Numerical Solutions of Schrödinger's Equation, TB2

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Abstract

A integration approach is taken to solve the eigenfunctions and eigenvalues of the Schrödinger Equation in a 1-Dimensional quantum well. The 'Shooting Method', and the Runge-kutta Method, are used to intergrate across the specified well, and calculate the eigenvalues. This will be applied to a Square Well (infinite, and finite), a $(cosh^2)^{-1}$ potential, and to a potential barrier. Where appropriate, results will be compared to expected analytical solutions.

Contents

1 Introduction

The numerical solution of Schrödinger's Equation for one or more particles is an important problem in the field of Quantum Mechanics, and, in most cases, is the only method we can use to obtain a usable solution. Scenarios involving such a solution generally involve some external potential felt by the particles, and interactions between the particles.

The aim of this project is to derive Eigenvalues (E) and Eigen-vectors (ψ) for the one-dimensional Schrödinger Wave Equation in a specified potential well. (e.g, an electron trapped in a semi-conductor of some kind). Some of the cases will also have correlating analytical solutions, which will enable us to check our numerical results.

2 The Infinite Square Well

2.1 Introduction

We begin by considering the simplied conditions of the infinite Square Well. As seen in the lecture notes, we can describe a 'time-independent' version of Schrödinger's Equation by:

$$(-\hbar^2/2m)\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi$$

Which correlates to:

$$\hat{H}\psi = E\psi$$

,
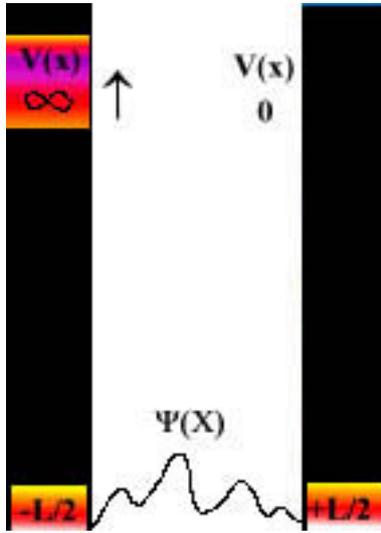
Figure 1: An Infinite Square Well Example

Where $\hat{H}$ is the Hamiltonian Operator, defined by $\hat{H} = ((-\hbar^2/2m)\nabla + V(x))$.

In the case of the Infinite Potential Well, as can be seen in the diagram, the wave function only exists between $-L/2 < x < +L/2$, where $V(x) = 0$.

(At all other points, V(x) is infinite, thus there is no probability of finding the wave here).

Therefore, we can simplify our original equation to:

$$\frac{d^2\psi}{dx^2} = -E\psi \tag{1}$$

(Note, we have let $(\hbar^2/2m) = 1$).

Where E are the eigenvalues we wish to calculate. From our above diagram we can also set the following boundary conditions for our equation, which will allow us to evaluate E:

$$\psi(-L/2) = 0, \psi(+L/2) = 0, E > 0 \tag{2}$$

2.1.1 The Analytical Solution

We now, to obtain an analytical solution, solve this like any other Differential Equation. First, we introduce the substitution $k^2 = E$, therefore our equation is now:

$$\frac{d^2\psi}{dx^2} = -k^2\psi$$

This has a solution which is a superposition of plane waves:

$$\psi(x) = Ae^{ikx} + Be^{-ikx}$$

..and, substituting our boundary conditions:

$$\psi(L/2) = Ae^{ikL/2} + Be^{-ikL/2}$$

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and..
$$\psi(-L/2) = Ae^{-ikL/2} + Be^{+ikL/2}$$

Which, substituting Cos and Sin functions, correlates to:

$$2[ACos(kL/2) + BCos(kL/2)] = 0$$

$$2i[ASin(kL/2) - BSin(kL/2)] = 0$$

These two equations have non-trivial solutions for:

$$A = B$$

$$cos(kL/2) = 0$$

Therefore:

$$k_n = (2n+1)\pi/L$$

with..

$$\psi(x) = 2Acos(k_n x)$$

Which is a Symmetrical 'even' Eigen-function.

Similarly, for

$$B = -A$$

$$Sin(kL/2) = 0$$

Therefore:

$$k_n = (2n)\pi/L$$

with..

$$\psi(x) = 2ASin(k_n x)$$

Which is a Symmetrical 'odd' Eigen-function.

Therefore, in general the Eigen-energy can be calculated analytically in our program (for comparison) by:

$$E(n) = (\hbar^2/2m)(n^2\pi^2)/L^2$$

(in our case, $(\hbar^2/2m) = 1$).

So, summing up, we wish to solve equation (1) for boundary conditions (2) numerically to give us successive Eigenvalues E that match those obtained for the analytical solution. (Afterwhich, we can extend the project to consider more realistic finite potential wells.)

2.2 The Shooting Method.

Generally, for a first or second order ODE, we use the 'Runge-Kutta' method to find specific solutions. We would feed in the ODE, and the initial conditions, and the Runga Kutta method would feed out successive 'stepped' values of the function for which we are solving ('Y', 'ψ', whatever). In our case, there is an unknown, 'E', for which we want to find values that will make our equation fit our BC's. This is known as a 'Two-point Boundary Value' problem, and can be solved using the 'Shooting Method'. [1]

We begin by considering the conditions at $x = 0$. We know our solutions are symmetrical, and therefore must be 'odd' or 'even'. (i.e., cos and sin functions...standing waves). Therefore, there are two possible conditions at $x = 0$:
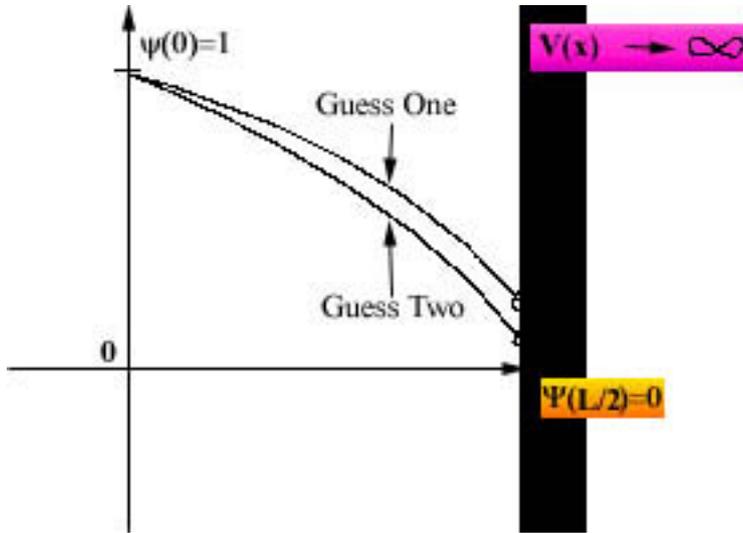
Figure 2: Shooting Method Example

Cos conditions:

$$\psi(0) = 1, \frac{d\psi(0)}{dx} = 0 \tag{3}$$

Sin conditions:

$$\psi(0) = 0, \frac{d\psi(0)}{dx} = 1 \tag{4}$$

We take these as our initial conditions. First, we consider only the cos (3) conditions. We next guess a value of 'E', put it in our ODE equation (1), and then feed this, and our initial conditions (3), into a 'Runga-kutta' function for $0 < x < +L/2$.

