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1) INTRODUCTION

In the early twentieth century, experimental evidence showed that atomic particles also exhibited wave-like properties in nature in addition to other known properties. For example, electrons have been found to give diffraction when passed through double slits, similar to those in light waves. Upon this discovery, it would make sense to create a mathematical wave equation that would demonstrate this newly discovered property of atoms.

Schrödinger was the first person to develop this type of equation. After this success of Schrödinger, voices of controversy arose around science about what this equation meant. The wave equation developed by Schrödinger can be written in the form of a matrix, and the eigenvalues of this matrix were equal to the energy levels of the quantum mechanical system, the simplest way to test the validity of this wave equation was to solve the energy levels of the Hydrogen atom. The results of the energy levels derived by the equation agreed with Rydberg's Law.
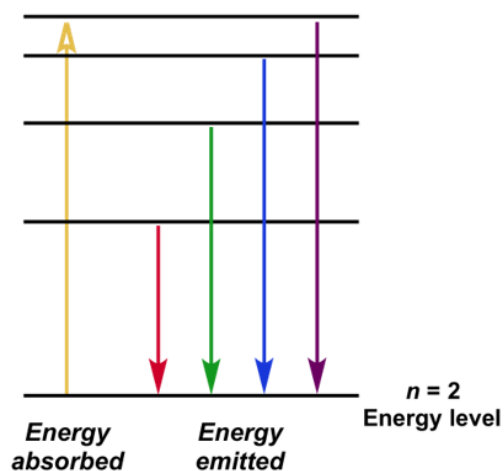

Figure.1: Hydrogen atom energy levels derived using Rydberg's Law
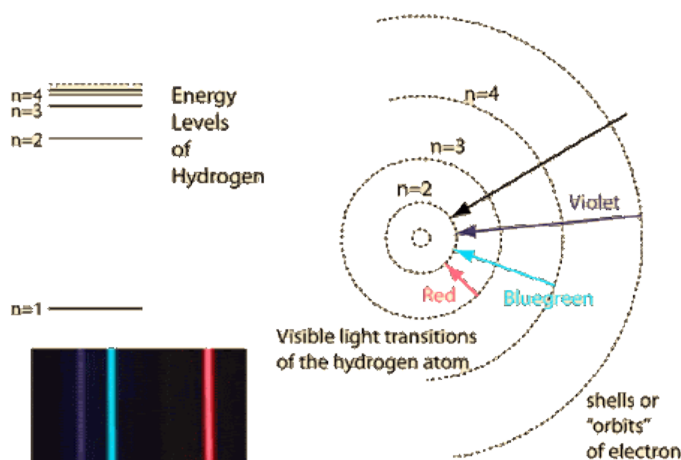

Figure.2: Wave nature of electrons of Hydrogen atom derived from Schrödinger's equation

It was difficult to understand what Schrödinger's wave function was in the beginning of the theory was released. After much discussion, the wave function is now considered to be a sort of probability distribution. The Schrödinger equation is used to find the energy levels of quantum mechanical systems such as atoms and transistors. The reason for this equation to be considered as a kind of probability distribution is that the wave function finds the probability of finding the particle at a certain position.

The solution to Schrödinger's equation is the wave describing the quantum aspects of the system. However, physically interpreting the wave is one of the fundamental philosophical problems of quantum mechanics and has led to many divergences among scientists.

For a given system, the wave function is replaced by individual series, each other's natural harmonics, an infinite series. Schrödinger discovered that replaced waves describe the individual states of the quantum system and that the amplitutes of these waves are of relative importance of that state to the entire system. The Schrodinger equation is the name of the fundamental non-relativistic wave equation used to explain the behaviour of a particle in a field of force in one version of quantum mechanics. There is the time-dependent(dynamic character) equation, applied to the motion of free particles, used to explain progressive waves. And the time-independent(static character) method used for representing standing waves in this equation. For a variety of simple systems, Schrodinger's time-independent equation can be solved analytically. In relation to the coordinates, the time-dependent equation is of the first order of time, not of the second order, so it is not consistent with relativity.Three quantum numbers, corresponding to three co-ordinates, give the solutions for bound systems, and an approximate relativistic correction is possible by adding the fourth spin quantum number.

2) METHODS-DISCUSSION

In quantum mechanics, there is no known definite position or velocity of the particle. All information about the system is instead stored in an entity that is called the wavefunction:

Ψ(x,t): wavefunction, wave function is a complex function of position(x) and time(t).

When the system is not measured, the system's behavior obeys the Schrödinger equation.

$$i\hbar\frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V(x)\Psi(x): Schr\ddot{o}dinger's\ equation$$

$\hbar$: Planck constant $(10^{-34}$ J.s$)$

m: The mass of the particle being described

$\frac{\partial^2}{\partial x^2}$: The 'operator' describes how the wavefunction(Ψ) changes from one place to another

V(x): This quantity describes the forces acting on the particle.

i: "Imaginary number", it is equal to the square root of minus one $\left(\sqrt{-1}\right)$.

$\frac{\partial \Psi}{\partial t}$: This quantity describes how Ψ changes its shape with time.

When one starts to measuring the system, the system stops obeying the Schrödinger's equation. Instead, the wavefunction collapses to one of the eigenstates of the operator corresponding to the measurement returning one of the eigenvalues which in turn is the result of the measurement wavefunction collapse is a probabilistic event, which is the particle behavior might be in an entity found. The probability of collapsing to a certain eigenstate is equal to norm square of the linear product(projection) of the wavefunction before the "collapse" to the relevant eigenstate. This interpretation is called Copenhagen Interpretation.

2.a) Numerical Solution

The entity mentioned before can be divided into small grids with grid numbers:
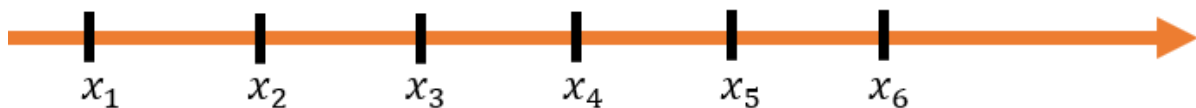
Therefore, the wavefunction can be thought of as a vector which can be shown in a matrix form.

$$\overline{\Psi} = \begin{bmatrix} \Psi(x_1) \\ \Psi(x_2) \\ \Psi(x_3) \\ . \\ . \\ . \\ \Psi(x_N) \end{bmatrix}$$

States are such vectors. On the other hand, the operators are the matrices that can "operate" on these vectors.

