QUANTUM MECHANICS

MAYANK

October 20, 2019

Subject	Scilab Report File(QM)
Date Submitted:	October 3,2019
Exam Roll no.	17036567058
College Roll no.	31730724
course	Bsc($\mathcal{H}$) Physics
semester	5
Instructor:	Dr. Pranav Kumar

Signature

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1 Simple Harmonic Motion

The equation of motion for a particle of mass m under the action of linear restoring force $\vec{F} = -k\vec{x}$, in a viscous medium of drag coefficient b and simultaneously under the external force of the form $\vec{F}(t) = \vec{F}_o cos(\omega_d t)$ is given by the following equation :

$$m\ddot{x} = -kx - b\dot{x} + F_o cos(\omega_d t) \quad (1)$$

The steady state solution to this equation is the following :

$$x_s(t) = Asin(\omega_d + \phi_o) \quad (2)$$

wherer A and ϕ_o depends on driving frequency ω_d by the following expression :

$$A(\omega_d) = \frac{F_o}{\sqrt{m^2(\omega_d^2 - \omega_o^2)^2 + b^2\omega_d^2}} \quad (3)$$

$$\phi_o(\omega_d) = \arctan\left(\frac{2\omega_d\omega_o\zeta}{\omega_d^2 - \omega_o^2}\right) \quad (4)$$

where ζ is called damping ratio :

$$\zeta = \frac{b}{2\sqrt{km}}$$

AIM: To solve the equation (1) differential equation numerically in scilab for $m = 1kg$ and obtain the following results :
(a) when $F = 0N, b = 0.5Nm^{-1}s, \omega_o = 3rads^{-1}$ obatin phase plot [1] ,$x(t), v(t)$
(b) when $F = 0.7N, b = 1.8Nm^{-1}s, \omega_o = 3rads^{-1}, \omega_d = 2.4rads^{-1}$ obtain phase plot [2] , $x(t), v(t)$
(c) Obtain Resonance curves [3] for the values $b = 0.2, 0.5, 0.8$ respectively.

