COMPACT OPERATORS AND THE SCHRÖDINGER EQUATION

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Thesis Prepared for the Degree of

MASTER OF ARTS

UNIVERSITY OF NORTH TEXAS

December 2006

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Kazemi, Parimah, Compact Operators and the Schrödinger Equation. Master of Arts (Mathematics), December 2006, 25 pp., 10 illustrations, bibliography, 5 titles.

In this thesis I look at the theory of compact operators in a general Hilbert space, as well as the inverse of the Hamiltonian operator in the specific case of $L^2[a,b]$. I show that this inverse is a compact, positive, and bounded linear operator. Also the eigenfunctions of this operator form a basis for the space of continuous functions as a subspace of $L^2[a,b]$. A numerical method is proposed to solve for these eigenfunctions when the Hamiltonian is considered as an operator on $\mathbf{R}^n$. The paper finishes with a discussion of examples of Schrödinger equations and the solutions.

CONTENTS

LIST OF FIGURES

CHAPTER 1

A BRIEF INTRODUCTION TO QUANTUM MECHANICS

The focus of this project is to solve the one-dimensional, time independent Schrödinger equation for particles under different potentials. The Schrödinger equation is

$$H\psi = e\psi \tag{1}$$

where H, the Hamiltonian operator is given by

$$H\psi = -\psi" + q\psi,$$

q is a real valued function that describes the potential and e is a positive number. The theory discussed in this paper deals with the case where q is non-negative and continuous on an interval.

Throughout this paper X will be the domain of H, where X is all members of $C^2[a, b]$ so that $u(a) = u(b) = 0$ and for $u, v \in X$ the inner product of u and v is $\int_a^b uv$. This implies that for $u \in X, \|u\|^2 = \int_a^b u^2$. The co domain of H, denoted by Y, will be the space consisting of the continuous functions on [a,b] with the same inner product and norm. The eigenfunctions of equation (1) will be the wave functions which describe the position and momentum of the particle. The eigenvalues of equation (1) will be the energy levels of the particle. The energy levels increase as the particle reaches higher quantum states. Now we give a brief discussion comparing and contrasting classical physics and quantum mechanics.

Classical physics states that a particle in motion follows a trajectory. This implies that at any given time the position and momentum of a particle can be found simultaneously. So particles are treated as discrete objects that follow certain paths. In the late 19th and early 20th century through a combination of experiments and theory, Plank, Einstein, Born, Heisenberg, and others showed that Newtonian Mechanics did not describe particles at the quantum level. Among their results were the following:

- Momentum and position of a particle in motion cannot both be known to a great degree of accuracy. Specifically $\Delta x \Delta p = h$, where h is Plank's constant and Δx, Δp are uncertainties in position and momentum. Hence, as Δx decreases, Δp increases and vice versa.
- Particles, in particular electrons, behave like waves in that if a beam of electrons is passed through a diffraction grating, it is possible to obtain a wavelength for the beam of electrons. This implies that electrons display the same wave behavior as light.
- Einstein showed that light behaves as if it consisted of discrete units called quanta each with energy $h\nu$, where $\nu = \frac{c}{\lambda}$, λ is the wavelength of light, and c is the speed of light.

Further information regarding these findings can be found in most quantum mechanics books, for example [5].

To account for the wave-particle duality of matter, a new theory was called for. This theory would use probability to describe the position of matter just as intensity is used to predict the probability of finding a photon in a region, but still take into account that light and matter behave like particles during emission and absorption of energy. In 1926 Erwin Schrödinger proposed equation (1). His equation uses the idea that the total energy of a particle, as described in classical physics, is the sum of its kinetic and potential energies. In the definition of H, $-\psi$" represents the kinetic energy of the particle and $q\psi$ represents the potential energy of the particle.

Unlike classical mechanics, the wave function does not predict exactly where the particle will be at a given time. Instead, from the wave function one can find the probability of finding the particle in a given region. This is known as Born's interpretation of the wave function. Born postulated that just as the probable position of a photon is given by the square of the amplitude of the electromagnetic wave, the probability of finding an electron in a region R is given by $\int_R \psi^* \psi$ where $\psi^* \psi = \psi^2$ if ψ is real valued [2].

CHAPTER 2

COMPACT OPERATORS AND THE SCHRÖDINGER EQUATION

In this chapter we discuss the development of compact operators which, as we will see, play a key role in finding eigenvalues and eigenvectors of H. $H : X \to Y$ will be given by $Hu = -u" + qu$, where q is continuous on $[a, b]$. We will specify when q is non-negative.

This section consists of a discussion showing that the Hamiltonian operator with zero boundary conditions has a compact, symmetric, positive, and continuous inverse T with domain all of Y.

2.1. Compact Operators

To show that H has an inverse consider the following

Definition 2.1. Let n be a positive integer. Define $L(\Re^n)$ to be the space of linear transformations from $\Re^n \to \Re^n$.

Lemma 2.2. *Let $Q : [a, b] \to L(\Re^n)$ be continuous. There exists $M : [a, b] \to L(\Re^n)$ so that $M' = -MQ$ and $M^{-1}(t)$ exists for all $t \in [a, b]$.*

Proof. Let

$$Q(t) = \begin{pmatrix} a_{1,1}(t) & \dots & a_{1,n}(t) \\ \vdots & & \vdots \\ a_{n,1}(t) & \dots & a_{n,n}(t) \end{pmatrix} \text{ and define } M(t) = \begin{pmatrix} b_{1,1}(t) & \dots & b_{1,n}(t) \\ \vdots & & \vdots \\ b_{n,1}(t) & \dots & b_{n,n}(t) \end{pmatrix}.$$