As seen in the diagram, we check the last value that comes out of the runge kutta functions, $\psi(L/2)$, and compare it with our final boundary condition (2): $\psi(L/2) = 0$. If they don't match, our guess was wrong... therefore we increase our value of E, and try again! We keep doing this until the $\psi(L/2)$ value returned is within a specified tolerance of 0, at which point we have an Eigenvalue solution for E!

We can continue doing this, for both initial conditions (3) and (4), for higher and higher values of E, obtaining more solutions for E (and ψ). (Note, in my program, we start at E=0, which is sensible, and use a bisection method to home in on the required 'root'. More on this below).

Now, to make use of both of our boundary conditions, and make sure we pick up every possible solution, we simply try each for each value of E. We hence find that our first successful solution, E(1) comes from our cos initial conditions, E(2) from our sin conditions, E(3) from our cos conditions...etc.. i.e, they alternate! See the following diagrams for graphs of some of the Psi functions, and some of the E values.

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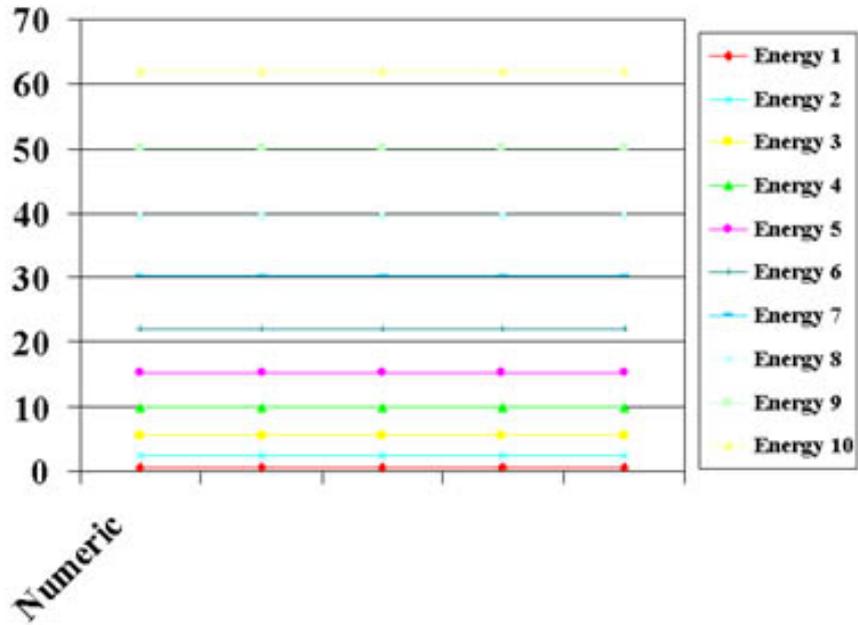
Figure 3: Infinite Energy Solutions
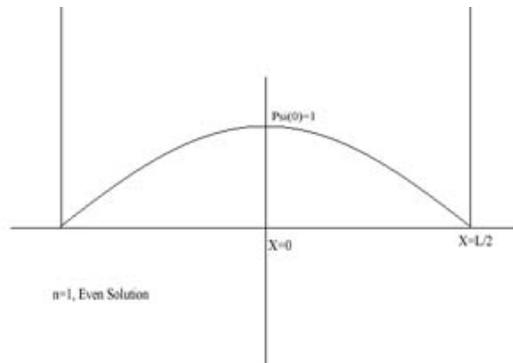
Figure 4: The first Even Solution

2.3 Root Finding

There are several approaches that can be taken to find the second boundary condition, so that we can find the Eigenvalue Energy to a given tolerance. The simplest is similar to the 'approximation' method used in 'root finding'. We specify the value by which we increase E after each loop, and check for $\psi(L/2) < root - tolerance$.

In general, we set this root-tolerance a factor of ten, or more, greater than the E-increment. Unfortunately, this method is very slow if we want to find
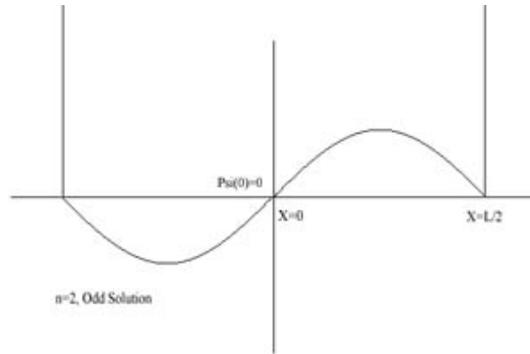
Figure 5: The First Odd Solution
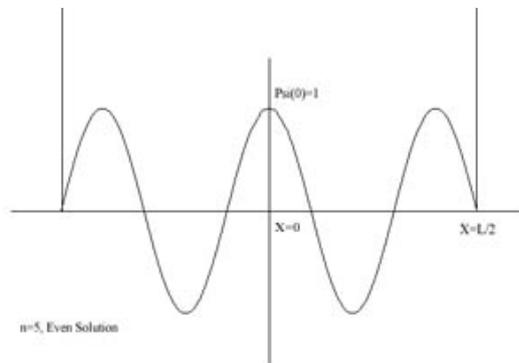
Figure 6: The Third Even Solution

E to any reasonable number of decimal points. A problem also arises which causes the program to pick up the same Eigenvalue more than once, or even skip certain results. The speed issue can be resolved to some extent by having a dynamic E-tolerance, but in general it is far more efficient to use a form of 'Bisection'.

The Bisection method involves beginning with a low E-increment, and then checking for a change in sign between consecutive values of $\psi(L/2)$. We then enter a loop, and continually decrease and swap the sign of the E-increment. This continues until we find $\psi(L/2) < root - tolerance$. This method is very fast, allowing us to obtain numerical results that match the expected analytical answer by up to 5 or 6 decimal points.