The position operator that corresponds to a position measurement in a matrix form:

$$\bar{\bar{X}} = \begin{bmatrix} x_1 & 0 & 0 & \cdots & 0 \\ 0 & x_2 & 0 & \ddots & 0 \\ 0 & 0 & x_3 & \ddots & 0 \\ \vdots & \vdots & \vdots & \ddots & 0 \\ 0 & 0 & 0 & \cdots & x_N \end{bmatrix}$$: Position operator as a matrix

The eigenvalues of this matrix are $x_1, x_2, x_3, \ldots, x_N$ while the corresponding eigenstates are:

$$\begin{bmatrix} 1 \\ 0 \\ . \\ . \\ . \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ . \\ . \\ . \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 1 \\ . \\ . \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ . \\ 1 \\ . \\ 0 \end{bmatrix}, \ldots, \begin{bmatrix} 0 \\ 0 \\ 0 \\ . \\ . \\ 1 \end{bmatrix}, \text{respectively}$$

If one measures the position of a particle with wavefunction $\bar{\Psi}^{old}$, s/he can get x_2 (for example) as a result with probability :

$$\left| \bar{\Psi}^{old\prime} * \begin{bmatrix} 0 \\ 1 \\ . \\ . \\ . \\ 0 \end{bmatrix} \right|^2 = \left| \bar{\Psi}^{old}(x_2) \right|^2$$

where $\bar{\Psi}^{old\prime}$ is the permission conjugate of $\bar{\Psi}^{old}$.

Probability of getting x_2 upon measurement. This multiplication is repeated for all eigenstates of the position operator matrix.

After getting the result x_2, the new wavefunction becomes $\bar{\Psi}^{new} = \begin{bmatrix} 0 \\ 1 \\ . \\ . \\ . \\ 0 \end{bmatrix}$.

This transformation of the wavefunction can be represented as below:
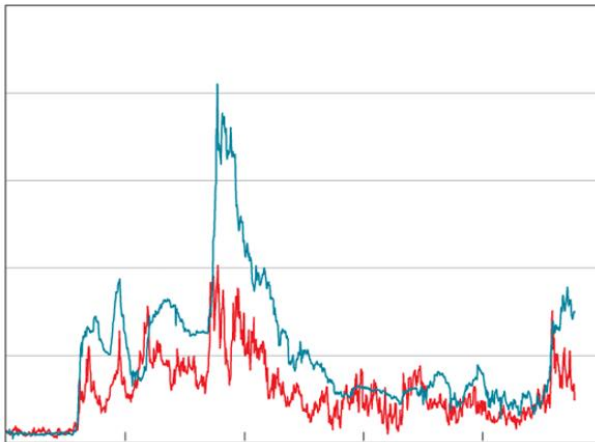
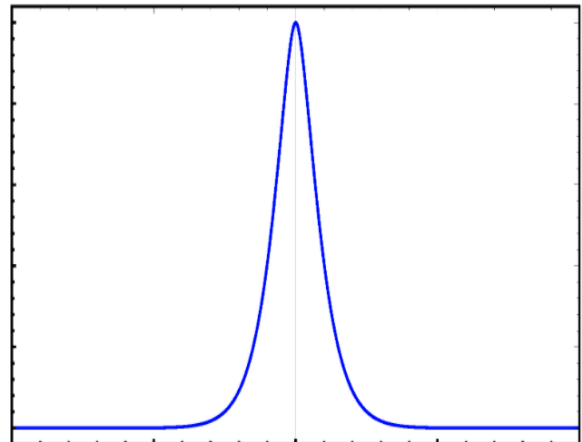Figure.3: Representation of old wavefunction, a strange plot due to complex term in wavefunction

Figure.4: Representation of new wavefunction, sharp peak at a certain point where the measurement is done

In quantum mechanics, the momentum operator is the operator associated with the linear momentum. The momentum operator is, in the position representation, an example of a differential operator. For the case of one particle in one spatial dimension, the definition is:

$$\hat{p} = -i\hbar\frac{\partial}{\partial x} \ or \frac{\hbar}{i}\frac{\partial}{\partial x} \qquad (-i = \frac{1}{i})$$

where $\hbar$ is Planck's reduced constant, i the imaginary unit, x is the spatial coordinate, and a partial derivative $\frac{\partial}{\partial x}$ is used instead of a total derivative $\frac{d}{dx}$ since the wavefunction is also a function of time. The "application" of the operator on a differentiable wave function is as follows:

$$\hat{p}\Psi = -i\hbar\frac{\partial\Psi}{\partial x}$$

In a basis of Hilbert space consisting of momentum eigenstates expressed in the momentum representation, the action of the operator is simply multiplication by p, i.e. it is a multiplication operator, just as the position operator is a multiplication operator in the position representation.

$\hbar$ is a small number$(10^{-34}$ J. s) that keeps quantum effects at nanoscale. The matrix form of momentum is:

$$\bar{\bar{p}} = \begin{bmatrix} 0 & 1 & 0 & 0 & \dots & 0 \\ -1 & 0 & 1 & 0 & \dots & 0 \\ 0 & -1 & 0 & 1 & \dots & 0 \\ 0 & 0 & -1 & \ddots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \ddots & \dots & 1 \\ 0 & 0 & 0 & 0 & -1 & 0 \end{bmatrix}\frac{\hbar}{i}\frac{1}{2\Delta x}, \text{where } \bar{\bar{p}} \text{ is the momentum operator as a matrix.}$$