$b_{i,j}(t)$ will be determined shortly . Then

$$M(t)Q(t) = \begin{pmatrix} \sum_{i=1}^n b_{1,i}(t)a_{i,1}(t) & \dots & \sum_{i=1}^n b_{1,i}(t)a_{i,n}(t) \\ \vdots & & \vdots \\ \sum_{i=1}^n b_{n,i}(t)a_{i,1}(t) & \dots & \sum_{i=1}^n b_{n,i}(t)a_{i,n}(t) \end{pmatrix}$$

Consider the equation

$$\begin{pmatrix} b'_{i,1}(t) \\ \vdots \\ b'_{i,n}(t) \end{pmatrix} = -Q^T(t) \begin{pmatrix} b_{i,1}(t) \\ \vdots \\ b_{i,n}(t) \end{pmatrix}$$

Write this system as $B'_i(t) = -Q^T(t)B_i(t)$ and choose $C_1 \neq 0 \in \Re^n$. By the fundamental existence theorem, there is a unique solution $B_1(t)$ so that $B_1(a) = C_1$ and $B'_1(t) = -Q^T(t)B_1(t)$. Suppose $C_2, \ldots C_n$ have been chosen so that $\{C_1, \ldots C_n\}$ is linearly independent. Then $B'_i(t) = -Q^T(t)B_i(t)$ has a unique solution satisfying $B_i(a) = C_i$ for all i with $1 \leq i \leq n$. Hence one can inductively solve for the rows of M and obtain the desired matrix. Furthermore since the rows of $M(a)$ were picked to be linearly independent, $M(a)$ has an inverse. In addition, it is a fact that if $M(c)^{-1}$ exists for some $c \in [a, b]$, then $M(t)$ has an inverse for all $t \in [a, b]$. It also follows from the fundamental existence theorem that the entries in M are continuous. See chapters 1 and 3 of [1]. □

LEMMA 2.3. *Suppose q is continuous and non-negative. Then H, the Hamiltonian is positive and injective.*

PROOF.

$$\begin{aligned} & \langle Hu, u \rangle \\ &= \int_a^b uHu \\ &= -u(b)u'(b) + u(a)u'(a) + \int_a^b (u'^2 + qu^2) \end{aligned}$$

Using the boundary conditions $u(a) = u(b) = 0$, we get

$\langle Hu, u \rangle \geq 0$

for all $u \in X$ and

$\langle Hu, u \rangle = 0$

iff $u = 0$. □

THEOREM 2.4. *Let q be a non-negative and continuous function on $[a,b]$. Suppose g is a continuous function on $[a,b]$ and there is $u \in X$ so that $Hu = g$. Then there is a continuous function k from $[a,b]^2$ to $\Re$ so that*

$$u(t) = \int_a^b k(s,t)g(s)ds$$

PROOF. Let

$$A = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \text{ and } B = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

Then if

$$\vec{u} = \begin{pmatrix} u \\ u' \end{pmatrix}$$

$$A\vec{u}(a) + B\vec{u}(b) = \vec{0}. \tag{2}$$

Also let

$$Q = \begin{pmatrix} 0 & 1 \\ q & 0 \end{pmatrix}$$

and

$$\vec{g} = \begin{pmatrix} 0 \\ -g \end{pmatrix}$$

Then

$$\vec{u}' = Q\vec{u} + \vec{g} \tag{3}$$

By lemma (2.2) there is a matrix M so that $M' = -MQ$ and $M(t)^{-1}$ exists for all $t \in [a,b]$. By multiplying both sides of equation (3) by M we get

$$M\vec{u}' = MQ\vec{u} + M\vec{g}$$

$$M\vec{u}' + M'\vec{u} = M\vec{g}$$

$$(M\vec{u})' = M\vec{g}$$

Thus, $\int_a^t (M\vec{u})' = \int_a^t M\vec{g}$.

Integrating and solving for $\vec{u}$(t) gives

$$\vec{u}(t) = M(t)^{-1}(M(a)\vec{u}(a) + \int_a^t M\vec{g}) \tag{4}$$

Let $t = b$ and we get

$$\vec{u}(b) = M(b)^{-1}(M(a)\vec{u}(a) + \int_a^b M\vec{g})$$

Now equation (2) becomes

$$A\vec{u}(a) + BM(b)^{-1}(M(a)\vec{u}(a) + \int_a^b M\vec{g}) = \vec{0}$$

which can be written as

$$(A + BM(b)^{-1}M(a))\vec{u}(a) = -BM(b)^{-1}\int_a^b M\vec{g} \tag{5}$$

Let $\Gamma = A + BM(b)^{-1}M(a)$. Suppose $\Gamma v = 0$ and let $\gamma(t) = M(t)^{-1}M(a)v$. Then $A\gamma(a) + B\gamma(b) = \vec{0}$ and $\gamma' = Q\gamma$. But since H is injective $\gamma(t)$ must be the zero function. Thus $v = \vec{0}$. This implies that the linear operator Γ is injective and has an inverse. Thus we can solve for $\vec{u}(a)$.

Now rewrite equation (4) as

$$\vec{u}(t) = M(t)^{-1}(-M(a)(A + BM(b)^{-1}M(a))^{-1}BM(b)^{-1}\int_a^b M\vec{g} + \int_a^t M\vec{g})$$

Which simplifies to

$$\vec{u}(t) = \int_a^t M(t)^{-1}D^{-1}AM(a)^{-1}M(s)\vec{g}(s)ds \; - \; \int_t^b M(t)^{-1}D^{-1}BM(b)^{-1}M(s)\vec{g}(s)ds$$

where $D = AM(a)^{-1} + BM(b)^{-1}$.