2.4   Comparing Results

The following table of data shows the first 10 results of a well of length '4', with a numerical results 'tolerance' of '0.000001'. The first few energies match the expected analytical results to 5 decimal points. As we go up in n-values, this accuracy diminishes.

n	E (Numeric)	E (Analytic)
1	0.6168514491	0.6168502752
2	2.467423466	2.467401101
3	5.551932058	5.551652477
4	9.871158188	9.869604404
5	15.42704192	15.42125688
6	22.22346924	22.20660991
7	30.2669709	30.22566349
8	39.56742819	39.47841761
9	50.1385235	49.96487229
10	61.99781171	61.68502752

2.5 The Infinite Well Program

The main program for the infinite well accepts the length of the Well, and the number of Eigen-energies to find. It returns the numerical Eigenvalue solutions, compared with the expected Analytical solution, and can be altered to return some of the 'ψ' values, which can then be used to plot graphs. (See Appendix 1 for a full copy of the code).

3 The Finite Square Well

3.1 Introduction

Now, we wish to extend our numerical solution to a slightly more complicated case. That of the finite potential well. Unlike the infinite well, we assign the potential outside of the well as:

$$V(x) = 0, x > L/2, x < -L/2$$

And within these limits:

$$V(x) = -V, L/2 > x > -L/2$$

(note, often the boundary is expressed in the form $-a < x < a$, but in this case I'm using the clementure I used in the infinite Square Well problem). Therefore, in the above boundary, our Schrodinger Equation is:

$$\frac{d^2\psi}{dx^2} = (-E + V)\psi$$

3.1.1 The Wave Functions

Our general solution of the SE (from the lecture notes [5]) gives the following Wave functions:

$$\psi(x) = a_1 e^{(\kappa x)} + b_1 e^{(-\kappa x)} for x < -L/2$$

$$\psi(x) = a_2 e^{(Kx)} + b_2 e^{(-Kx)} for -L/2 < x < L/2$$

$$\psi(x) = a_3 e^{(\kappa x)} + b_3 e^{(-\kappa x)} for x > L/2$$
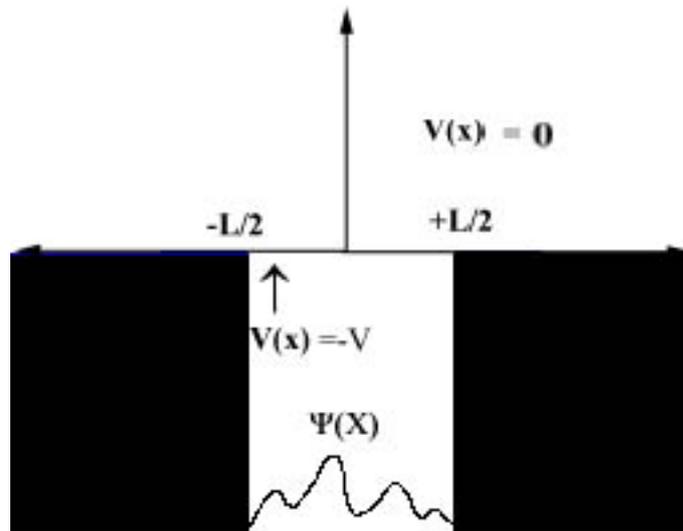
Figure 7: Finite Well Example

Where the constants K, and κ, are given by:

$$K = \sqrt{(-|E| + V)}$$

$$\kappa = \sqrt{(|E|)}$$

(not forgetting that we have set $2m = \hbar = 1$).

As we can see from the Figure 7, the wave function must vanish as $x \to \pm\infty$, therefore $b1 = a3 = 0$. The central wave functions, as in the case of the infinite square well, give us symmetrical cos and sin functions! (See the notes on Parity in lectures, and in the Infinite Square Well section above). Therefore we have even solutions of the form:

$$\psi(x) = a_1 e^{(\kappa x)},$$

$$\psi(x) = a_2 cos(Kx),$$

$$\psi(x) = a_1 e^{(-\kappa x)}$$

(for each boundary), and odd solutions of the form:

$$\psi(x) = -A_1 e^{(\kappa x)},$$

$$\psi(x) = A_2 sin(Kx),$$

$$\psi(x) = A_2 e^{(-\kappa x)}$$

3.2 Changing the Shooting Method

At each boundary, we want the ψ wave function, and it's derivative, $\frac{d\psi}{dx}$, to be continous. Therefore, at the right boundary condition (for the even functions, for example):

$$a_2 cos(K(L/2)) = a_1 e^{(-\kappa(L/2))} \tag{5}$$

and, the derivative:

$$-ka_2 sin(K(L/2)) = -\kappa a_1 e^{(-\kappa(L/2))} \tag{6}$$

Looking at the right hand side of this equation gives us the simple relation:

$$\frac{d\psi(L/2)}{dx} = -\kappa\psi(L/2)$$

and therefore:

$$\frac{d\psi(L/2)}{dx} + \kappa\psi(L/2) = 0$$

This gives us a simple boundary condition we can insert into our current infinite square well code, along with the initial conditions, which still apply:

Even Solns:

$$\psi(0) = 1, \frac{d\psi(0)}{dx} = 0$$

Odd Solns:

$$\psi(0) = 0, \frac{d\psi(0)}{dx} = 1$$

Therefore, as in the infinite square well situation, we integrate from $x = 0$ to $x = L/2$, using the above initial condition, and check the above boundary condition at L/2. As before, we home in on the condition using a form of 'Bisection'.

3.3 Alternative Transcendent Method

We can check these results by performing another numerical calculation based on the following 'transcendental' equations (derived by dividing (6) by (5) (for the even solution), and the same for the appropriate boundary condition equations for the odd solution).:

$$-\kappa = -Ktan(Ka) \tag{7}$$

(From (6)/(5), the even solution)

$$-\kappa = Kcot(Ka) \tag{8}$$

(From the equivalent odd Boundary Conditions) Remember:

$$K = \sqrt{(-|E| + V)}$$

$$\kappa = \sqrt{(|E|)}$$

We now perform a substitution of $x = ka, y = ka$ to make our equations dimensionless, and define:

$$x^2 + y^2 = r^2 = (L/2)^2 V \tag{9}$$

Even Solution:

$$y = xtan(x) \tag{10}$$

Odd Solution:

$$y = -xcot(x) \tag{11}$$

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We solve these three equations numerically by finding where (7) and (8), or (7) and (9) intersect. These points define a finite number of Eigen-energies, En, via our previous definition of κ and K.

