENRQ and those with phase speed between 1540 m/s and 1545 m/s (modes that propagate in the surface duct) are shown in Table 4.1. The wavenumbers obtained using KRAKENRQ are the same as those obtained using KRAKENC upto 10 significant digits and the latter are not shown. The absorption coefficients (imaginary part of the wave numbers) estimated using KRAKEN are higher by an order or two. The mode functions corresponding to the first wave number in the table are shown in Figure 4.3. The mode function estimated by KRAKEN is clearly a leaky one as the mode propagates down to the sediment, whereas the mode function estimated by KRAKENRQ reveals that this mode has an evanescent part along with the oscillatory part in the sediment (below the dotted line), hence its absorption coefficient reduces and it propagates to longer ranges. The transmission loss ($TL(r,z) = 20\log|p(r,z)|$) curves for a receiver depth of 10 m computed using these methods are compared in Figure 4.4 with the wave number integration model SCOOTER. KRAKENRQ matches well with the reference model whereas KRAKEN over estimates the transmission loss. Further, assuming a shear speed of 412 m/s for the sediment half-space, wave numbers are computed for frequencies 250 Hz, 500 Hz, 1000 Hz, 2000 Hz, 4000 Hz, 6000 Hz, 8000 Hz and 10000 Hz using KRAKENC and KRAKENRQ. The number of modes with phase speed between 1540 m/s and 1550 m/s estimated by these methods and time taken for computations are compared in Table 4.2. As frequency increases, the performance of KRAKENC degrades. The inefficiency of the complex root finding algorithm of KRAKENC is reflected in the abrupt increase of the computational time for frequencies 2 kHz or more. At 10 kHz, KRAKENC fails to estimate any mode that propagates in the surface duct. In Figure 4.5, the transmission loss curve for a source and receiver located at 10 m and for a frequency of 10 kHz generated using KRAKENRQ is compared with that obtained using SCOOTER. There is very good agreement.

Sr. No.	KRAKEN			KRAKENRQ		
	κ	α	Ph. speed	κ	α	Ph. speed
1	1.019700157	-0.1295605987E-02	1540.449235	1.019885629	-0.7825041727E-04	1540.169096
2	1.019410309	-0.1384937310E-02	1540.887229	1.019555378	-0.7789829795E-04	1540.667982
3	1.019122738	-0.1265879079E-02	1541.322030	1.019227565	-0.7706828608E-04	1541.163506
4	1.018837197	-0.1012276735E-02	1541.754002	1.018906080	-0.7447556976E-04	1541.649773
5	1.018573947	-0.6832964203E-03	1542.152468	1.018609016	-0.6266672656E-04	1542.099375
6	1.018379062	-0.4574282480E-03	1542.447587	1.018399378	-0.4435236748E-04	1542.416817
7	1.018151412	-0.5801742797E-03	1542.792465	1.018168673	-0.6649788690E-04	1542.766310
8	1.017866423	-0.5716413779E-03	1543.224427	1.017867779	-0.7361347405E-04	1543.222371
9	1.017568476	-0.5518612214E-03	1543.676286	1.017554135	-0.7466114353E-04	1543.698042
10	1.017268549	-0.5628397106E-03	1544.131418	1.017238901	-0.7478672826E-04	1544.176422
11	1.016969026	-0.6131027071E-03	1544.586203	1.016923261	-0.7500525979E-04	1544.655714

TABLE 4.1: Wave numbers with phase speed between 1540 m/s and 1545 m/s computed using KRAKEN and KRAKENRQ for a frequency of 250 Hz. KRAKENC gives the same results as KRAKENRQ.

Frequency (Hz)	KRAKENC		KRAKENRQ	
	# modes	Comp. time (sec)	# modes	Comp. time (sec)
250	20	0.066	21	0.096
500	41	0.273	42	0.434
1000	83	1.144	84	1.949
2000	166	104.78	168	8.177
4000	299	707.0	335	65.02
6000	430	2963.0	504	142.3
8000	583	4891.0	672	264.1
10000	didn't converge	—-	842	409.3

TABLE 4.2: Number of modes with phase speed between 1540 m/s and 1550 m/s estimated by KRAKENC and KRAKENRQ and time taken for its computation for different frequencies.



(a) (b)

FIGURE 4.3: The portion below 2000 m depth of the mode function corresponding to the first wave number in Table 4.1 estimated by (a) KRAKEN and (b) KRAKENRQ. Dotted line indicates the water-sediment interface.