Let

$$K_1(s,t) = M(t)^{-1}D^{-1}AM(a)^{-1}M(s) \text{ if } a \le s \le t$$

$$K_2(s,t) = -M(t)^{-1}D^{-1}BM(b)^{-1}M(s) \text{ if } t \le s \le b$$

Note $K_1(t,t) - K_2(t,t)$ is the identity. Define $k(s,t)$ to be the upper right entry of $K_1(s,t)$ for all s $\in [a,t]$ and $k(s,t)$ to be the upper right entry of $K_2(s,t)$ for all s $\in [t,b]$. Observe that k is well defined and continuous at $s = t$. Also the entries in $M(t)$ are continuous, thus all the entries in K_1 and K_2 are continuous, so k is continuous.

□

Now for $g \in Y$ define

$$(Tg)(t) = \int_a^b k(s,t)g(s)ds,$$

where k is the function from Theorem 2.4.

Proposition 2.5. *k from Theorem 2.4 is unique, and T is H^{-1}.*

Proof. For $g \in Y$, let $u(t) = \int_a^b k(s,t)g(s)ds$, if we work backwards in the proof of theorem 2.4 we see, $u \in X$ and $-u" + qu = g$. Thus for each $g \in Y$, $Tg \in X$ and $H(Tg) = g$. Suppose there is a continuous functions $j : [a,b] \to \Re$ that satisfies the same properties as k, for $x \in [a,b]$ let $g_x(s) = k(s,x) - j(s,x)$, and $v_x(t) = \int_a^b j(s,t)g_x(s)ds$. Then $Hv_x = H(Tg_x)$ so $v_x = Tg_x$. This implies $0 = \int_a^b (k(s,t) - j(s,t))(k(s,x) - j(s,x))ds$ for all $t \in [a,b]$, thus if we let $x = t$ then $k(s,x) - j(s,x) = 0$ for all $s \in [a,b]$. Because x was arbitrary then $k(s,t) = j(s,t)$ for all $s,t \in [a,b]$.

Thus T has domain all of Y and for $g \in Y, H(Tg) = g$. For $u \in X, Hu \in Y$, let $\widehat{u} = \int_a^b k(s,t)Hu(s)ds$, then $H\widehat{u} = Hu$, $\widehat{u} = u$, and $T(Hu) = u$. □

From now on T with domain all of Y will denote H inverse. To show that T is compact consider the following

Definition 2.6. Let $W \in L(F, K)$, where F and K are inner product spaces. W is compact if whenever $\{x_n\}_{n\geq 1} \subseteq F$ is bounded then $\{Wx_n\}_{n\geq 1}$ has a convergent subsequence in K.

Definition 2.7. $D \subseteq C[a, b]$ (with sup norm) is equicontinuous at $x \in [a, b]$ if for all $\epsilon > 0$ there exists $\delta > 0$ so that if $|x - y| < \delta$ then $|f(x) - f(y)| < \epsilon$ for all $f \in D$. D is equicontinuous if it is equicontinuous at every point of $[a, b]$.

Proposition 2.8. *If $\{g_n\}_{n\geq 1} \subseteq Y$ is bounded, then $\{Tg_n\}_{n\geq 1} \subseteq X$ is an equicontinuous and bounded subset of $C[a, b]$.*

Proof. Since k is continuous on $[a, b]^2$, k is bounded on $[a, b]^2$. Say $|k(s, t)| \leq C$ on $[a, b]^2$, so if $g \in Y$

$$sup_{t\in[a,b]}|\int_a^b k(s,t)g(s)ds| \leq$$
$$sup_{t\in[a,b]}\int_a^b |k(s,t)||g(s)|ds \leq$$
$$C\int_a^b |g(s)|ds$$

Suppose $\|g_n\|_Y = \int_a^b g_n^2 \leq \widehat{C}$ for all $n \geq 1$ then by the Cauchy-Schwarz inequality for inner product spaces

$$\int_a^b |g_n| \leq (\int_a^b g_n^2 \int_a^b 1)^{1/2} \leq ((b-a)\widehat{C})^{1/2}$$

Now,

$$sup_{t\in[a,b]}|Tg_n(t)| \leq C(\widehat{C}(b-a))^{1/2}$$

Thus, one has $\{Tg_n\}_{n\geq 1}$ is a subset of $C[a, b]$ that is bounded in the sup norm. But since

$$\|Tg_n\|_X = \int_a^b (Tg_n)^2 \leq C^2\widehat{C}^(b-a)^2$$

$\{Tg_n\}_{n\geq 1}$ is bounded in X also. Note the above implies that T is continuous, since if $\|g\|_Y \leq 1$ then $\|Tg\|_X \leq C^2(b-a)$.

To show $\{Tg_n\}_{n\geq 1}$ is equicontinuous, let $x \in \Re$ and $\epsilon > 0$, $0 < \bar{\epsilon} < \frac{\epsilon}{((b-a)\widehat{C})^{1/2}}$. Choose $\delta > 0$ so that if

$$|s-x| < \delta \text{ then } |k(s,t) - k(x,t)| < \bar{\epsilon}.$$

Then

$$\begin{aligned}|Tg_n(s) - Tg_n(x)| &= \\ \left|\int_a^b (k(s,t) - k(x,t))g_n(t)dt\right| &\leq \\ \int_a^b |k(s,t) - k(x,t)||g_n(t)|dt &\leq \\ \bar{\epsilon}\int_a^b |g_n| &\leq \\ \bar{\epsilon}((b-a)\widehat{C})^{1/2} &< \epsilon\end{aligned}$$

□

By the following (Arzela-Ascolli Theorem), T is compact. See page 5 of [1].

THEOREM 2.9. *Every bounded equicontinuous subset of C[a,b] has a limit point.*

Also if $sup_{t\in[a,b]}|f(t) - Tg_n(t)| \to 0$, then $\int_a^b (f - Tg_n)^2 \to 0$. Thus f is the limit of $\{Tg_n\}_{n\geq 1}$ in X if it is the limit of $\{Tg_n\}_{n\geq 1}$ in $C[a,b]$.