In the program, we set $y^2 = r^2 - x^2$, and find, again using the bisection method, where: For the even solution:

$$\sqrt{(y^2)} - \sqrt{(x^2)}tan(\sqrt{(x^2)}) = 0$$

and, for the Odd solution:

$$\sqrt{(y^2)} + \sqrt{(x^2)}cot(\sqrt{(x^2)}) = 0$$

For the y-value which fits either of these conditions, we define the Eigen-energy as:

$$E_n = -y^2/(L/2)^2$$

3.4 Comparing Results

Again, as in the infinite square well, the first eigenfunction solution (for Eigen-value E(1)) is even, and the subsequent solutions oscillate between even and odd. The data obtained from both solutions fits this pattern, and the following table compares the results from the 'shooting method' with the results from the 'transcendent equation' method (note, this is for $V = -10$, Shooting method root tolerance= 0.000001, TE X-increment= 0.001 and $L = 4$).

n	E (TE)	E (SM)
1	-9.541	-9.541064623
2	-8.17675	-8.176890575
3	-5.95375	-5.953834945
4	-2.99875	-2.998487614
5	-0.0135	-0.01340610705

3.5 Finite Square Well Programs

The Finite Square Well program accepts a value of 'Well Length', L, and a potential Depth, V. It calculates the Eigen-energies to a tolerance (attempted accuracy) of 0.000001. (This can be altered manually in the code, by changing the constant 'tol'). It performs the intergration with a step-length proportional to the Well Length, and outputs the Eigen-energy, and value of $\psi(L/2)$. It will then output the corresponding values calculated from the 'Transcendantal Equations'. (See Appendix 2 for a full copy of the code).

4 The Inverse Cosh Potential

4.1 Introduction

The Inverse $cosh^2$ potential is an interesting function, somewhat similar to the Harmonic Well. It has been solved numerically, using Legendre Polynomials, and is covered in "Theoretical Physics Volume 3: Quantum Mechanics" by Landau and Lifshitz. [4] The Potential, V, is described by:

$$V(x) = -V_0/(cosh^2(\alpha x))$$
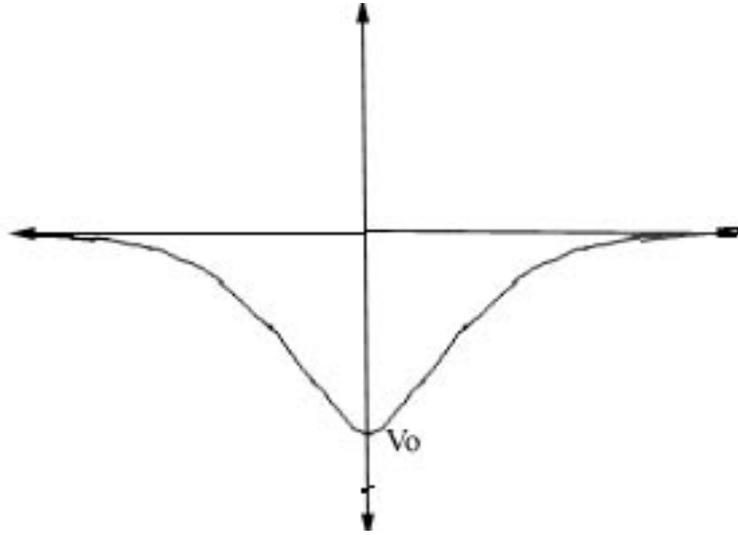
Figure 8: Landau-Lifshitz Potential

This function describes a negatic 'harmonic' well, of depth V_0 , width scaled by α, and:

For:

$$x- > \pm\infty, V(x)- > 0$$

(This can be seen in diagram 4).

We begin to solve this by making the following substitution for 'x':

$$\xi = tanh(\alpha x)$$

This quite simply maps the entire x-axis, from $-\infty$ to $+\infty$ onto ± 1. This enables us to perform the integration as if we were integrating to infinity, with the boundary condition:

$$Psi(x) = 0, x \rightarrow \pm\infty$$

and therefore..

$$Psi(\xi) = 0, \xi \rightarrow \pm 1 \tag{12}$$

4.2   Changing the Program, and solving

Obviously, this is a very powerful mapping tool. To use it in our integration program, we first have to rearrange the Schroginger Equation in terms of this new variable. Remember, we are using $\hbar^2 = 2m = 1$, and schrodinger's equation (in terms of x) is:

$$\frac{d^2\psi}{dx^2} + (E + V_0/(cosh^2(\alpha x)))\psi = 0$$

The derivatives of $\psi(x)$ in terms of the new variable, ξ are:

$$\frac{d\psi}{dx} = \frac{d\psi}{d\xi}\frac{d\xi}{dx}$$

where..

$$\frac{d\xi}{dx} = \alpha sech^2(\alpha x)$$

$$\frac{d\xi}{dx} = \alpha(1 - \xi^2)$$

Therefore..

$$\frac{d\psi}{dx} = \frac{d\psi}{d\xi}\alpha(1 - \xi^2)$$

and...

$$\frac{d^2\psi}{dx^2} = \alpha^2(1 - \xi^2).((1 - \xi^2)\frac{d^2\psi}{d\xi^2} - 2\xi\frac{d\psi}{d\xi}) \qquad (13)$$

Next, we look at the energy terms of our SE, and make the following substitutions:

$$\epsilon = \sqrt{-E/\alpha}$$

and..

$$s(s + 1) = V_0/\alpha^2$$

Now, we can re-arrange the energy terms in our SE to give:

$$\alpha^2(1 - \xi^2)[s(s + 1) - \epsilon^2/(1 - xi^2)] \qquad (14)$$

Which, combined with our equation for $\frac{d^2\psi}{dx^2}$ gives us:

$$\frac{d^2\psi}{d\xi^2} = 2\frac{d\psi}{d\xi}/(1 - \xi^2) - [s(s + 1)/(1 - xi^2) - \epsilon^2/(1 - xi^2)^2]\psi \qquad (15)$$

Now, it is a trivial task to alter the code from our previous potentials. We simply insert the above equation into our function for $\frac{d^2\psi}{d\xi^2}$, and integrate from our central Even and Odd boundary conditions (which still hold), and check that, as described above, $\psi(1) = 0$.

Even though our shooting is now dependant on our substitution ϵ, we still use increments on 'E' in both the calculation and bisection functions. This is because it is slightly easier to increment 'E' from $E = -V_0 \rightarrow E = 0$ than it is to increment ϵ from $\epsilon = sqrts(s + 1) \rightarrow \epsilon = 0$, or somesuch.