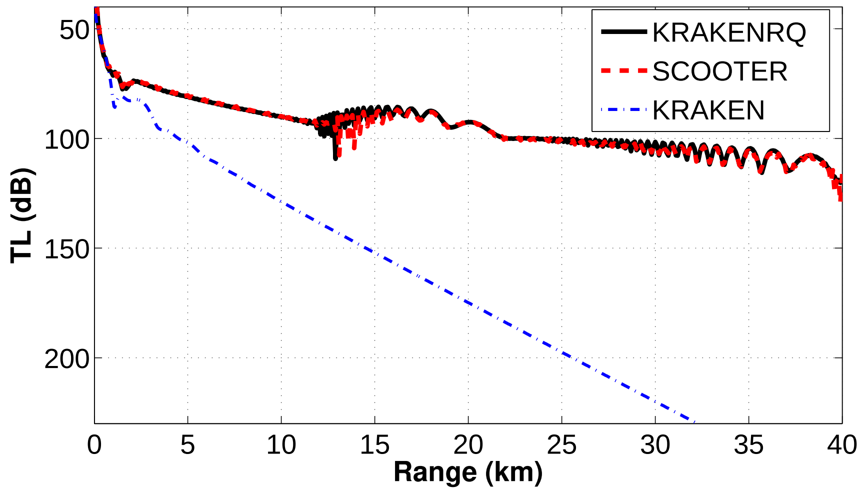


FIGURE 4.4: Transmission loss curves computed using KRAKENRQ and SCOOTER for a source and receiver at 10 m, frequency 250 Hz.

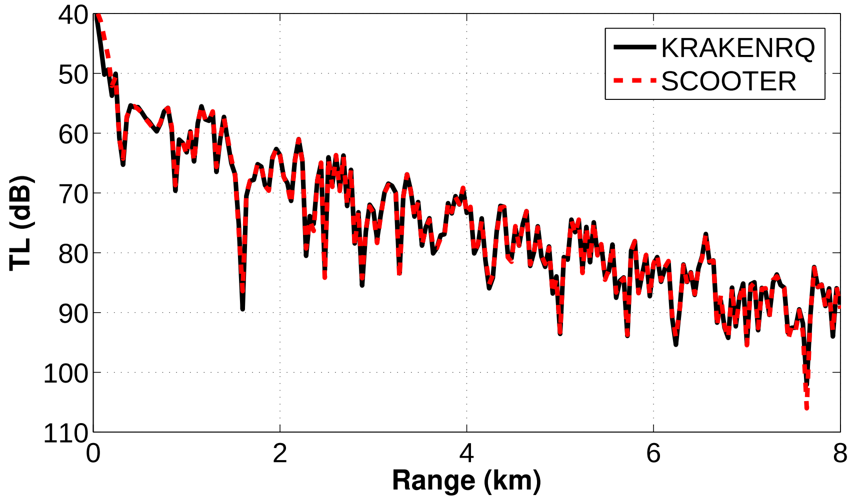


FIGURE 4.5: Transmission loss curves computed using KRAKENRQ and SCOOTER for a source and receiver at 10 m, frequency 10 kHz. The modes that are dominant in the surface duct (phase speed between 1530 m/s and 1550 m/s) are considered.

Chapter 5

Summary

Our research work concentrated on the discrete spectrum of non-selfadjoint Schrödinger operator defined in $L^2(0,\infty)$ with compactly supported potential. This class of operators are coming under the category of operators which are relative compact perturbations of self-adjoint Schrödinger operator. The work started with an extensive survey of research articles in this field. The survey on few important such articles are included in Chapter 2. These articles are mainly concentrated on the distributions of discrete spectrum in the complex plane. Some of these articles are concerned with the boundedness and finiteness of the discrete spectrum. Some others are about convergence of discrete elements towards the essential spectrum $[0,\infty)$. Rate of convergence is measured using Lieb-Thirring type inequalities and there are a number of articles discussing estimate for $\sum\limits_{\lambda\in\sigma_{\mathrm{d}}(H)} \mathrm{dist}(\lambda,[0,\infty))^p$ under different conditions on potential.

5.1 Theoretical Study

Chapters 3 and 4 are mainly documentation of our work. Theoretical work is covered in Chapter 3. We have considered Schrödinger operator valued function $H(z) = -\frac{d^2}{dx^2} + V_0 + zV_1$ defined on the complex plane with compactly supported V_0, V_1 in Section 3.3. Evolution of discrete spectrum of $H(z)$ as z varies in a path in $\mathbb{C}$ is studied.