To show that T is symmetric, we will show H is symmetric. Since H is bijective this will imply that T is symmetric. Let u and v be in the domain of H. Then

$$\langle Hu, v\rangle - \langle Hv, u\rangle =$$

$$\int_a^b (-u" + qu)v - (-v" + qv)u =$$

$$\int_a^b -u"v + v"u$$

An integration by parts gives that this equals

$$-(vu')(b) + (vu')(a) + (uv')(b) - (uv')(a)$$

With zero boundary condition on u and v, the above equation is zero. So $\langle Hu, v\rangle = \langle Hv, u\rangle$.

Finally to show that T is positive, suppose $g \in Y$ and $Tg = u$. Then $g = Hu$ and so

$$\langle Tg, g\rangle = \langle u, Hu\rangle \geq 0.$$

To show that H has an eigenvalue, note that if

$$Tu = \lambda u$$

then

$$Hu = \frac{1}{\lambda}u.$$

λ is real as T is positive, and $\lambda \neq 0$ since T is injective.

Thus, to show H has an eigenvalue it suffices to show T has an eigenvalue.

THEOREM 2.10. *Suppose F is an inner product space and W is a compact, symmetric, and non-negative member of $L(F, F)$. Then $|W|$ is an eigenvalue of W.*

PROOF. Since W is bounded, one can define

$$|W| = \text{ lub } \{\|Wx\| : x \in F, \|x\| = 1\}$$

It is known that

$$|W| = \text{ sup } \{\langle Wx, x\rangle : x \in F \text{ and } \|x\| = 1\}.$$

For each $n \geq 1$ choose $x_n \in F$ so that $\|x_n\| = 1$ and

$$|W| - \langle Wx_n, x_n \rangle < \frac{1}{n}$$

Then since $\{x_n\}_{n\geq 1}$ is bounded, $\{Wx_n\}_{n\geq 1}$ has a convergent subsequence $\{Wx_{n_i}\}_{i\geq 1}$. Let x be the limit of this subsequence. Then

$$\begin{aligned}
\lim_{i\to\infty} \|Wx_{n_i} - |W|x_{n_i}\|^2 &= \\
\lim_{i\to\infty} \langle Wx_{n_i} - |W|x_{n_i}, Wx_{n_i} - |W|x_{n_i} \rangle &= \\
\lim_{i\to\infty} \|Wx_{n_i}\|^2 - 2|W|\langle Wx_{n_i}, x_{n_i} \rangle + \|x_{n_i}\|^2|W|^2 &\leq \\
\lim_{i\to\infty} 2|W|^2 - 2|W|\langle Wx_{n_i}, x_{n_i} \rangle &= 0 \\
\text{since } \lim_{i\to\infty} \langle Wx_{n_i}, x_{n_i} \rangle &= |W|. \\
\text{Thus } x = \lim_{i\to\infty} |W|x_{n_i} &\text{ and} \\
Wx = W \lim_{i\to\infty} |W|x_{n_i} &= \\
|W| \lim_{i\to\infty} Wx_{n_i} &= \\
&|W|x
\end{aligned}$$

□

Let $\lambda_1 = |T|$ and let ψ_1 be an eigenvector for λ_1. Then T restricted to the orthogonal complement of ψ_1, ψ_1^p, is a compact, symmetric, non-negative, and continuous linear transformation. So $T|_{\psi_1^p}$ has an eigenvlaue $\lambda_2 = |T|_{\psi_1^p}|$ and a corresponding eigenvector ψ_2. $\lambda_2 \leq \lambda_1$ as

$$|T|_F| = \sup \{\langle Tx, x \rangle : x \in F \text{ and } \|x\| = 1\}.$$

Where $F = \psi_1^p$. By continuing this process we can generate more eigenfunctions and eigenvalues. Because the dimension of the eigenspace of λ_1 is finite, we must generate a new eigenvalue after a finite number of runs through the above process. Hence we can generate a countable set of eigenfunctions that span X.

CHAPTER 3

NUMERICAL SCHEME

3.1. Numeric Scheme

The numerical scheme makes use of the Rayleigh quotient to find the eigenvectors and eigenvalues. See pages 172-178 of [3]. Here is a brief description of the algorithm.

Let n be a positive integer and divide $[a, b]$ into $n + 1$ equal sections. Let H_n be the matrix

$$\begin{pmatrix} \alpha + v_1 & \beta & 0 & \ldots 0 \\ \beta & \alpha + v_2 & \beta & \ldots 0 \\ \ldots & & & \\ 0 & \ldots & -1 & \alpha + v_n \end{pmatrix}$$

where

$$\begin{pmatrix} v_1 \\ \vdots \\ v_n \end{pmatrix}$$

is the discrete version of v, the potential, on $[a+1/(n+1), b-1/(n+1)]$, $\alpha = 2(n+1)^2$, and $\beta = -(n+1)^2$.

H_n is the discrete version of the Hamiltonian with zero boundary conditions. For v non-negative, the determinant of this matrix will be greater that or equal to $(\frac{\beta}{\alpha+c})^n$, where c is an upper bound to v on $[a, b]$. Thus H_n is invertible if v is non-negative, hence we can define T_n to be H_n^{-1}. Also since H_n is symmetric, H_n is diagnolizable. So let P be an orthonormal basis of eigenvectors of H_n for $\Re^n$.

For the remainder of this section $\langle ., . \rangle$ and $\|.\|$ will denote the standard norm and inner product on $\Re^n$.