Derivation of momentum operator matrix:

$$\hat{p}\Psi_5 = \frac{\hbar}{i}\frac{\partial\Psi_5}{\partial x}(at\ x = x_5) = \frac{\hbar}{i}\frac{\Psi_6 - \Psi_5}{\Delta x} = \frac{\hbar}{i}\frac{\Psi_6 - \Psi_4}{2\Delta x}$$

$$\begin{bmatrix} & & & & & \dots & \dots \\ & & & & & \dots & \dots \\ & & & & & \dots & \dots \\ & & & \ddots & \ddots & \vdots & \dots \\ & & & \frac{-\hbar}{i2\Delta x} & 0 & \frac{\hbar}{i2\Delta x} & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \dots \\ & & & & & & \vdots \end{bmatrix}\begin{bmatrix} \cdot \\ \cdot \\ \Psi_3 \\ \Psi_4 \\ \Psi_5 \\ \Psi_6 \\ \cdot \\ \cdot \\ \cdot \end{bmatrix} \longrightarrow \hat{p}\Psi_5 = \frac{\hbar}{i}\frac{\Psi_6 - \Psi_4}{2\Delta x}$$

$$\underbrace{\phantom{\begin{bmatrix} & & & & & & \end{bmatrix}}}_{\bar{\bar{p}}}$$

Deriving kinetic energy:

$P = mv$ where P is the momentum, m is the mass, v is the velocity of mass and T is the kinetic energy

$$T = \frac{mv^2}{2} \longrightarrow T = \frac{p^2}{2m}$$

putting $\frac{\hbar}{i}\frac{\partial}{\partial x}$ for p:

$$T = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$$

$since \ \dfrac{\partial\Psi_5}{\partial x} = \dfrac{\Psi_6 - \Psi_4}{2\Delta x} \ ---\rightarrow$

$$\frac{\partial^2\Psi}{\partial x^2}(at\ x = x_5) = \frac{\dfrac{\partial\Psi_6}{\partial x} - \dfrac{\partial\Psi_5}{\partial x}}{\Delta x} = \frac{\dfrac{\Psi_6 - \Psi_5}{\Delta x} - \dfrac{\Psi_5 - \Psi_4}{\Delta x}}{\Delta x} = \frac{\Psi_6 + \Psi_4 - 2\Psi_5}{\Delta x^2}$$

Therefore T(kinetic energy) in matrix form can be represented as follows:

$$\overline{\overline{T}} = \begin{bmatrix} 2 & 1 & 0 & 0 & \dots & 0 \\ -1 & 2 & 1 & 0 & \dots & 0 \\ 0 & -1 & 2 & 1 & \dots & 0 \\ 0 & 0 & -1 & \ddots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \ddots & \dots & 1 \\ 0 & 0 & 0 & 0 & -1 & 2 \end{bmatrix} \frac{\hbar^2}{2m\Delta x^2} \ , \text{where } \overline{\overline{T}} \text{ is the kinetic energy operator in matrix form}$$

Similarly, potential energy operator in matrix form:

$$\overline{\overline{V}} = \begin{bmatrix} V(x_1) & 0 & 0 & \dots & 0 \\ 0 & V(x_2) & 0 & \ddots & 0 \\ 0 & 0 & V(x_3) & \ddots & 0 \\ \vdots & \vdots & \vdots & \ddots & 0 \\ 0 & 0 & 0 & \dots & V(x_N) \end{bmatrix}$$

Total energy is usually named Hamiltonian and denoted by H:

$\overline{\overline{H}} = \overline{\overline{T}} + \overline{\overline{V}}$ (Total energy = Kinetic energy + Potential energy)

Notice that:

$$i\hbar\frac{\partial\Psi}{\partial x} = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\Psi$$

Hence, Schrödinger's equation becomes:

$$\frac{\partial\overline{\Psi}}{\partial x} = \frac{\overline{\overline{H}}}{i\hbar}\overline{\Psi}$$

This equation can be solved numarically using fourth-order Runge Kutta method.

- Before the solution of Schrödinger's equation, it is benefical to give background about fourth-order Runge Kutta method.

Given following inputs,
- An ordinary differential equation that defines value of dy/dx in the form x and y.
- Initial value of y, i.e., y(0)

Thus it is given below:

$$\frac{dx}{dy} = f(x, y), y(0) = y_0$$

The task is to find value of unknown function y at a given point x.

The Runge-Kutta method finds approximate value of y for a given x. Only first order ordinary differential equations can be solved by using the Runge Kutta 4th order method.

Below is the formula used to compute next value y_{n+1} from previous value y_n. The value of n are 0, 1, 2, 3, …(x-x_0)/h. Here h is step height and $x_{n+1} = x_0 + h$. Lower step size means more accuracy.

$$K_1 = hf(x_n, y_n)$$

$$K_2 = hf(x_n + \frac{h}{2}, y_n + \frac{k_1}{2})$$

$$K_3 = hf\left(x_n + \frac{h}{2}, y_n + \frac{k_2}{2}\right)$$

$$K_3 = hf(x_n + h, y_n + k_3)$$

$$y_{n+1} = y_n + \frac{k_1}{6} + \frac{k_2}{3} + \frac{k_3}{3} + \frac{k_4}{6} + O(h^5)$$

The formula basically computes next value y_{n+1} using current y_n plus weighted average of four increments.
- k_1 is the increment based on the slope at the beginning of the interval, using y
- k_2 is the increment based on the slope at the midpoint of the interval, using y + $hk_1/2$.
- k_3 is again the increment based on the slope at the midpoint, using using y + $hk_2/2$.
- k_4 is the increment based on the slope at the end of the interval, using y + hk_3.

The method is a fourth-order method, meaning that the local truncation error is on the order of $O(h^5)$, while the total accumulated error is order $O(h^4)$.