Our major finding is that if the path traced by a discrete spectral element $\kappa(z)$ of $H(z)$ as z moves along a path terminates, then this terminal point lies on the essential spectrum $[0, \infty)$. We have further extended this result and proved that any discrete spectral element of the nonself-adjoint operator $H(i) = -\frac{d^2}{dx^2} + V_0 + iV_1$ is evolved from either a discrete spectral element or a resonance of the self-adjoint Schrödinger operator $H(0) = -\frac{d^2}{dx^2} + V_0$ as z varies from 0 to i.

In Section 3.4, a more general case is discussed where the potential V_0 and V_1 satisfy $\int_0^\infty xV_j dx < \infty$. Here we have proved that any discrete spectral element of $H(i)$ is evolved from either a discrete element of $H(0)$ or a spectral singularity of $H(it_0)$ for some $0 < t_0 < 1$. An estimate for lower bound of the number of discrete spectral elements of self-adjoint Schrödinger operator is derived based on this analysis.

An example is provided in Section 3.5 to illustrate our theoretical study. Evolution of discrete spectral elements and resonances are demonstrated for $H(z) = -\frac{d^2}{dx^2} + V_0 + zV_1$, where V_0, V_1 are constants on their support $[0, 1]$. The spectral elements or resonances are evaluated using the characteristic equation, which is an analytic expression. A scheme for estimating complex resonance of self-adjoint Schrödinger operator from real resonance (antibound states) of another operator, with a potential whose values on its support shifted to the negative side, is explained. In a similar way a scheme for estimating eigenvalues of a nonself-adjoint Schrödinger operator that are lying on the right half-plane from the real eigenvalues of a self-adjoint Schrödinger operator is also explained. This method is used in Chapter 4 to devise a new numerical scheme for estimating eigenvalues of a Schrödinger operator.

5.2 Application in Acoustic Modelling

In Chapter 4, a new numerical approach is derived for underwater acoustic modelling through normal mode method. Normal mode method requires estimation of eigenvalues of a nonself-adjoint Schrödinger operator. Eigenvalues of this Schrödinger operator are classified as those corresponding to water trapped and leaky modes. This classification is purely based on the position of these eigenvalues. Those which are lying on the left half-plane correspond to trapped modes and lying on the right half-plane correspond to leaky modes. Leaky modes are evolved from the resonances of the corresponding self-adjoint Schrödinger operator. To estimate this, the method described in the last paragraph of Section 3.5 is used.

This method is implemented in FORTRAN and is named as KRAKENRQ, as it is obtained by modifying a well known normal mode implementation KRAKEN. In this implementation, wave numbers (or eigenvalues) and mode functions (eigenfunctions) are estimated initially without considering absorption in the acoustic medium, *that is*, ignoring the imaginary part or considering the self-adjoint operator. If the sediment half-space is a soft bottom, it is replaced with a harder one. *That is* to say that the potential is moved further to the negative side. The real eigenvalues (or wave numbers) of the resulting operator are estimated, then the wave numbers that are evolved from these real wave numbers, as the potential continuously changes to take the original value, are obtained. Here the evolution is completed in few steps (mostly single step) as the imaginary part is very small and at each step Rayleigh quotient iteration is used. For better accuracy, solving the vertical wave equation is repeated for few more, finer discretisations and Richardson extrapolation is applied. Examples are provided to show that KRAKENRQ performs better than the existing implementation KRAKEN and KRAKENC and it works even at relatively higher frequencies.

5.3 Suggestions for Future Study

The analysis on nonself-adjoint Schrödinger operators for its spectral characteristic is an active topic. The articles covered in our survey (Chapter 2) contains very recent works. The research work covered under this document concentrated mainly on methods of estimating the discrete spectral elements. Even though the numerical scheme derived using our study to model underwater acoustic propagation is effective, some more theoretical study is required to make it a fool-proof numerical scheme. For example, the following questions need to be answered.

1. What should be the discretization used in each step to estimate an eigenvalue κ_1 of $H(i)$ which is evolved from eigenvalue κ_0 of $H(0)$?