Choose $x_0 \neq 0 \in \Re^n$ and Define x_k as

$$x_k = q_k T_n x_{k-1}$$

$$q_k = \frac{\|x_{k-1}\|^2}{\langle T_n x_{k-1}, x_{k-1}\rangle}$$

PROPOSITION 3.1. *Let x_k be defined as above then*

1) $\lim_{k\to\infty} q_k = |T_n|$ *if* $\langle T_n x_0, x_0\rangle \neq 0$

2) $x = \lim_{k\to\infty} x_k$ *exists*

3) $T_n x = |T_n| x$

PROOF. To show 1) note that

$$q_k = \frac{(q_1 \dots q_{k-1})^2 \|T_n^{k-1} x_0\|^2}{(q_1 \dots q_{k-1})^2 \langle T_n^k x_0, T_n^{k-1} x_0\rangle} = \frac{\|PD^{k-1}C\|^2}{\langle PD^k C, PD^{k-1}C\rangle} = \frac{\|D^{k-1}C\|^2}{\langle D^k C, D^{k-1}C\rangle}$$

where $P^{-1}x_0 = C$.

So if $C = \begin{pmatrix} c_1 \\ \vdots \\ c_n \end{pmatrix}$ and the diagonal entries of D are $d_1, \dots d_n$ then

$$\lim_{k\to\infty} q_k = \lim_{k\to\infty} \frac{d_1^{2k} c_1^2 + \dots d_n^{2k} c_n^2}{d_1^{2k+1} c_1^2 + \dots d_n^{2k+1} c_n^2} \tag{6}$$

Let $|T_n| = d_1$ and assume $d_i \geq d_{i+1}$. By dividing top and bottom of (6) by d_1 and taking the limit on k one gets that (6) equals $|T_n|^{-1}$.

To show 2) start by writing x_k as

$$(\prod_{i=1}^{k} q_i) T^k x_0 =$$

$$(\prod_{i=1}^{k} q_i) PD^k C =$$

$$P(\prod_{i=1}^{k} q_i D)C$$

Then

$$\begin{aligned}\|x_k - x_l\|^2 = \\ \|(\prod_{i=1}^{k}(q_i D) - \prod_{i=1}^{l}(q_i D))C\|^2 \leq \\ (\sum_{j=1}^{n}(\prod_{i=1}^{k}(q_i d_j) - \prod_{i=1}^{l}(q_i d_j))^2)c_M\end{aligned}$$

where c_M is $\max(c_1^2, \ldots c_n^2)$.

$$q_{i+1}d_1 = \frac{c_1^2 + \ldots \alpha_n^{2i} c_n^2}{c_1^2 + \ldots \alpha_n^{2i+1} c_n^2}$$

where $\alpha_i = \frac{d_i}{d_1} \leq 1$ and $\alpha_i \geq \alpha_{i+1}$. Also $q_i d_1 \geq 1$ so $1 \leq \prod_{i=1}^{k}(q_i d_1)$ for all k and $\{\prod_{i=1}^{k}(q_i d_1)\}_{k \geq 1}$ is increasing. To show this sequence is bounded will show $\{\sum_{i=1}^{k}(q_i d_1 - 1)\}_{k \geq 1}$ is bounded (see following proposition for explanation).

$$\begin{aligned}q_{i+1}d_1 - 1 = \\ \frac{c_1^2 + \ldots \alpha_n^{2i} c_n^2}{c_1^2 + \ldots \alpha_n^{2i+1} c_n^2} - 1 = \\ \frac{c_1^2 + \ldots \alpha_n^{2i} c_n^2 - (c_1^2 + \ldots \alpha_n^{2i+1} c_n^2)}{c_1^2 + \ldots \alpha_n^{2i+1} c_n^2} \leq \\ c_M \frac{\alpha_2^{2i}(1-\alpha_2) + \ldots \alpha_n^{2i}(1-\alpha_n)}{c_1^2 + \ldots \alpha_n^{2i+1} c_n^2} \leq \\ \frac{c_M(n-1)\alpha_2^{2i}(1-\alpha_n)}{c_1^2} = M\beta_i\end{aligned}$$

where $M = \frac{c_M(n-1)(1-\alpha_n)}{c_1^2}$ and $\beta_i = \alpha_2^{2i}$.

$\sum_{i=1}^{k} M\beta_i$ is bounded for all k, hence $\{\prod_{i=1}^{k}(q_i d_1)\}_{k \geq 1}$ converges and as $k, l \to \infty$, $\prod_{i=1}^{k}(q_i d_1) \to \prod_{i=1}^{l}(q_i d_1)$.

Now $d_j = d_1(d_j/d_1)$ so

$$\prod_{i=1}^{k} q_i d_j = (d_j/d_1)^k \prod_{i=1}^{k} q_i d_1 \to 0$$

as k $\to \infty$. So one has $\|x_k - x_l\| \to 0$ as k and l go to infinity , which makes $\{x_k\}_{k\geq 1}$ a cauchy sequence in $\Re^n$. So it is converges.

To show 3), note that

$$|T|\, x =$$
$$\lim_{n\to\infty} \frac{1}{q_{n-1}} \lim_{n\to\infty} x_{n-1} =$$
$$\lim_{n\to\infty} \frac{1}{q_{n-1}} x_{n-1} = \lim_{n\to\infty} \frac{1}{q_{n-1}} q_{n-1} T x_{n-2} =$$
$$\lim_{n\to\infty} T x_n = T \lim_{n\to\infty} x_n = Tx.$$

□

Proposition 3.2. *If $\{\sum_{i=1}^{k} a_i\}_{k\geq 1}$ is bounded, then $\{\prod_{i=1}^{k}(1+a_i)\}_{k\geq 1}$ is bounded .*

Proof.

$$ln(1+a_i) \leq a_i \text{ so}$$
$$\sum_{i=1}^{k} ln(1+a_i) \leq \sum_{i=1}^{k} a_i$$

□

3.2. Numerical Results

Numerical results were obtained for four different potentials. In three of the four cases the potential q was non-negative and continuous on an interval symmetric about the origin. So the theory discussed in the section regarding compact operators applies to these potentials. In the fourth example, the potential was positive on an interval symmetric about the origin, but unbounded.