- Back to solution of the Schrödinger's equation:

Let, $\bar{\bar{U}} = \dfrac{\bar{\bar{H}}}{i\hbar}$

$$k_1 = \Delta t \bar{\bar{U}} \bar{\Psi}^t$$

$$k_2 = \Delta t \bar{\bar{U}} \left(\bar{\Psi}^t + \frac{k_1}{2}\right)$$

$$k_3 = \Delta t \bar{\bar{U}}(\bar{\Psi}^t + \frac{k_2}{2})$$

$$k_4 = \Delta t \bar{\bar{U}}(\bar{\Psi}^t + k_3)$$

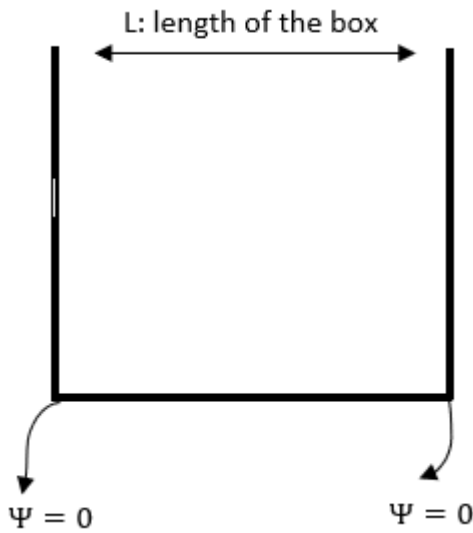Therefore, $\bar{\Psi}^{t+1} = \bar{\Psi}^t + \dfrac{k_1 + 2k_2 + 2k_3 + k_4}{6}$

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Figure.5: Simple presentation of the box

Figure.6: Grid interpretation for the length of the box

The box includes one particle and it is free to move in it(up-down and left-right). The box has a length of L. At the ends, the wavefunctions are equal to zero.

Operator has eigenvalues and for each eigenvalue, yhe operator matrix has eigenvectors.

Operator →
$$e = \begin{bmatrix} \bar{e}_1 & \bar{e}_2 & \bar{e}_3 & ... \\ \vdots & \vdots & \vdots & ... \\ \vdots & \vdots & \vdots & ... \\ \vdots & \vdots & \vdots & ... \\ \vdots & \vdots & \vdots & ... \end{bmatrix}$$
and corresponding eigenvalues are $\lambda_1, \lambda_2, \lambda_3, ...$ respectively

$$\bar{f} = \sum_{i=1}^{n=N} c_i \, \bar{e}_1,$$ where $\bar{f}$ is the initial function c_i is the constant number and e_i is the eigenvector

$c_i = \bar{e}_1' \, \bar{f}$, where $\bar{e}_1'$ is the permission conjugate of $\bar{e}_1$

$$\begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ . \\ . \\ . \end{bmatrix} = \bar{\bar{e}}_1' \, \bar{f}$$

Therefore:

$|c_1|^2 : probability\ of\ collapsing\ into\ \bar{e}_1$

$|c_2|^2 : probability\ of\ collapsing\ into\ \overline{e_2}$

$|c_3|^2 : probability\ of\ collapsing\ into\ \overline{e_3}$

The ground state is described as the lowest energy state of an atom or other particle. Therefore, the plot at the ground state is expected to one and only one peak.

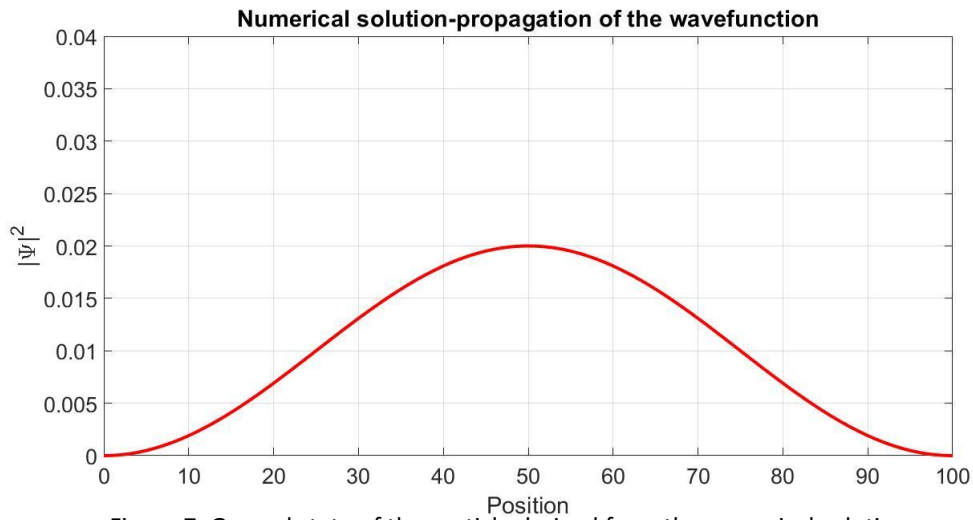**Numerical solution-propagation of the wavefunction**

Figure.7: Ground state of the particle derived from the numerical solution

Here the length of the box(L) is taken as 100, m is taken as 1, the number of grids(N) is taken as 200, grid size is taken as length divided by the grid intervals which is N+1=201. Here the measured energy is 0.99998 which is very close to 1 as expected since when one looks at the energy levels of an atom s/he will see that the energy difference between the first orbit and the second orbit is only one E (1^2).

On the other hand, excited state means that an electron from an orbital absorbs incoming radiation or a photon that corresponds to its energy level and hence is elevated to a higher energy level. First excited state describes the the electron is elevated by one energy state, hence two visible peaks in the plot.

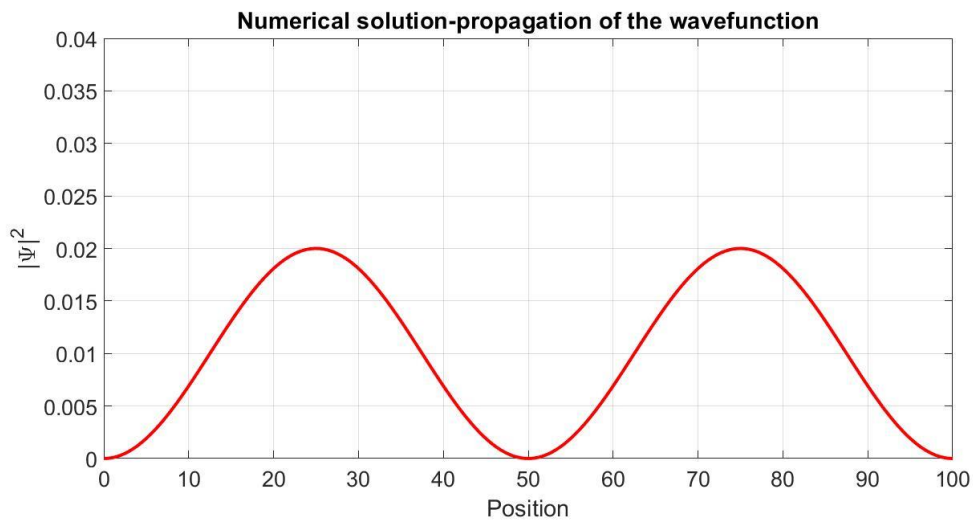**Numerical solution-propagation of the wavefunction**

Figure.8: The first excited state of the particle derived from the numerical solution

Here the length of the box(L) is taken as 100, m is taken as 1, the number of grids(N) is taken as 200, grid size is taken as length divided by the grid intervals which is N+1=201. Here the measured energy is 3.9997 which is very close to 4 as expected since when one looks at the energy levels of an atom s/he will see that the energy difference between the first orbit and the the third orbit is two E (2^2).