2. How much the value of the potential on its support need to be shifted to the negative side to obtain all the eigenvalues? *That is*, if V_0, V_1 are compactly supported on $[0, \infty)$ then to find out eigenvalues of $H(i) = -\frac{d^2}{dx^2} + V_0 + iV_1$ that are evolved from the resonances of $H(0) = -\frac{d^2}{dx^2} + V_0$ how much the value of the potential V_0 on its support need to be shifted to the negative side?

Answering these greatly improve our numerical scheme and avoid any ambiguity in the scheme. The first question is about choosing discretization so that we may not miss any eigenvalue, particularly if two or more eigenvalues are collapsing to form an eigenvalue of multiplicity more than one. Lemma 3.4 proved in Chapter 3 characterizes such a situation where two or more curves traced by eigenvalues of $H(z)$ meet at z. Thus $\int\limits_0^\infty \phi^2(z,x)dx$, $\phi(z,x)$ is the eigenfunction corresponding to the eigenvalue $\kappa(z)$ of $H(z)$, can be treated as a measure to determine the closedness of two such curves. Or if $\int\limits_0^\infty \phi^2(z,x)dx$ is close to zero, then one should take special care in choosing the discretization Δz to find the evolved eigenvalue $\kappa(z + \Delta z)$. The second question, to some extent, can be answered using physical consideration of the problem at hand and the same is explained in Section 4.3. But here too how much the value of V_0 on its support should be shifted to the negative side to get V_0' so that all the eigenvalues of $H(i) = -\frac{d^2}{dx^2} + V_0 + iV_1$ can be found out from the real eigenvalues of $-\frac{d^2}{dx^2} + V_0'$ is not known.

There are further studies and extensions possible to the acoustic modelling application. The current version of KRAKENRQ works better than the existing model KRAKEN. The model can also be used for relatively high frequency applications, but it is not computationally efficient at these frequencies. A modification is planned in which $k(z)$ is approximated as piece-wise linear and hence the eigenfunction can be obtained analytically (Airy or exponential functions). This will improve the accuracy and computational time and an efficient acoustic modelling for higher frequency applications may be possible. Another possible area is to study the randomness in acoustic modelling due to random behavior of $k(z)$. This is driven by the physical nature of the problem. The dynamical nature of sound speed $c(z)$ of the ocean medium forces to treat $k(z) = 2\pi f/c(z)$ as random. Theoretical study needs to be carried out to obtain statistics of discrete spectral elements and eigenfunctions of the random Schrödinger operator with compactly supported potentials that are drawn from an appropriate probability space.

Appendix A

Appendix

A.1 Linear Perturbation Theory

Let H_0 be a linear operator in the Hilbert space $\mathscr{H}$, and (λ_0, f_0) an eigenpair of H_0. Let the perturbed operator H be

$$H = H_0 + \epsilon H_1 + \epsilon^2 H_2 + \cdots \tag{A.1}$$

and assume it has an eigenpair (λ, f) such that

$$\lambda = \lambda_0 + \epsilon\lambda_1 + \epsilon^2\lambda_2 + \cdots \tag{A.2}$$

and

$$f = f_0 + \epsilon f_1 + \epsilon^2 f_2 + \cdots . \tag{A.3}$$

For a first order (linear) approximation to the eigenvalue λ, use $Hf = \lambda f$, and A.1, A.2 & A.3 to get

$$(H_0 - \lambda_0 I) f_1 = (-H_1 + \lambda_1 I) f_0 \tag{A.4}$$

If we assume H_0 is self-adjoint (so is $H_0 - \lambda_0 I$) and if f_1 satisfies A.4, then

$$\begin{aligned} < f_0, (-H_1 + \lambda_1 I) f_0 > &= < f_0, (H_0 - \lambda_0 I) f_1 > \\ &= 0 \end{aligned}$$

rearrange and solve for λ_1,

$$\lambda_1 = \frac{< H_1 f_0, f_0 >}{< f_0, f_0 >}.$$

A.2 Rayleigh Quotient Estimate

Let H be an operator on the Hilbert space $\mathscr{H}$, and let $f \in \mathscr{H}$ and assume f is near to some eigenfunction of H, then the best estimate for the corresponding eigenvalue is $< f, Hf > /\|f\|^2$. To prove this claim, let $\lambda = \lambda_1 + i\lambda_2 \in \mathbb{C}$ and define

$$g(\lambda_1, \lambda_2) \quad = \quad \|Hf - \lambda f\|^2.$$

And from preliminary calculus, for a minimum of g

$$\frac{\partial g}{\partial \lambda_1} = 0 \Longrightarrow$$

$$\lambda_1 = \text{real}\left(\frac{< Hf, f >}{\|f\|^2}\right)$$

and

$$\frac{\partial g}{\partial \lambda_2} = 0 \Longrightarrow$$

$$\lambda_2 = \text{imag}\left(\frac{< Hf, f >}{\|f\|^2}\right)$$

or

$$\lambda = \frac{< Hf, f >}{\|f\|^2}$$

. So $\|Hf - \lambda f\|$ is minimum or Hf is *close* to λf, if $\lambda = < Hf, f > /\|f\|^2$.