The particle in a box is the case where $q = 0$. This describes the situation where a particle is confined to a box of finite length. Within these walls there is no force imposed on the particle but at the walls the potential rises to infinity. The harmonic oscillator is the case where $q(x) = x^2$. This potential describes the situation where the particle undergoes a restoring force proportional to its displacement which keeps the particle in the equilibrium

position. The double well is given by $q(x) = 25(x-1)^2(x+1)^2$ and $q(x) = 50(x-1)^2(x+1)^2$. This potential describes a particle confined to a region where there is a dip in the potential in a region to the left of the origin and in a symmetric region to the right of the origin, but there is a barrier at the origin. These describe the positive and continuous potentials. The coulomb potential describes the behavior of an electron around the nucleus. This potential is given by $q(x) = |x|^{-1}$. On a symmetric interval about the origin this potential is unbounded but positive. So the theory above does not cover this case.
Now a brief discussion of each of the potential and the solutions obtained.

3.2.1. *Particle in the Box*

The problem of the particle in the box can be solved explicitly. The solutions with the imposed zero boundary conditions are

$$\psi_n(x) = c \sin \frac{n\pi x}{L}$$

where L is the length of the box and c is usually the normalization constant. From this one gets that the energies or eigenvalues are $(n\pi L^{-1})^2$. Note that the difference in energy between the n and $n+1^{st}$ level is $(2n+1)\pi L^{-1}$. So the energy levels rise as the square of the integers. If one examines the wave functions, one observes that the number of nodes increases as the particle reaches higher quantum states (a node represents a position where there is no electron density). This suggests that the wavelength of the particle is decreasing. Einstein's equation of light states that energy is inversely proportional to wavelength so this suggests that the kinetic energy of the particle increases as it reaches higher states. This is consistent with the increasing eigenvalues. The energy levels start at $n = 1$. This implies that the ground state energy of the particle is positive. One explanation of this is the uncertainty principle. Since one knows the particle is confined to within a box of length 2L, one can use that $\Delta p \Delta x = h$ to estimate the momentum of the particle which is nonzero. One then uses the relationship between kinetic energy and momentum to conclude that since the momentum of the particle is non-zero then the lowest possible energy must be positive[5]. Another way of looking at this is that since the Hamiltonian is injective for non-negative potentials, then $Hu = 0$ only has the trivial solution which can not be an eigenvector. See figures 3.1 and 3.2.

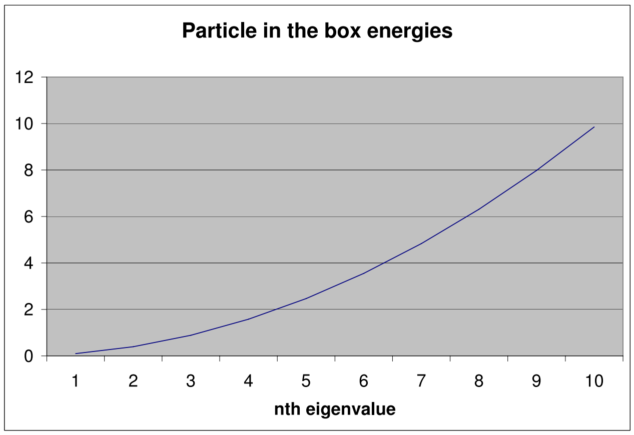

FIGURE 3.1. Particle in Box Energy Levels

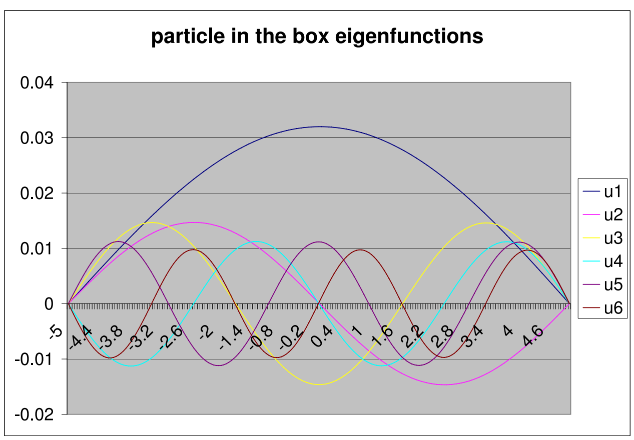

FIGURE 3.2. Particle in Box Eigenfunctions

3.2.2. *Harmonic Oscillator*

The problem of the harmonic oscillator can also be solved for explicit solutions. The wave functions are the product of a constant (usually the normalization constant) the exponential function

$$f(x) = e^{-\frac{x^2}{2}}$$

and a hermite polynomial. The first few hermite polynomials are are

$$\begin{aligned} 1 \\ 2x \\ 4x^2 - 2 \\ 8x^3 - 12x \\ 16x^4 - 48x^2 + 12 \\ 32x^5 - 160x^3 + 120x \end{aligned}$$

These solutions can be obtained by supposing that a solution of the form

$$e^{-\frac{x^2}{2}} f(x)$$

exists and plugging such a solution into the Schrödinger equation. The energy levels of the harmonic oscillator are given by

$$\frac{(2n+1)\hbar\omega}{2} \text{ where } \omega = \sqrt{\frac{k}{m}} \text{ and k is the force constant, n is a positive integer}$$

One notes that the differences in energy levels are $\hbar\omega$ so the energy levels increase at a constant rate. Furthermore, the harmonic oscillator has positive ground state energy. This can again be explained by the uncertainty principle or by the Hamiltonian being injective. It is also worth noting that if the force constant is small or the particle is massive, then the first few energy levels of the harmonic oscillator are negligible. In the case of atoms however the energy levels become important [2]. See figures 3.3 and 3.4.