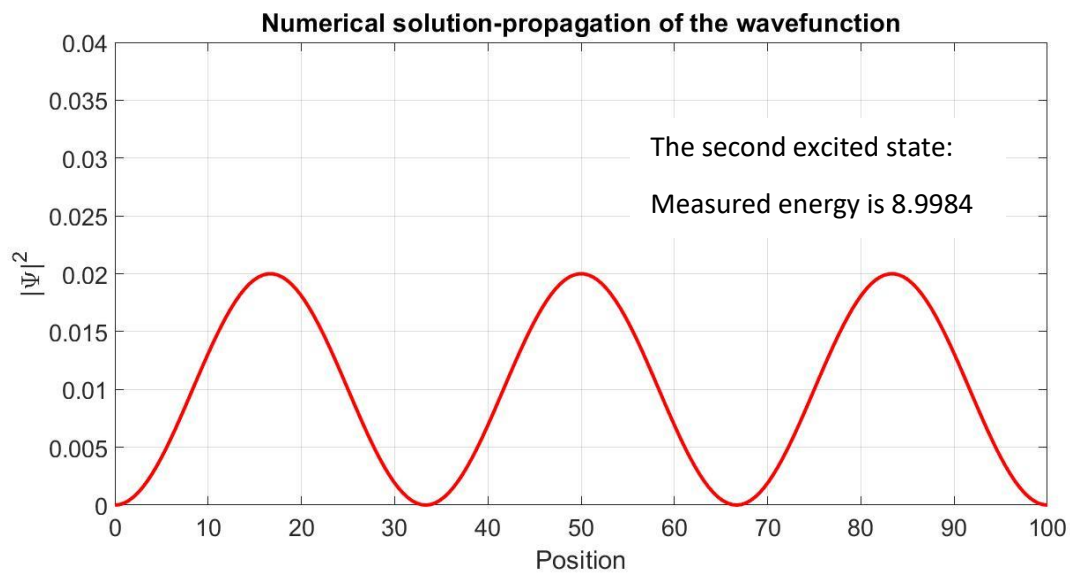Other excited levels can be derived from the oscillation behavior of the particle:

Numerical solution-propagation of the wavefunction

The second excited state:

Measured energy is 8.9984

Figure.9: The second excited state of the particle derived from the numerical solution

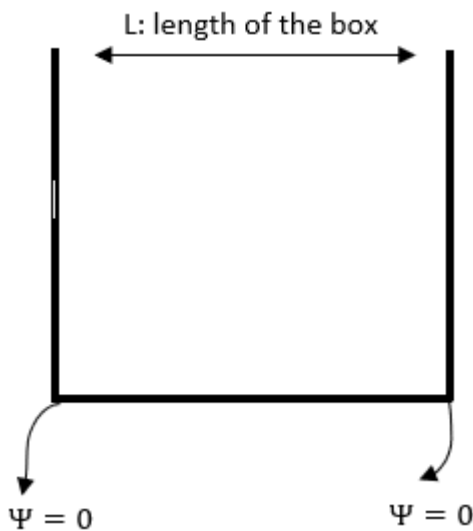## 2.b) Analytical Solution

L: length of the box

Figure.5: Simple presentation of the box

The box includes one particle and it is free to move in it(up-down and left-right). The box has a length of L. At the ends, the wavefunctions are equal to zero.

$\Psi = 0$ $\Psi = 0$

$i\hbar \dfrac{\partial \Psi}{\partial x} = -\dfrac{\hbar^2}{2m}\dfrac{\partial^2 \Psi}{\partial x^2}$, original Schrödinger's equation as derived before

$\Psi(x,t) = \Phi(x)\varphi(t)$, where $\Phi(x)$ is the function of space and $\varphi(t)$ is the function of time

$i\hbar \dfrac{\partial \varphi}{\partial x} = E\varphi$, coming from the time part

$-\dfrac{\hbar^2}{2m}\dfrac{\partial^2 \Phi}{\partial x^2} = E\Phi$, which is also called time $-$ independent Schöredinger's equation.
coming from the space(position) part, where E is an energy constant, a numerical value.

Time equation gives:

$$\varphi = e^{\frac{-iEt}{\hbar}}$$

Space equation gives:

$$\Phi = \sin\left(\frac{n\pi x}{L}\right), \text{where } n = 1,2,3,4 \dots$$

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}, \text{where } E_n \text{ is the energy constant changing according to n.}$$

If the eigenvalues are divided by E_n, the results will be 1,4,9,16...(square of integers)

Overall, the general solution of the Schrödinger's equation for a particle in a box:

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \sin\left(\frac{n\pi x}{L}\right) e^{-i\frac{n^2\pi^2\hbar}{2mL^2}t}$$

Quantum Harmonic Oscillator:

$$V(x) = \frac{kx^2}{2} \longrightarrow -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V(x)\Psi(x) = E\Psi(x)$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + \frac{kx^2}{2}\Psi(x) = E\Psi(x)$$