If $H = H_0 + \epsilon H_1$, and (λ_0, f_0) is an eigenpair of the operator H_0, then the Rayleigh quotient estimate for the eigenvalue of the linearly perturbed operator H, taking f_0 as an eigenfunction approximation, is

$$\lambda = \frac{< Hf_0, f_0 >}{< f_0, f_0 >} = \lambda_0 + \epsilon \frac{< H_1 f_0, f_0 >}{< f_0, f_0 >}$$

. This is the same as the linear perturbation approximation obtained with the additional condition of self-adjointness on the operator H_0. From this we can draw the following conclusion. If the linear perturbation approximation fails, then the eigenfunction f_0 of the unperturbed operator H_0 is not a good estimate for the perturbed operator H.

A.3 Inverse Iteration

Let H be an operator in the Hilbert space $\mathscr{H}$, and let $\lambda_1, \lambda_2, \dots$ are its eigenvalues $f_1, f_2, \dots$ are the respective eigenfunctions. Further assume that $\lambda_i \neq \lambda_j$ for $i \neq j$ and that any vector f in $\mathscr{H}$ can be expressed as a linear combination of the eigenfunctions. Let μ be close to λ_i such that $|\lambda_i - \mu| < |\lambda_j - \mu|$ for all $j \neq i$ and let $f = \sum_j a_j f_j$ with $a_i \neq 0$. Now

$$
\begin{aligned}
(H - \mu I)^{-1} f &= \sum_j a_j (\lambda_j - \mu)^{-1} f_j \\
&= \frac{1}{\lambda_i - \mu} \left(\sum_{j \neq i} a_j \frac{\lambda_i - \mu}{\lambda_j - \mu} f_j + a_i f_i \right) \\
(H - \mu I)^{-k} f &= \frac{1}{(\lambda_i - \mu)^k} \\
&\quad \left(\sum_{j \neq i} a_j \left(\frac{\lambda_i - \mu}{\lambda_j - \mu} \right)^k f_j + a_i f_i \right).
\end{aligned}
$$

Thus $(H - \mu I)^{-k} f$, for large values of k, is approximately a multiple of f_i. Or $\frac{(H-\mu I)^{-k} f}{\|(H-\mu I)^{-k} f\|}$ converges to f_i. This is the philosophy behind inverse iteration.

Given an estimate μ, the eigenfunction f corresponding to the eigenvalue λ which is closest to μ of the operator H can be found using the following iterative process:

Start with a vector f_0 and in each step a better estimate of the eigenfunction is obtained by solving the equation $(H - \mu I) f_{k+1} = f_k$.

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Publications

1. *S. Satheesh Kumar*: **A modified numerical approach for leaky mode computation**, Acta Acustica united with Acustica 103(5) (2017), pp. 767–771.

Abstract

Acoustic modelling using normal mode approach is examined in Indian Ocean environment with a soft sediment bottom. Computing leaky modes is critical in modelling the acoustic field in these environments. Normal mode programs KRAKEN and KRAKENC are applied to these environments and their instability in determining some of the leaky modes is pointed out. Rayleigh quotient iteration is proposed in place of inverse iteration in KRAKENC for determining the dominant complex modes. This approach provides better estimate of all the dominant modes and is found to be stable even at higher frequencies.

2. *M. N. N. Namboodiri and S. Satheesh Kumar*: **On continuous movement of the discrete spectrum of Schrödinger operators** (pre-print)

Abstract

Continuous movement of discrete spectrum of the Schrödinger operator $H(z) = -\frac{d^2}{dx^2} + V_0 + zV_1$, with $\int_0^\infty x|V_j(x)|dx < \infty$, on the half-line is studied as z moves along a continuous path in the complex plane. The analysis provides information regarding the members of the discrete spectrum of the non-selfadjoint operator that are evolved from the discrete spectrum of the corresponding selfadjoint operator.

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