4.3   The Legendre Analytical Solution

The analytical solution, described by Landau and Lifshitz in chapter 3 of their book "Quantum Mechanics" is interesting in itself. It suggests an alternative direction, using legendre polynomials, we could take in solving these Eigenvalue equations numerically (This is covered in the final chapter of this report).

As quoted, details on Landau and Lifshitz solution can be found in their book. Briefly, they solve the problem by turning it into a general Legendre function with another substitution of:

$$\psi = (1 - \xi^{\epsilon/2})\omega(\xi)$$

and the temporary substitution:

$$u(1 - u)\frac{d\omega}{d\xi} + (\epsilon + 1)(1 - 2u)\acute{\omega} - (\epsilon - s)(\epsilon + s + 1)\omega = 0$$

We can use finite methods with this equation to compare our expected result for ψ when $\xi = 1$, (i.e., $x = \infty$), and when $\xi = -1$. This shows that, for these conditions:

$$s = \epsilon + n, n = 1, 2, 3...$$

therefore..

$$E_n = -\alpha^2/4[-(1+2n) + \sqrt{1 + 4V_0/\alpha^2}]^2$$

Now, we can use this equation in our program to compare with our numerical results.

4.4 Comparing Results

I have displayed below results for four different well 'depths'. This is to show a slightly unusual error that occurs in the higher energies for some depths. In all four cases, $\alpha = 1$, root finding tolerance is '0.000001', and the Energy increment Tolerance is '0.001'.

	nth result:	Numeric Energy:	Analytic Energy
For $V_0 = -10$	0	-7.298664802	-7.298437881
	1	-2.891326433	-2.895313644
	2	-0.2888599662	-0.4921894064
	nth result:	Numeric Energy:	Analytic Energy
For $V_0 = -15$	0	-11.5950479	-11.59487516
	1	-5.785451677	-5.784625486
	2	-1.943378701	-1.97437581
	nth result:	Numeric Energy:	Analytic Energy
	0	-16.00013563	-16
For $V_0 = -20$	1	-9.000954813	-9
	2	-3.997725357	-4
	3	-0.8346578926	-1

What we have discovered is the limitation on our shooting method, for solving these Eigenvalue problems. What seems to occur is, as the Eigen-energies approach 0, the solutions become more frequent. Therefore, especially in this complex mapping case, the integration routines find it harder to obtain accurate solutions because of the high frequency, and narrow gaps between these Eigen-energies.

4.5 The Inverse Cosh Program

The program for this potential asks the user for the 'depth' of the well, as well as the scale factor, or width, α of the potential. Again, the accuracy of the program is controlled by the variables 'Etol' and 'tol'. It will output (either in table or report format) the results, along with the corresponding analytical solutions, up to $E = 0$, after which our boundary conditions no longer apply. (See Appendix 3 for a full copy of the code).
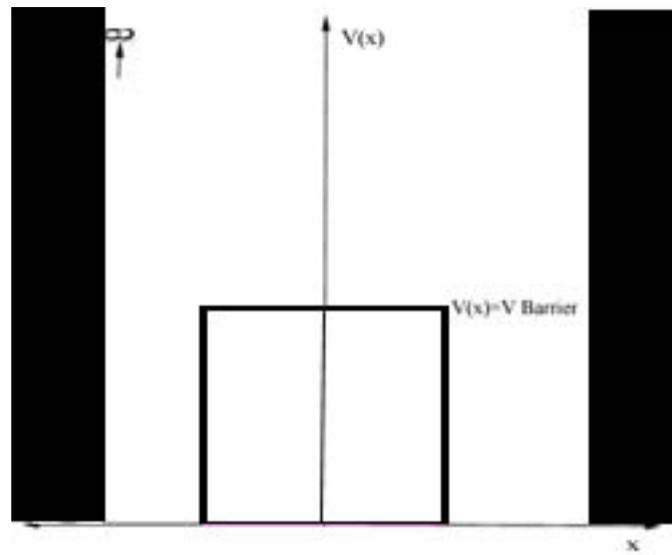
Figure 9: A Potential Barrier

5 The Potential Barrier

5.1 Introduction

The final potential configuration we will investigate, is that of the 'Symmetric Potential Well Barrier within two Infinite Potential Walls' (Sometime referred to as a two-level system). While the changes required to our program are almost trivial, the potential provides us with a way to investigate some of the most important, and fascinating, aspects of Quantum Mechanics.

The potential of the system (as shown in the diagram), can be expressed as:

$$x < -(L/2), V(x) \to \infty$$

$$-(L/2) < x < -(a/2), V(x) \to 0$$
$$-(a/2) < x < (a/2), V(x) \to V_{bar}$$
$$(a/2) < x < (L/2), V(x) \to 0$$
$$x > (L/2), V(x) \to \infty$$

5.2 Analytical Solution

We can begin to caclulate an analytical solution, based on our work on the solutions for the Infinite Potential Well and our class work on Scattering Resonances. Unfortunately, this does not lead us to a general analytical solution for

any barrier potential height or width. It can, though, provide us with a solution for some 'limiting cases', which we can use to test the accuracy of our program.

Because we have defined our barrier potential to be symmetric around the origin, we can state that our Eigen-functions must have odd or even parity. (Just like all the other potentials we have investigated, thus enabling us to still use our cos and sin initial conditions when we approach it numerically).

We also know that between the barrier, and the Infinitely high walls, we must have a some superposition of plane waves that vanishes at those walls. Therefore, we define:

$$\psi_\pm(x) = \psi_L(x) + \phi_\pm(x) \pm \psi_R(x),$$

$$\psi_L(x) := A sink(x + L/2) = -L/2 < x < -a/2$$

$$\psi_R(x) := A sink(L/2 - x) = a/2 < x < L/2$$

Where ψ_L is confined within the left part of the well ($x < -a/2$), ψ_R is confined within the right side of the well, and ϕ is some exponential function within our potential barrier, connecting both sides. (Note, the + and - notation represents the even and odd solutions respectively, and $k = \sqrt{(2m/\hbar^2)E}$ as usual).

Because both sides are binded by the part of the wave function which tunnels through this barrier, we can call on the transfer matrix formulisation used in the calculations for a wave packet tunneling through a similar barrier. This will enable us to calculate the allowed Eigen-energies, E.