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega, \text{where } n = 1,2,3,4 \dots \text{ and } \omega \text{ is the frequency of the system} \left(\sqrt{\frac{k}{m}}\right)$$
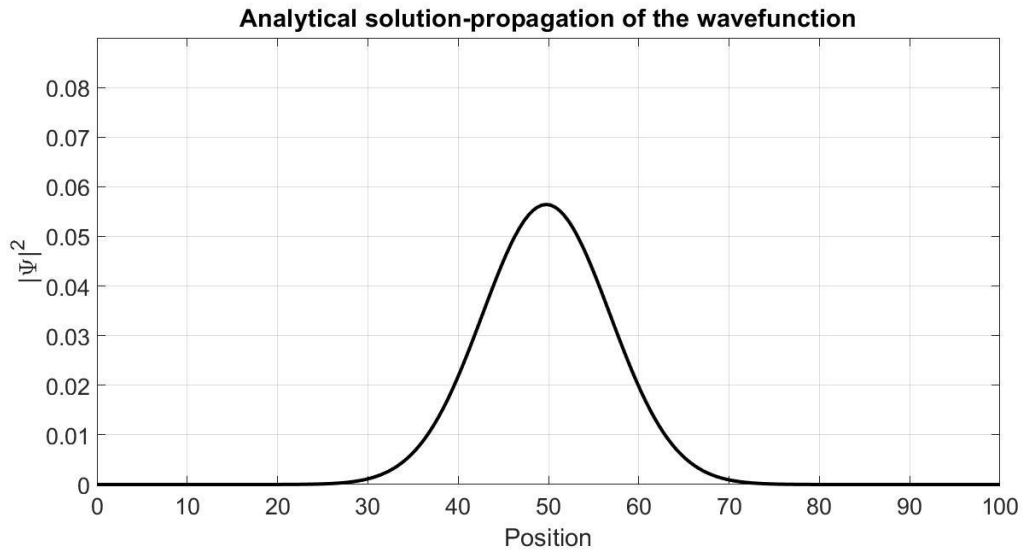

Figure.10: Ground state of the particle derived from the analytical solution

Ground state from the analytical solution. Here the length of the box(L) is taken as 100, m is taken as 1, the number of grids(N) is taken as 200, grid size is taken as length divided by the grid intervals which is N+1=201, all as in the numerical solution. Here the measured energy is 0.49992 which is not close to 1. This caused by the interpretation of $E_n = \left(n + \frac{1}{2}\right)\hbar\omega$. Here n = 0 so the result shall be half of 1. The analytical solution includes some experimental results in it to be more accurate and include nature effect.

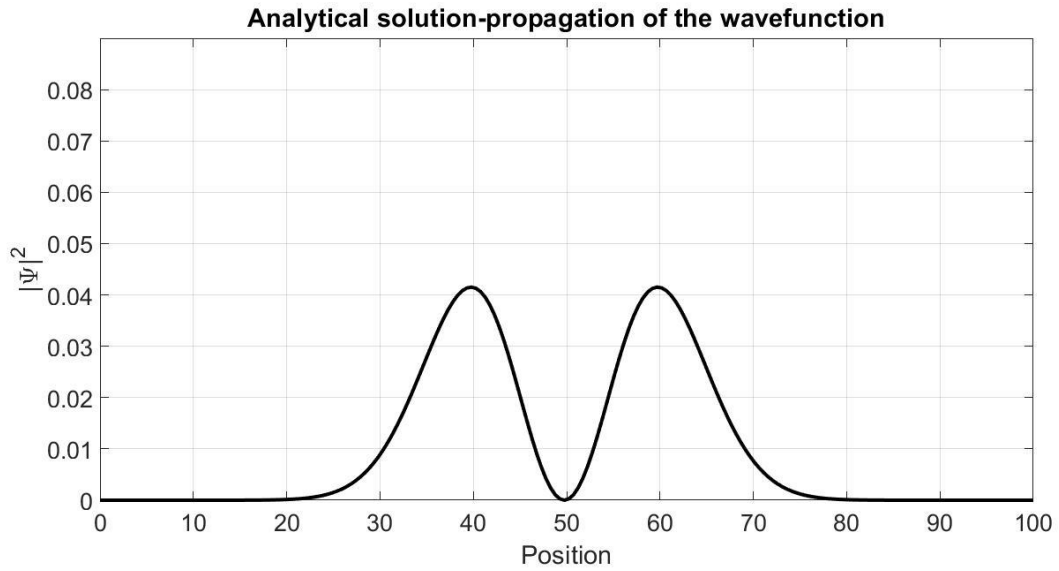**Analytical solution-propagation of the wavefunction**

Figure.11: The first excited state of the particle derived from the analytical solution

First excited state from the analytical solution. Here the length of the box(L) is taken as 100, m is taken as 1, the number of grids(N) is taken as 200, grid size is taken as length divided by the grid intervals which is N+1=201, all as in the numerical solution. Here the measured energy is 1.4996. This caused by the interpretation of $E_n = \left(n + \frac{1}{2}\right)\hbar\omega$. Here n = 1 so the result shall be 3/2 times of 1. The analytical solution includes some experimental results in it to be more accurate and include nature effect.

The other states can be derived as well:

Analytical solution-propagation of the wavefunction

The second excited state:

Measured energy is 2.499
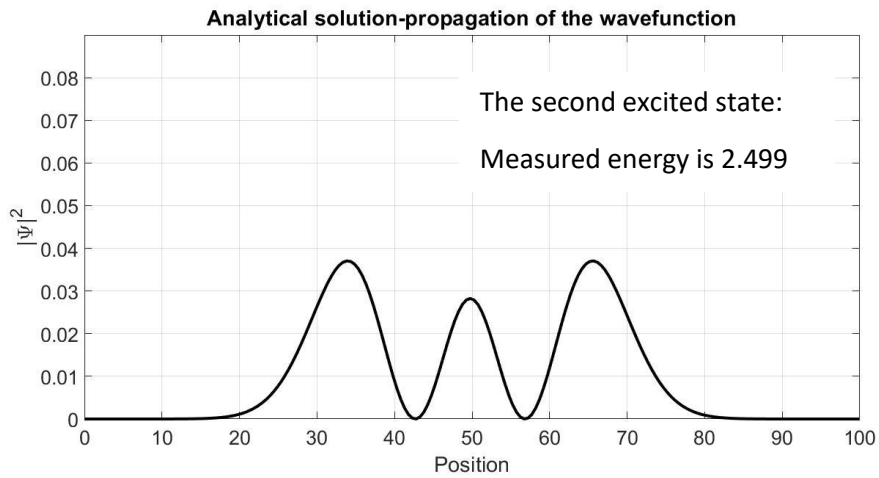
Figure.12: The second excited state of the particle derived from the analytical solution