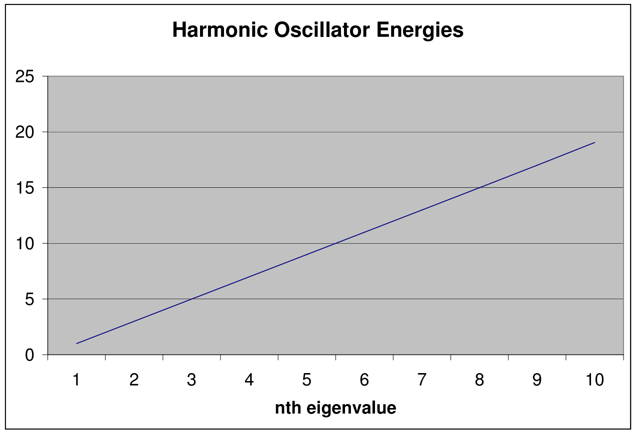

FIGURE 3.3. Harmonic Oscillator Energy Levels

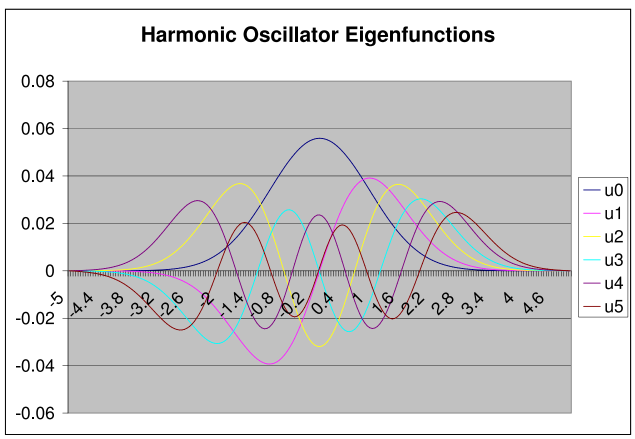

FIGURE 3.4. Harmonic Oscillator Eigenfunctions

3.2.3. *Double Well and Coulomb Potentials*

The numerical results obtained for the double well were probably the most interesting. If one examines the energy level, it is apparent that the energy levels are close to being pairwise degenerate before the particle has sufficient energy to overcome the barrier at the origin. But after the barrier is overcome, the energy levels of the particle rise almost linearly in a similar manner as the harmonic oscillator. This was the case when the barrier at the origin was 25 and 50.

The eigenfunctions of a particle under this potential also displayed different behaviors before and after the particle had sufficient energy to escape the barrier. Before the energy barrier is overcome, there is a dip at the origin in the n^{th} eigenfunctions where n is odd. This corresponds to a lower probability of finding the particle there. After the energy barrier is overcome, the eigenfunctions resemble those of the harmonic oscillator. See figures 3.5 to 3.8.

For the Coulomb potential a cut off value of 10^{16} was used at the origin. The numerical results obtained for the Coulomb potential indicate that the first ten eigenvalues are pairwise degenerate. The overall rise in the energy levels does not seem to be linear. The eigenfunctions indicate that the probability of finding the particle at a region, R, about the origin goes to zero as the diameter of R goes to zero. Away from the origin, the results indicates that the particles is equaly likely to be on the left or the right. This is what one would expect as the potential is symmetric. See figures 3.9 and 3.10.

For this potential the eigenfunctions obtained from the code did not have a first or second derivative at the origin. As mentioned before, the theory discussed in this paper does not deal with this situation. The reference below discusses how to deal with this situation. The suggestion is to divide up the problem of solving the Hamiltonian on the interval $[-a, a]$ into a two interval problem. So seek solutions on the interval $[-a, 0]$ and $[0, a]$. Then form the direct product of the spaces $L^2[-a, 0]$ and $L^2[0, a]$ and obtain an operator on this new space from the direct sum of the operators on each of $L^2[-a, 0]$ and $L^2[0, a]$. For a detailed explanation see chapter 13 of [4]. For the problem of the singularity at the origin see part 4 of [4].