The above two equations, for the ψ function on either side of the barrier, are connected via a transfer matrix, which gives us the following two linear equations (using complex exponentials instead of sin functions):

$$\pm e^{ikL/2} = -M_{11}e^{-ikL/2} + M_{12}eikL/2$$

$$\mp e^{-ikL/2} = -M_1^* 2 e^{-ikL/2} + M_{22}e^{ikL/2}$$

These therefore give us the condition for k, and subsequently the Eigenenergies E, by:

$$\pm 1 = -M_{11}(k)e^{ikL} + M_{12}(k) \tag{16}$$

Therefore, by defining the two transer matrix elements for several limiting cases, we can determine the appropriate eigenenergies for those potentials. The simplest is of course, for $V(x) = 0$, where we find:

$$M_{11} = 1,$$

$$M_{12} = 0$$

Therefore:

$$\pm 1 = -e^{ikl} \rightarrow k = n\pi/L$$

$$n = 1, 2, 3....etc$$

Which is what we expect for an infinite potential well.

Now, we can define our transfer matrix M for a tunnel barrier using the solution we found for a scattering barrier in class. We can then attempt to solve

our k-dependant equation for these matrix elements for some further limiting cases.

$$M_{11} = e^{ika}[cosh(\kappa a) + i\epsilon_-/2sinh(\kappa a)]$$

$$M_{12} = i\epsilon_+/2sinh(\kappa a)$$

$$\epsilon_\pm := \kappa/k \pm k/\kappa, k := \sqrt{(2m/\hbar^2)E}, \kappa\sqrt{(2m/\hbar^2)(V-E)}$$

Now, we can perform some algebra using this, and the equation we derived for calculating 'k', and seperating the real and imaginary parts (both of which can be shown to give the same result), we obtain: For the Even solutions:

$$1 = \kappa/k tan(K(a-L)/2)tanh(\kappa a/2) \tag{17}$$

..and for the odd solutions:

$$1 = \kappa/k tan(K(a-L)/2)coth(\kappa a/2) \tag{18}$$

We can now test this using $V(x) = \infty$, and then see if we can obtain an analytical result for the case of V(x) being finite, but still very large.

As $V(x) \to \infty, \kappa \to \infty$, and:

$$k/\kappa = 0 = tan(k(a-L)/2), \to k(L-a)/2 = n\pi$$

$$n = 1, 2, 3...etc$$

These are the same energies we'd expect for the two completely seperate infinite potential wells (both of width (L-a)/2).

Now, we can let $V < \infty, V >> 0$. As we mentioned earlier, with a finite barrier the two sides of the well will become 'coupled', hence our use of the 'transfer matrix' method. We begin by introducing two dimensionless variables (something unneccessary in the numerical solution):

$$x = ka/2, \alpha := \sqrt{ma^2V/2\hbar^2}$$

Substituting these into equations [17] and [18] gives us:

$$-1 = \sqrt{\alpha^2 - x^2}/x tan x [tanh(\sqrt{\alpha^2 - x^2}]^{\pm 1}$$

By performing a taylor expansion of this for $\alpha >> 1$ around the lowest eigen-energy solution for $V \to \infty$, (i.e. $x_1 = pi, \to x = x_1 + y, y << 1$), we obtain:

$$x \approx \pi(1 - 1/\alpha[tanh(\alpha)]^{\pm 1})$$

Which, using our earlier definition of 'x', gives us the two wave vectors for the lowest eigen-energy solution!:

$$k_+ \approx 2\pi/a[1 - 1/(\alpha tanh(alpha))] \tag{19}$$

$$k_- \approx 2\pi/a[1 - tanh(\alpha)/\alpha] \tag{20}$$

We have obtained two slightly different 'k', and thus Energy, ($E = \hbar^2 k^2 / 2m$), solutions for what should be the lowest single 'k' solution (at least for an equivalent infinite potential well). This is known as 'level splitting', and is an important consequence of coupling two regions in space via the 'tunnel effect'. We will discuss this further in the results section, as it is interesting to observe how these energies split under different conditions.

Now that was have these 'limiting case' solutions, we can use them as a 'bench mark' to see what our program produces under similar conditions. Later, we will also plot some of our solutions graphically, and see how it compares with what we expect for these 'coupled' wave functions.

5.3 Program Modifications

As mentioned in the introduction, the modifications to our infinite potential well program are trivial. Our two-boundary conditions still hold, for both even and odd solutions: Even conditions:

$$\psi(0) = 1, \frac{d\psi(0)}{dx} = 0$$

Odd conditions:

$$\psi(0) = 0, \frac{d\psi(0)}{dx} = 1$$

Even though our wave function for the origin is 'within' the barrier, these conditions still hold because our potential is symmetric. (In effect, within the barrier the even functions are Cosh functions, and the odd functions are Sinh functions). As before, we then integrate to our +L/2 boundary to match an 'E' value to:

$$\psi(L/2) = 0$$

We now only have to change the Differential equation that we feed into Runga Kutta. We simply set the condition (again, $\hbar^2 = 2m = 1$!):

For $L/2 > |x| > a/2$:

$$\frac{d^2\psi}{dx^2} = -E\psi \tag{21}$$

and, for $a/2 > |x| > 0$:

$$\frac{d^2\psi}{dx^2} = (V - E)\psi \tag{22}$$

We don't have to worry about matching 'continuity' while passing from the barrier, to the zero potential area, as it is done automatically via our integration.

5.4 Comparing Results

I have arranged my program so that it will display the most relevant analytical solution to compare with each numerical result. For example, if the length of the well is twice the length of the barrier (L=2a), it will calculate and display the above analytical solution for large V(x) for the first two lowest states, (n_1, n_2.

If $L! = 2a$, or $n > 2$ it will display the approriate 'closest' infinite square well Energy (because each 'infinite well energy' has been split in two!), for the well width $(L - a)/2$.

Finally, if $E > V_{barrier}$, it will display the infinite square well result (without the splitting) for a well of width L.

