Part I
Numerov

The following Note is on the Mathematics of our Quantum mechanics lab.

1 Schrödinger Equation (1D)

The time-independent Schrödinger equation is given by

$$E\psi = \frac{p^2}{2m}\psi + V(x)\psi \qquad \left(p = -i\hbar\frac{d}{dx}\right)$$

$$(E - V(x))\psi = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}, \qquad \text{set } \hbar = 1,\ m = 1.$$

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

So, we obtain a differential equation of the form

$$y'' = K(x)\, y$$

Hence we shall use Numerov method to solve this.

2 Numerov formula:

$$y_{n+1} = \frac{2\left(1 + \frac{5h^2}{12}K_n\right)y_n - \left(1 - \frac{h^2}{12}K_{n-1}\right)y_{n-1}}{1 - \frac{h^2}{12}K_{n+1}}$$

$$\text{here } K(x) = 2\big(V(x) - E\big).$$

To use the Numerov formula , we first need to first make a grid of say N points. Let's say we want to make a grid of x from point a to b with N number of points for our numeric solving of TISE, then

$$x_i = ih + a$$

where, $h = \frac{b-a}{N}$

$$x_i = ih + b$$

Now, in our Syllabus, we have only two kinds of equations that we need to solve using the Numerov technique

2.1 Schrödinger equation (Time independent)

as defined above:
The various potentials and their respective range are given as follows:

1. $V(x) = \frac{1}{2}Kx^2$; harmonic oscillator; $x \in [-5, 5]$
2. $V(x) = \frac{1}{2}kx^2 + \frac{1}{4}\beta x^2$; anharmonic oscillator; $x \in [-5, s]$
3. $V(x) = \frac{-1}{x}$; Conlomb potential; $x \in [0.1, 10]$
4. $V(x) = -\frac{e^{-\lambda x}}{x}$; Scanning $CP; x \in [0.1, 10]$
5. $V(x) = \frac{1}{2}kx^2 + \frac{1}{4}\beta x^4$; harmonic with a quintic term ' $x \in [-10, 10]$

2.2 Radial Equation

$$\frac{d^2u(r)}{dr^2} + \left[2\big(E - V(r)\big) - \frac{\ell(\ell+1)}{r^2}\right] u(r) = 0$$
$$\Rightarrow \frac{d^2u(r)}{dr^2} = \left[2\big(V(r) - E\big) + \frac{\ell(\ell+1)}{r^2}\right] u(r)$$

The wave function R(r)=rU(r) and the Normalisation integral is

$$\int R^2(r)dr = A^2$$

Now , r=x (as per our previous notation) Here also , the V(r) can have two different kind of functional forms:

1. $V(r) = \frac{-1}{r}$; Conlomb potential; $x \in [0.1, 10]$
2. $V(r) = -\frac{e^{-\lambda r}}{r}$; Scanning $CP; x \in [0.1, 10]$

In our exams we could be asked to perform the following using operations:

2.3 Normalize the wave function.

To do this, we will just use Riemann integration.

$$A^2 = \int \psi^*(x)\psi(x)dx = \int \psi^2(x)dx = \sum_{i=1}^{N} \psi^2(x_i)\, h.$$

So, Normalized Ware function is

$$\psi'(x_i) = \frac{\psi(x_i)}{A}$$

To plot the probability function , just plot the square of the function in all of the above cases.

2.4 Bisection

Numerov is a very sensitive numerical integration technique,If the value of E that is being used in there is not exactly equal to the Eigen-value of the equation , we shall observe diveregence.
So , the condition that Numerov has converged is

$$\psi(x = b) = 0$$

Now, More often than not , this condition is not plausible in computation endeavours. so we set the condition for convergence as

$$\psi(x = b) \leq 10^{-n}$$

where n is the order of tolerance. Now, to use the bisection method, we shall consider a range for E (say $\in [E_{min}, E_{max}]$), Hence, The end point at the tail of our wavefunction can be considered a function of our energy, hence we have

$$y(E) = \psi(x = b)|_E$$

and we have to find the point, $E = E_{eigen}$ such that,

$$y(E_{eigen}) \approx 0$$

or ,

$$y(E_{eigen}) \leq 10^{-n}$$

Rest work is standard bisection algorithm.