Analytical solution-propagation of the wavefunction

The third excited state:
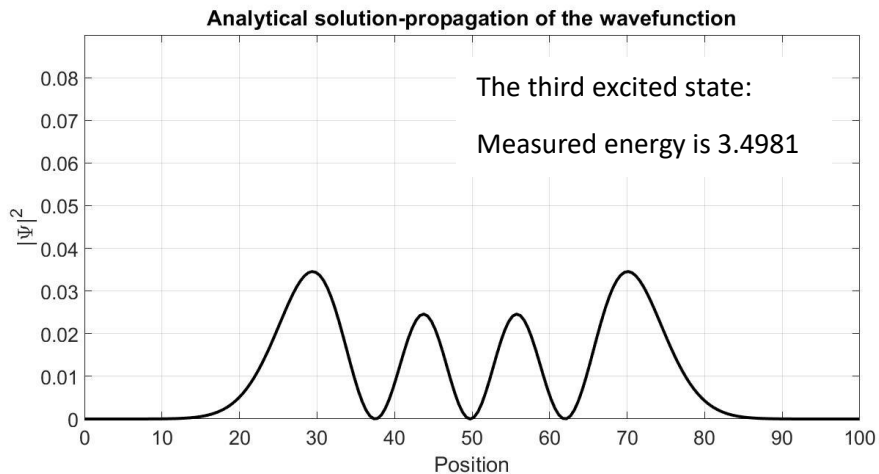
Measured energy is 3.4981

Figure.13: The third excited state of the particle derived from the analytical solution
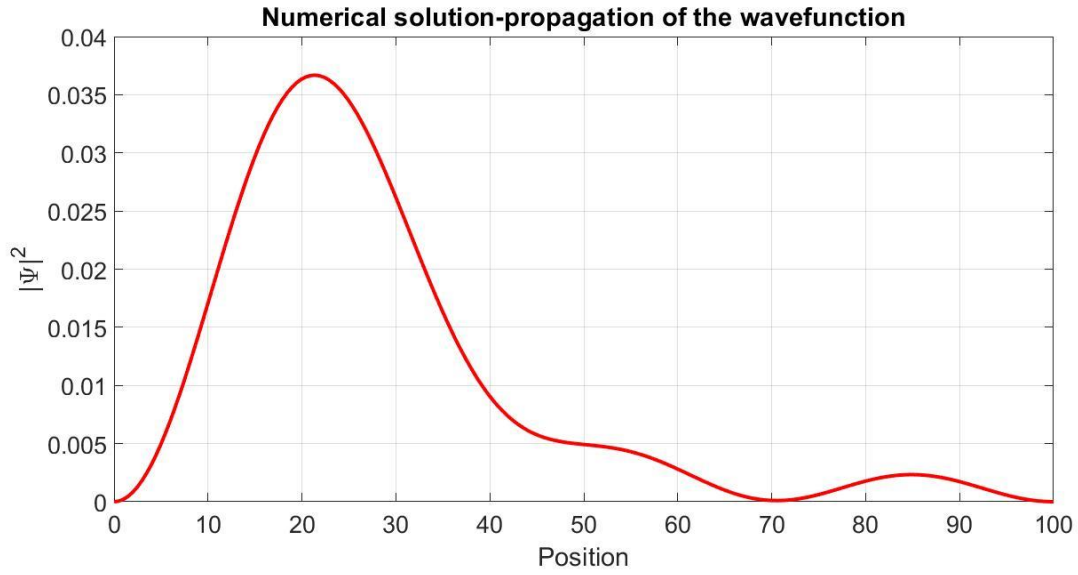
3) COMPARISON of TWO DIFFERENT SOLUTIONS

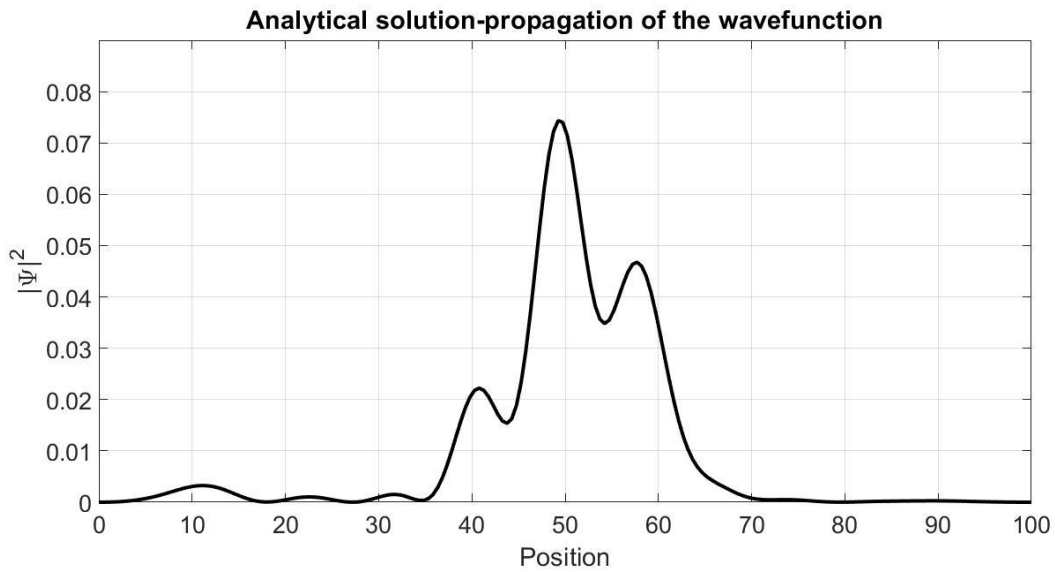Figure.14: Behavior of the partical at t = 1 according to numerical solution

Figure.15: Behavior of the partical at t = 1 according to analytical solution

The results of the numerical solution obeys stability more than the analytical solution. When one looks at the plot derived from different methods, s/he will see that the peak points in numerical solution have same magnitude. On the other hand, the peak values of the energy states in analytical solution results, while the middle ones are the same as each other and also, the end peaks are the same as each other, middle and end peaks are not the same. Also, the oscillation from the analytical solution is more stable, which is they do not have much noise in their motion. The above plots were taken for the same time. The stability difference between results from two different methods is caused by the equation used to solve the system. In analytical solution, the method is mainly interpreting the previous result. However, even if the previous results are used, the equation $E_n = \left(n + \frac{1}{2}\right)\hbar\omega$ makes the behavior far from a nice stability.