5.4.1 Diagrams

The graph of energies should hopefully illustrate this more clearly

- The Diagram to the right illustrates the first 6 energies which exist 'beneath' a barrier of height 100.
- The lines on the left show the actual numerical solutions, and are grouped into very close 'pairs'.
- These values are 'split' from the equivalent infinite square well, shown on the right.
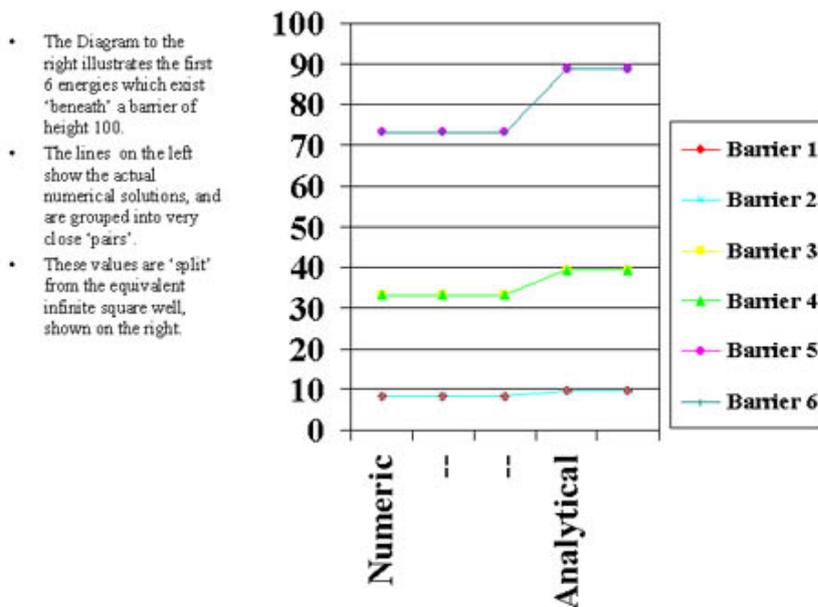
Figure 10: Eigen-energy Solutions

The two wave-function pictures illustrate the two lowest Eigen-functions for a barrier of potential 10, Well length 4, and Barrier Width 2. (They were taken from the graphical program, with a 'y-magnification factor' of 20).
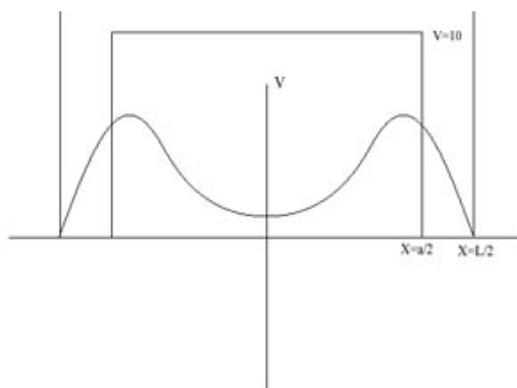
Figure 11: The first Cos solution
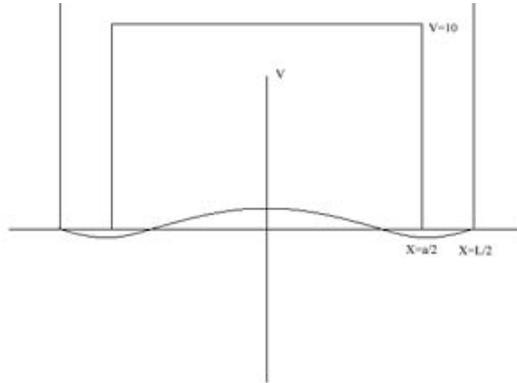
Figure 12: The first Sin solution

5.4.2   Data

The following are the results for the first two eigenenergies for three different 'Depths' of well. The other parameters of the calculation are the same as used for the above graphs. ($L = 4, a = 2, Tolerance = 0.0001$).

Potential Barrier height of '10':

nth result:	Numeric Energy:	Analytic Energy
1	5.453921598	4.599169126
2	5.53971392	4.629759292

Potential Barrier height of '50':

nth result:	Numeric Energy:	Analytic Energy
1	7.726374401	7.275447353
2	7.726387615	7.275454269

Potential Barrier height of '150'

nth result:	Numeric Energy:	Analytic Energy
1	8.646448765	8.323702116
2	8.646448765	8.323702116

In all three cases, the analytical energies have been given by our even and odd analytical equations [17] and [18]. The interesting thing to note, is how as the potential 'height' increases, the 'matching' between the numerical and analytical values increase. This is because we derived the equations [17] and [18] for the case of $V < \infty, V >> 0$.

Another aspect our results we can observe quite easily, is the differences between the 'split' energies, and the 'source' infinite potential well energies. For example, the following data shows the first 10 eigen-energies for a barrier of height '100', and the other parameters as before:

nth result:	Numeric Energy:	Analytic Energy
1	8.353770507	7.99437956
2	8.353770532	7.994379574
3	33.16472528	39.47841761
4	33.16472411	39.47841761
5	73.15418593	88.82643963
6	73.15488671	88.82643963
7	102.1779417	30.22566349
8	108.13675	39.47841761
9	116.09675	49.96487229
10	123.92375	61.68502752

As you may notice, the first two analytical solutions are again given using our limiting case equations. The solutions for $n = 3 \rightarrow n = 6$ are compared with the corresponding energy for an Infinite Potential well of width: $L_well = (L - a)/2$. As you can see, the 'split' energies, are all slightly lower than equivalent Infinite well energies.

As the Eigen-energies become greater than the height of the barrier, it becomes difficult to match them to an equivalent analyitical solution. ($n > 6$ in this case). Fortunately, we can say that if we were allow our program to continue to calculate higher and higher Eigen-energies ($E >> V_{barrier}$), the solutions will tend towards those of a normal infinite potential well of width 'L'. (These are the values we have included in the analytical column for $n > 6$).

5.5   The Barrier Programs

As mentioned before, the code for this potential is very similar to the infinite potential well. (So much so that it is used to produce both types of graphs in the graphical program, discussed in the next chapter).

The program prompts the user for the width between the Infinite Potential walls, the width of the potential barrier, and the potential 'height' of that barrier. It also asks how many Eigen-energies to find. This is so we can observe the nature of the Eigen-energies for $E >$ The Height of the Barrier. (See Appendix 4 for a full copy of the code).

Unfortunately, due to the nature of our shooting method, the program will most likely crash for large well 'widths'. It is a matter of trial and error, to 'increase the accuracy' of the Energy-increment tolerance (i.e., decrease the value of Etol), to reduce the large 'jumps' in $\psi(L/2)$ (which would take the Bisection function a large amount of time to bisect), while trying to reduce the time it takes to 'count' up in these increasingly small increments.

If more time were available, it would be feasible to create normalised dynamic 'tolerances', which modify themselves according to the dimensions of the well. Unfortunately, this would take a large amount of time for testing and finding the neccessary boundaries and parameters for the different tolerances to operate under.

6 The Graphical Program

6.1 Overview

I have produced a short graphical program which calculate the ψ functions for both the infinite potential well, and for the potential barrier. For variety, and speed, the code has been altered to use a simple 'approximation method' (as discussed in the first chapter), which only finds the solutions for a relatively low eigen-energy accuracy. Fortunately, this makes very little difference to the appearence of the function.