Part II
Tri-diagonalization

The second numerical technique that we use in our Quantum Mechanics lab is based on discretizing the Schrödinger equation directly and rewriting it in a matrix form. This method converts the differential equation into an eigenvalue problem, where the allowed energy levels appear naturally as eigenvalues of a Hamiltonian matrix.

3 Discretization of the Time-Independent Schrödinger Equation

We again start with the one-dimensional time-independent Schrödinger equation

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

As before, we set

$$\hbar = 1, \qquad m = 1$$

so that the equation becomes

$$-\frac{1}{2}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$

To solve this equation numerically, we discretize the spatial coordinate x. Let the interval $[a, b]$ be divided into N equally spaced points such that

$$x_i = a + ih, \qquad i = 1, 2, \ldots, N$$

where

$$h = \frac{b-a}{N}$$

At each grid point x_i, the wavefunction is written as

$$\psi(x_i) = \psi_i$$

4 Finite Difference Approximation

The second derivative of the wavefunction is approximated using the central finite difference formula:

$$\frac{d^2\psi}{dx^2}\Big|_{x=x_i} \approx \frac{\psi_{i+1} - 2\psi_i + \psi_{i-1}}{h^2}$$

Substituting this into the Schrödinger equation gives

$$-\frac{1}{2}\frac{\psi_{i+1}-2\psi_i+\psi_{i-1}}{h^2}+V_i\psi_i=E\psi_i$$

where $V_i = V(x_i)$.

Rearranging the above expression, we obtain

$$-\frac{1}{2h^2}\psi_{i+1}+\left(\frac{1}{h^2}+V_i\right)\psi_i-\frac{1}{2h^2}\psi_{i-1}=E\psi_i$$

This equation holds for every interior grid point $i = 1, 2, \ldots, N$.

5 Construction of the Hamiltonian Matrix

We now define a column vector consisting of the wavefunction values at each grid point:

$$\boldsymbol{\psi}=\begin{pmatrix}\psi_1\\ \psi_2\\ \vdots\\ \psi_N\end{pmatrix}$$

Using the finite difference equation at each grid point, the system of linear equations can be written in matrix form as

$$\mathbf{H}\boldsymbol{\psi}=E\boldsymbol{\psi}$$

Here, $\mathbf{H}$ is the Hamiltonian matrix of order N, given by

$$\mathbf{H}=\begin{pmatrix}\alpha_1 & \beta & 0 & \cdots & 0\\ \beta & \alpha_2 & \beta & \cdots & 0\\ 0 & \beta & \alpha_3 & \cdots & 0\\ \vdots & \vdots & \vdots & \ddots & \beta\\ 0 & 0 & 0 & \beta & \alpha_N\end{pmatrix}$$

where

$$\alpha_i=\frac{1}{h^2}+V(x_i),\qquad \beta=-\frac{1}{2h^2}$$

Thus, the Hamiltonian matrix is a symmetric tridiagonal matrix.

6 Eigenvalue Interpretation

The matrix equation

$$\mathbf{H}\boldsymbol{\psi}=E\boldsymbol{\psi}$$

is an eigenvalue equation.

Hence,

- The allowed energy levels E_n are the eigenvalues of the Hamiltonian matrix $\mathbf{H}$.
- The corresponding eigenvectors give the discrete values of the wavefunction $\psi_n(x_i)$.

Therefore, solving the time-independent Schrödinger equation numerically is equivalent to diagonalizing the Hamiltonian matrix.

7 Usage

The TQL2 algorithm that is being used , only returns eigen values and eigen states. And also the wavefunctions are normalised.

Part III
Two -state problem (Time evolution)

8 Two-State Quantum System

A two-state system is the simplest non-trivial quantum mechanical system, in which the Hilbert space is two-dimensional.

8.1 State Vector Representation

Let $\{|1\rangle, |2\rangle\}$ be an orthonormal basis of the two-dimensional Hilbert space. An arbitrary state of the system can be written as a linear superposition of these basis states:

$$|\psi(t)\rangle = c_1(t)|1\rangle + c_2(t)|2\rangle$$

where $c_1(t)$ and $c_2(t)$ are complex probability amplitudes.
The normalization condition of the state vector is given by

$$|c_1(t)|^2 + |c_2(t)|^2 = 1$$

8.2 Hamiltonian of a Two-State System

In the basis $\{|1\rangle, |2\rangle\}$, the Hamiltonian operator is represented by a 2×2 Hermitian matrix:

$$\mathbf{H} = \begin{pmatrix} E_1 & V \\ V^* & E_2 \end{pmatrix}$$

Here E_1 and E_2 represent the energies of the basis states, while V denotes the coupling between the two states. Hermiticity of the Hamiltonian ensures that the energy eigenvalues are real.