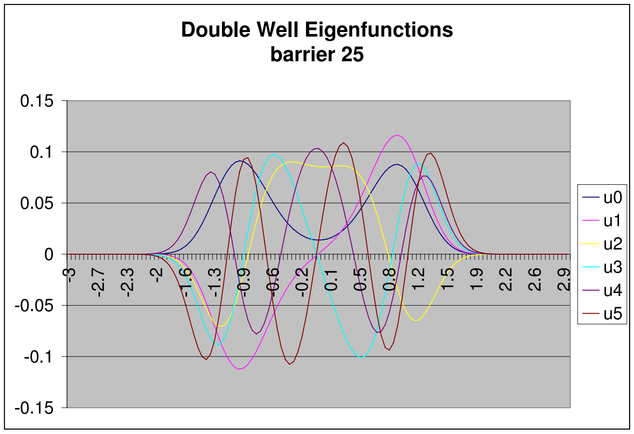

Figure 3.5. Double Well Energy Levels with Barrier of 25

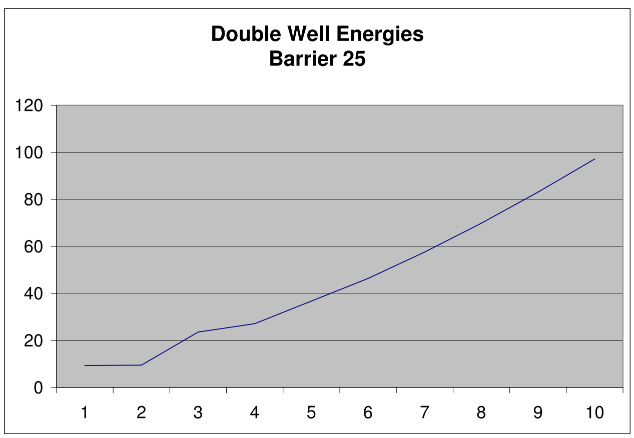

Figure 3.6. Double Well Eigenfunctions with Barrier of 25

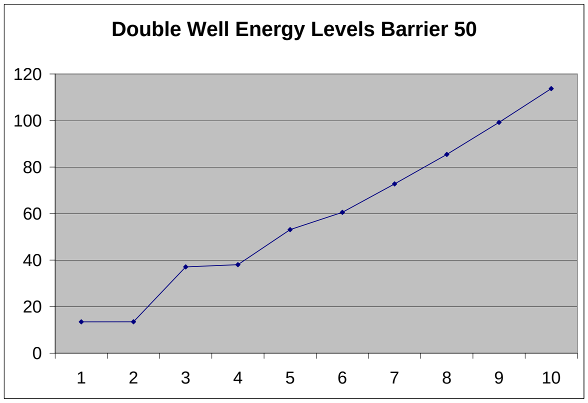

FIGURE 3.7. Double Well Energy Levels with Barrier of 50

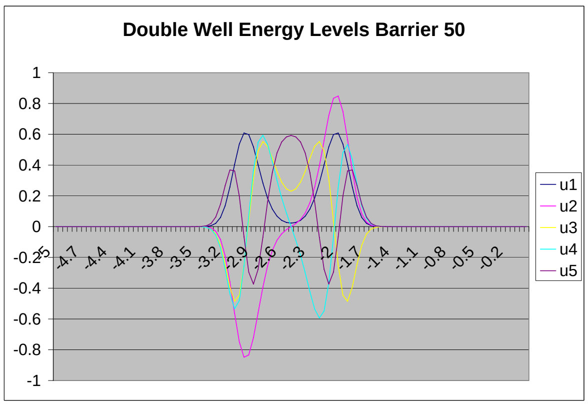

FIGURE 3.8. Double Well Eigenfunctions with Barrier of 50

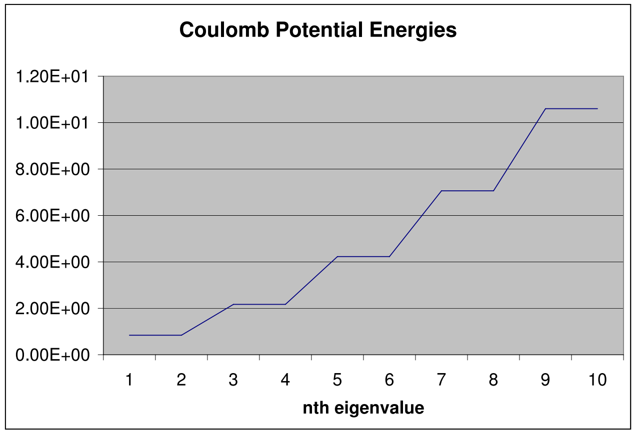

Figure 3.9. Coulomb Potential Energy Levels

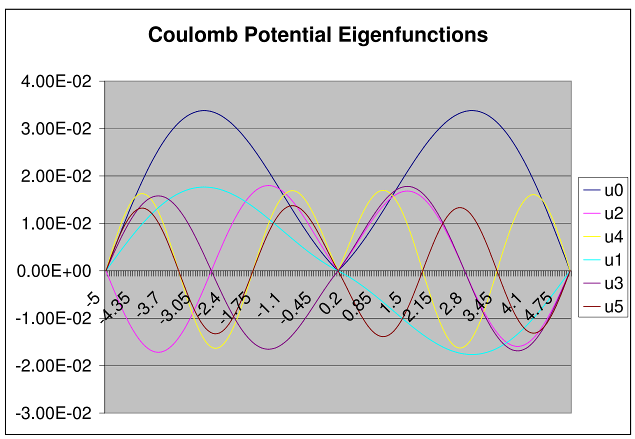

Figure 3.10. Coulomb Potential Eigenfunctions

CHAPTER 4

CONCLUSIONS

In this paper the goal of solving the one-dimensional time independent Schrödinger equation was accomplished completely in the case where the potential acting on the particle is non-negative and continuous. The theory on compact operators in a Hilbert space showed the existence of a discrete set of solution to $H\psi = \lambda\psi$ and the code found the solutions. One of the potential that was used in the code, the coulomb potential, was positive but not bounded on a symmetric interval about the origin. Although numerical solutions were obtained, the eigenfunctions did not have a second derivative everywhere. The theory about compact operators does not directly apply to this case to show that solutions must exist. Even so the solutions obtained seem to give meaningful information about a particle under this potential. As a follow up to this paper one might be interested in looking at topics such as:

- If compact operators in a Hilbert space can be extended to include operators with unbounded potentials.
- How the problem of singularity at the origin can be interpreted. Reference [4] gives a description of this.
- If Hilbert space theory applies when one replaces the one-dimensional time independent Schrödinger equation with the three dimensional time dependent Schrödinger equation.

It is probably also worth noting that all the theory developed in this paper used the incomplete $C[a, b]$ as a subset of $L_2[a, b]$. So completeness of a Hilbert space was not needed or used anywhere in this paper.

BIBLIOGRAPHY

[1] Coddington and Levinson, *Theory of ordinary differential equations*, McGraw-Hill Book Company, 1955.

[2] Peter Atkins, *Physical chemistry*, 6 ed., W. H. Freeman and Company, 1998.

[3] J. H. Wilkinson, *The algebraic eigenvalue problem*, Oxford University Press, 1965.

[4] Anton Zettl, *Strum-Liouville theory*, American Mathematical Society, 2005.

[5] Klaus Zoick, *Basic quantum mechanics*, John Wiley and Sons, Inc. 1969.