Unfortunately, it is not possible to change the parameters during runtime. It is preset to calculate 10 solutions for an infinite well of length '4', and performs the intergration over 400 steps (and hence a steplength of 0.01) to obtain a smooth curve plot. To introduce a potential barrier, simply alter the initial values of the variables 'Hbri', for the potential height of the barrier, and 'Lbri', for the width of the barrier.

The main graphical function draws the x and y (ψ) axes, two lines to represent the infinitely high walls, and (if one exists) a 'reduced' approximation of the barrier. It then draws the positive part of the ψ functions, and a symmetrical image (Odd or Even, depending on the solution 'type') for the negative part.

The final important new variable is 'yfac'. This alter's the magnification, or reduction, scale of the y-part of the ψ function. For an infinite well, it is satisfactory to leave it at it's default value of '100'. For the barrier potential, it may be neccessary to reduce it by a factor of 10, depending of the dimensions of the problem.

(This program was used to produce all of the Eigen-vector plots in this report).

6.2 Compiling the Graphical Program

The graphical program uses Borland's C++ OWL library. This enables us to create, and modify 'Windows' objects, and perform rudimentary graphical representations. Unfortunately, it is incredibly awkward and fiddly.

To compile the Graphical code provided with this report in Borland C++ V4.5+, it is neccessary to create a new project of type 'Win32 Application', and the OWL selection must be included in the 'Standard Libraries' selection box. Then goto 'Options'-'Project', and add the 'bin' directory to the 'Intermediate' and 'Final' boxes under 'Directories'-'Output Directories'. (See Appendix 5 for a full copy of the code).

7 Conclusion

We have developed the basics of solving the sublime Schrödinger's Equation, and applying it to some interesting, and practically useful potentials. In particular, the finite barrier potential has provided us with a tool to investigate the use of such structures in semi-conductors, and even gives us a glimpse of yet another future in the form of Quantum Computing. The idea of quantum 'binding' between the two wells by the electron 'tunneling' through an intervening potential, and the energy level-splitting that ensues, forms the foundation of the concept of 'qubits', or quantum bits.

We have also been able to investigate the limitations of our shooting method, via the propagation of errors in the potentials with corresponding analytical solutions, and the loss of accuracy with the Landau-Lifshitz potential. While we can be fairly certain this won't occur with our finite barrier potential, it could still be a problem if we wanted to apply this shooting method to an application which involves similar 'high-frequency' errors as Landau's Cosh potential.

7.1 Alternative Methods

This causes us to give a brief consideration to possible alternatives, especially if we wanted to simply increase the speed, and accuracy, of solving this kind of problem. There are many possible routes to take, all of which require a large amount of description. I will simply give a brief overview, and if applicable, a reference to a corresponding text.

7.1.1 Matrix-based Integration

All of the methods I will describe involve the manipulation of the problem via some kind of matrix-based method. After all, we are considering Schrödinger's in essence as an Eiganvalue problem.

In most mathematical integration problems, the traditional method of intergration is converted into a matrix problem. In some sense, it reduces the whole integration calculation into the 'diagonlisation' of the said matrix.

For example, the equation we use in Runga-Kutta (and most finite-step intergration routines) can be expressed as:

$$f''(x) = \frac{f(n+1) - 2f(n) + f(n-1)}{2\Delta^2} = g(x)$$

So we can convert this 'equation', or what effectively is a group of simultaneous equations in 'n', into a matrix, much like we would any other group of simultaneous equations. We could then solve it using any freely available matrix diagonlisation routines from a text book, or the internet.

This is covered in great detail in "Numerical Recipes: The art of Scientific Computing" by William. H. Press, et al. [1] and "Computational Physics", by J.M.Thijssen, Cambridge University Press. [2]

7.1.2 Finite Difference Methods

Another very common way of manipulating Boundary-value problems, and solving our differential equations is via what is known as "Finite Differences". It involves discretising the equation onto a 'straight line', or in the case of a 2D problem, a square lattice. The equation is manipulated in this new 'form', using the 'Relaxation Method', so that it in essence becomes another type of initial value problem. This is because, by 'discretising' the problem, any solution ψ_{ij} must be equal to the average of it's four neighbours, plus some function of x. This enables us to start with trial functions of ψ^0 and develop a sequence of possible solutions.

Again, this method is widely used for all forms of boundary value problems, and can be modified for increased efficiency using several different iterative

methods. It also leads on to the even more interesting method of solving such PDE's via Fast Fourier Transforms, which we won't discuss here.

(See Appendix A.7 of "Computational Physics", by J.M.Thijssen, Cambridge University Press). [2]

7.1.3 Sturm-Liouville Problems

Our Schrödinger's Equation can also be expressed as a 'Self-Adjoint Sturm Liouville' problem, similar to the steps we took to solve the Landau-Lifshitz potential analytically. Briefly, it involves re-arranging our equation to the form:

$$-(p\acute{y})' + qy = \lambda\omega y$$

.. and then to calculate the Eigenvalues, and Eigenfunctions of the said equation for some regular or singular boundary conditions. There are many texts on this subject, as it is a very general problem throughout numerical physics. One such recomended text is: Q. Kong, and A. Zettl, "Eigenvalues of regular Sturm-Liouville problems", J.Differential Equations, V. 131, no. 1, (1996), 1-19. [3]

7.1.4 Variational Calculas

The Variational Calculas is called into use when the problem involves solving Schrödinger's Equation in realistic electronic structure calculations, and a huge number of grid points are called in to play. Also, like most finite methods, it mainly used to calculate the grounds states of such complex systems

This method involves restricting the possible solutions to a subset of Hilbert Space, and in this subspace the best solutions are found. In general, the subspace of 'Linear Variational Calculas' is used, and Schrödinger's Equation is once again formulated as an eigen-value problem using this Orthonormal basis. Once again, the matrix methods described above are used to find the Eigenvalues of this new equation.

(See Chapter 3 of "Computational Physics", by J.M.Thijssen, Cambridge University Press). [2]

References

[1] "Numerical Recipes: The art of Scientific Computing" by William. H. Press, et al. Cambridge University Press.

[2] "Computational Physics", by J.M.Thijssen, Cambridge University Press.

[3] Q. Kong, and A. Zettl, "Eigenvalues of regular Sturm-Liouville problems", J.Differential Equations, V. 131, no. 1, (1996), 1-19.

[4] "Course in Theoretical Physics Volume 3: Quantum Mechanics" by L.D. Landau, E.M. Lifshitz. Butterworth-Heinemann.

[5] "Quantum Mechanics 1 Lecture Notes" By Dr T. Brandes, http://bursill.phy.umist.ac.uk/QM/qm1.html