8.3 Time Evolution

The time evolution of the system is governed by the time-dependent Schrödinger equation:

$$i\hbar\frac{d}{dt}|\psi(t)\rangle = \mathbf{H}|\psi(t)\rangle$$

Substituting the state expansion, we obtain the coupled differential equations:

$$\frac{dc_1}{dt} = \frac{E_1c_1 + Vc_2}{i\hbar} = f_2(t)$$

$$\frac{dc_2}{dt} = \frac{Vc_1 + E_2c_2}{i\hbar} = f_2(t)$$

These equations show that the occupation probabilities of the two states change with time due to the coupling between them. Now , the aboce equations are to be solved using Euler method: Where the boundary conditions are

$$c_1(t = 0) = 0$$

$$c_2(t = 0) = 1$$

The formula for euler method is :

$$y_i = y_{i-1} + f(t_i)dt$$

8.4 Measurement and Probabilities

If a measurement is performed in the $\{|1\rangle, |2\rangle\}$ basis, the probability of finding the system in a particular state is given by the square of the corresponding probability amplitude:

$$P_1(t) = |c_1(t)|^2, \qquad P_2(t) = |c_2(t)|^2$$

In the most general case that we solve for , the plot of these probabilities are sinusoidal curves with an exact phase difference of $\frac{\pi}{2}$

Part IV
Stern-Gerlach Experiment

9 Two-Dimensional Stern–Gerlach Experiment

we consider a two-dimensional Stern–Gerlach setup in which the translational motion of the particle and the magnetic field gradient act along different spatial directions.

9.1 Physical Configuration

Consider a beam of neutral particles entering the Stern–Gerlach apparatus with an initial velocity along the y-direction:

$$\vec{v} = v_y \, \hat{y}$$

The particles pass through an inhomogeneous magnetic field whose dominant component is along the x-direction:

$$\vec{B} = B_z(x) \, \hat{x}$$

with a nonzero spatial gradient

$$\frac{dB_z}{dx} \neq 0.$$

The magnetic field is assumed to vary only along the x-direction and to be uniform along the y-direction.

9.2 Magnetic Moment and Interaction Hamiltonian

Each particle possesses a magnetic moment $\vec{\mu}$ associated with its intrinsic spin. The interaction between the magnetic moment and the magnetic field is described by the Hamiltonian

$$\hat{H}_{\text{int}} = -\vec{\mu} \cdot \vec{B}.$$

For a spin-$\frac{1}{2}$ particle, the magnetic moment is proportional to the spin operator:

$$\vec{\mu} = \gamma \vec{S},$$

where γ is the gyromagnetic ratio.

Since the magnetic field is directed along the x-axis, the interaction Hamiltonian reduces to

$$\hat{H}_{\text{int}} = -\gamma \hat{S}_x B_z(x).$$

Thus, the magnetic field couples specifically to the x-component of the spin.

9.3 Force on the Particle

A magnetic moment placed in an inhomogeneous magnetic field experiences a force given by

$$\vec{F} = \nabla(\vec{\mu} \cdot \vec{B}).$$

In the present configuration, the force has only an x-component:

$$F_z = \mu_z \frac{dB_z}{dx}.$$

For a spin-$\frac{1}{2}$ particle, the eigenvalues of the spin operator $\hat{S}_x$ are

$$S_z = \pm \frac{\hbar}{2}.$$

Therefore, the force acting on the particle can take two discrete values:

$$F_z = \pm\frac{\gamma\hbar}{2}\frac{dB_z}{dx}.$$

taking all the constants as 1 we get:

$$F_z = \pm\frac{1}{2}\frac{dB_z}{dx}.$$

This shows that the force depends on the spin projection along the x-axis.

9.4 Two-Dimensional Motion of the Particle

Now , assume a function for B_z and take it's derivative using central difference formula. Then, find the displacement of the particle along it's z axis using our highschool formula:

$$\frac{dv_z(t)}{dt} = \frac{F_z(t)}{m}$$

$$\frac{dz(t)}{dt} = v_z(t)$$

Solve the above using Euler method. Repeat this many time and obtain a histogram of z.