4) CONCLUSION

The results obtained from the two different methods are also similar. Analytical solution gives more accurate results because it is safer to reach the solution thanks to the equations derived from some experiments and theories. The oscillation and behavior of a particle can never be exactly determined due to the porobability distrubution caused by nature's influence and uncertainty, so some noise can be expected in the plots, which is more similar to the result given by the analytical solution.

Changing the initial conditions directly affects the behavior of the particle. For example, the behavior of the particle becomes more regular and stable when it is created with initial condition of only a ground state instead of creating with the initial condition from a ground state and also a first excited state.

5) CODE REVIEW

```
1 -    clc;
2 -    clear;
3 -    clear all;              The length of the box, mass of the particle, grid number,
4 -    L = 100;                time step and grid size are described.
5 -    m = 1;
6 -    hbar = 1;
7 -    N = 200;
8 -    dt = 0.25;
9 -    dx = L/(N+1);

11 -   f0 = sin(pi*(1:N)'/(N+1)) + sin(2*pi*(1:N)'/(N+1)) + sin(3*pi*(1:N)'/(N+1));
12 -   f0 = f0/norm(f0)/sqrt(dx);    Initial function is determined and three harmonic
13 -   f = f0;                       behaviors are added to make things more complicated.

14 -   V = zeros(N,N);
15 -   X = zeros(N,N);
16 -   P = zeros(N,N);               Spaces for potential energy operator, position operator,
17 -   T = zeros(N,N);               momentum operator and kinetic energy operator are
18 -   X(1,1)  = 1/(N+1)*L;          opened. Momentum operator and position operator are
19 -   P(1,2)  = hbar/2i/dx;         defined.
20 -   T(1,1:2) = [2/dx^2*hbar^2/2/m -1/dx^2*hbar^2/2/m];
21 -   for n = 2 : N - 1
22 -        X(n,n)  = n/(N+1)*L;
23 -        P(n,n+1) = hbar/2i/dx;        In addition to initial values, other elements
24 -        P(n,n-1) = -hbar/2i/dx;       of the operator matrices are determined.
25 -        T(n,n-1) = -1/dx^2*hbar^2/2/m;
26 -        T(n,n)  = 2/dx^2*hbar^2/2/m;
27 -        T(n,n+1) = -1/dx^2*hbar^2/2/m;
28 -   end
```

```
29 -      X(N,N) = N/(N+1)*L;
30 -      P(N,N-1) = -hbar/2i/dx;
31 -      T(N,N-1:N) = [-1/dx^2*hbar^2/2/m 2/dx^2*hbar^2/2/m];
32 -      H = T + V;
33 -      U = H/hbar/1i;

35 -      fig = figure;
36 -      set(fig,'KeyPressFcn',@dummy);
37 -      for t = 1 : 1000000
38 -          k1 = dt*U*f;
39 -          k2 = dt*U*(f + k1/2);
40 -          k3 = dt*U*(f + k2/2);
41 -          k4 = dt*U*(f + k3);
42 -          f = f + (k1 + 2*k2 + 2*k3 + k4)/6;

43 -          if (mod(t,100) == 1)
44 -              if (fig.CurrentCharacter == 'h')
45 -                  fig.CurrentCharacter = '~';
46 -                  [f,value] = measure(H,f,dx);
47 -                  display(['Measured energy is ' num2str(value/(pi^2*hbar^2/2/m/L^2))]);
48 -              elseif (fig.CurrentCharacter == 'x')
49 -                  fig.CurrentCharacter = '~';
50 -                  [f,value] = measure(X,f,dx);
51 -                  display(['Measured position is ' num2str(value)]);
52 -              elseif (fig.CurrentCharacter == 'p')
53 -                  fig.CurrentCharacter = '~';
54 -                  [f,value] = measure(P,f,dx);
55 -                  display(['Measured momentum is ' num2str(value)]);
56 -              elseif (fig.CurrentCharacter == 'r')
57 -                  fig.CurrentCharacter = '~';
58 -                  f = f0;
59 -                  disp('Wavefunction was reset');
60 -              end
```

Pressing "h" will show current energy level. Here is the part that one can demonstrate ground state and excited states.
Pressing "x" will show current position of the particle.
Pressing "p" will show current momentum that the particle has.
Pressing "r" will reset the plot and behavior.

```
61 -              plot(L*(0:N+1)/(N+1),[0; conj(f).*f; 0],"r",'LineWidth',3);
62 -              axis([0 L 0 0.04]);
63 -              set(gca,'FontSize',20);
64 -              xlabel('Position');
65 -              ylabel('|\Psi|^2');
66 -              title("Numerical solution-propagation of the wavefunction")
67 -              grid on
68 -              drawnow;
69 -          end
70 -      end

73   function [f,value] = measure(Operator,f,dx)
74 -      [evec,eval] = eig(Operator);
75 -      c = evec'*f;
76 -      c2 = conj(c).*c/(c'*c);
77 -      r = rand;
78 -      s = 0;
79 -      for n = 1 : size(f,1)
80 -          s = s + c2(n);
81 -          if (s > r)
82 -              break
83 -          end
84 -      end
```

Hamiltonian equation is described as the summation of the kinetic energy and the potential energy.

Fourth order Runge Kutta method application

Plotting the behavior of particle and wavefunction

Measurement of the operator is done and eigenvectors and eigenvalues of operator matrix are found. Then, new random size is determined.

15

```matlab
85 -      f = evec(:,n);
86 -      f = f/norm(f)/sqrt(dx);
87 -      value = eval(n,n);
88 -    end
89    function dummy(~,~,~)
90 -    end
```

This determines collapse of the wavefunction and returns measurement results.