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[1] Particle in phase plot of figure 1. loses all energy under the action of damping force
[2] Particle in phase plot of figure 2. doesn't collapse because of the action of sinusoidal external force
[3] The Resonance curves in figure 2. refers to equation (3) for various values of b

```scilab
funcprot(0)
function dx=f(t,x)
    dx(1)=x(2)
    dx(2)=-gamm*x(2)-(w^2)*x(1) + (fo/m)*cos(wd*t)
endfunction
fo=input("enter the amplitude of force = ")
wd=input("enter the driving frequecy = ")
b=input("enter the value of damping constant  = ")
w=input("enter the value of natural frequency = ")
m=input("enter the value of m = ")
to=0
gamm=b/m
xo=[0;5]
t=0:0.01:100
sol=ode(xo,to,t,f)
  subplot(221)                            //PHASE SPACE PLOT
    plot(sol(1,:),sol(2,:))
    xtitle( "$\huge Phase \medspace Plot  $")
    xlabel("$\huge P(t) \medspace (momentum)$")
    ylabel("$\huge x(t) \medspace (position)$")

    subplot(222)                          //VELOCITY PLOT
    plot(t,sol(2,:))
    if(fo==0)  then
       break
    else
    xtitle( "$\huge v(t)=-A \omega cos(\omega t \medspace + \medspace \phi) $")
    end
    xlabel("$\huge time \medspace t(s)$")
    ylabel("$\huge v(t) \medspace (ms^{-1})$")
    xstring(60,3.5,["$\large m=1kg$"])
    if(fo==0) then
    xstring(60,3,["$\large b=0.5Nm^{-1}s$"])
    else
    xstring(60,3,["$\large b=1.8Nm^{-1}s$"])
    end
    if(fo==0) then
    xstring(60,2.5,["$\large F_{o} = 0N$"])
     else
    xstring(60,2.5,["$\large F_{o} = 0.7N$"])
    end
    xstring(60,2,["$\large \omega_{o}=3 \medspace rad\medspace s^{-1} \medspace
                      \omega_{d} = 2.4\medspace rad\medspace s^{-1}$"])
        subplot(223)                      //POSITION PLOT
    plot(t,sol(1,:))
    if(fo==0) then
       break
    else
    xtitle("$\huge x(t)=Asin(\omega t \medspace + \medspace \phi) $")
    end
    xlabel("$\huge time \medspace t(s)$")
    ylabel("$\huge x(t) \medspace (meters)$")
    xstring(60,0.98,["$\large m=1kg$"])
    if(fo==0) then
    xstring(60,0.85,["$\large b=0.5Nm^{-1}s$"])
    else
    xstring(60,0.85,["$\large b=1.8Nm^{-1}s$"])
    end
    if(fo==0) then
    xstring(60,0.7,["$\large F_{o} = 0N$"])
    else
    xstring(60,0.7,["$\large F_{o} = 0.7N$"])
    end
```

```
   xstring(60,0.55,["$\large \omega_{o}=3 \medspace rad\medspace s^{-1} \medspace
                         \omega_{d} = 2.4\medspace rad\medspace s^{-1}$"])

//DEFINING AMPLITUDE FUNCTION
    function amp=f(x)

    amp=fo/(sqrt(m^(2)*(x^(2)-w^(2))^(2) + b^(2)*x^(2)))

    endfunction
                //AMPLITUDE PLOT
    if(fo==0) then
       break
       else
    subplot(224)
    xtitle("$\huge Resonance \medspace Curve $")
    xlabel("$\huge Driving \medspace frequency \medspace \omega  $")
    ylabel("$\huge Amplitude $")
    for k=1:3
    B=[0.2,0.5,0.8]

    b=B(k)
    x(1)=2
    for i=2:200
        x(i)=0.01 + x(i-1)
        plot(x(i),f(x(i)),'.')
    end
    if(k==1) then
    xstring(2.9,0.1,["$\large b=$"])
    xnumb(3,0.1,B(k))
    elseif(k==2) then
    xstring(2.9,0.3,["$\large b=$"])
    xnumb(3,0.3,B(k))
    else
    xstring(2.9,0.7,["$\large b=$"])
    xnumb(3,0.7,B(k))
    end
    end
    end
```
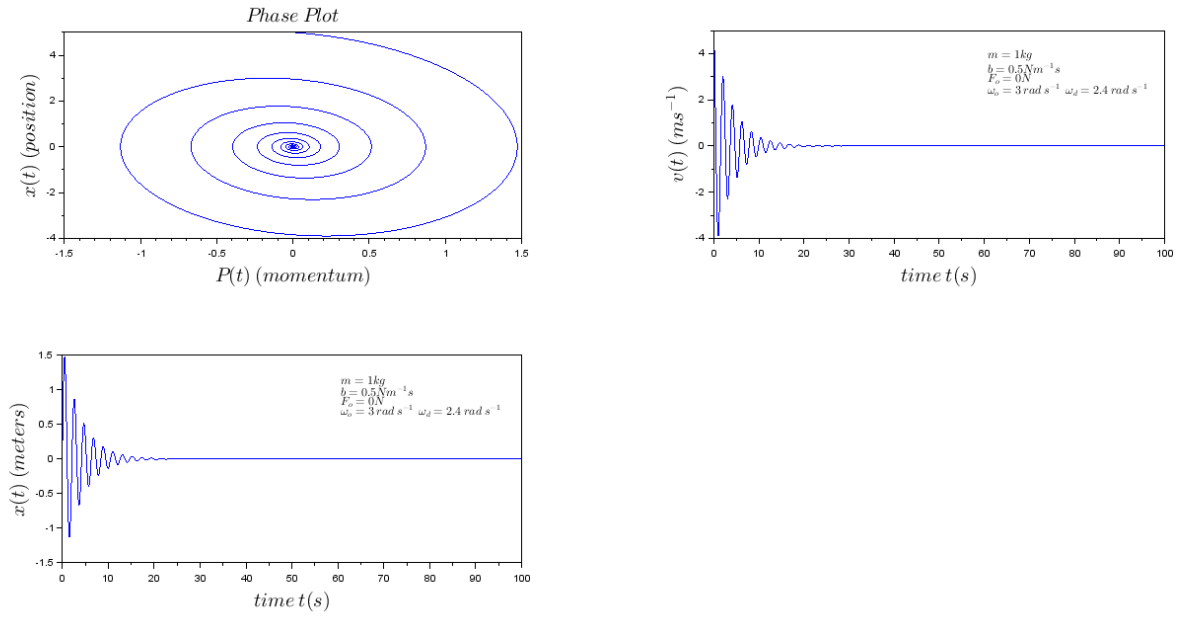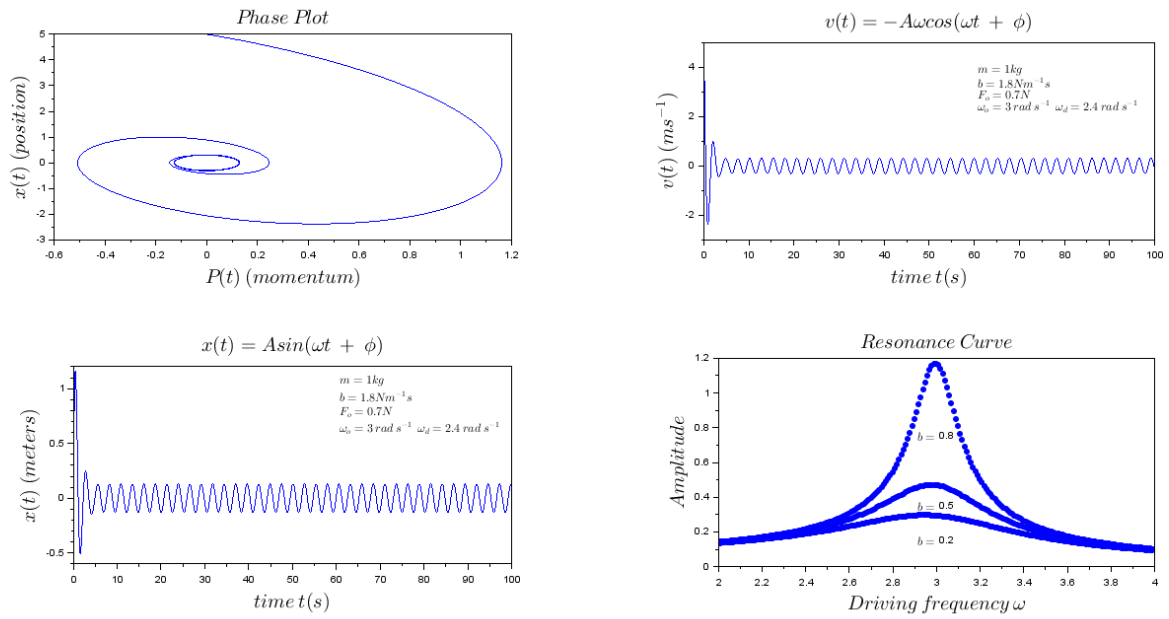
Figure 1: $F_o = 0N$, *damped harmonic oscillator*

Figure 2: $F_o = 0.7N$, *forced harmonic oscillator and resonance curves*

2 Probability Distribution

2.1 Quantum Harmonic Oscillator

Consider a quantum particle of mass m for which the hamiltonian is given by :

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\hat{x}^2$$

Therefore the time-independent schrödinger equation is given by

$$\hat{H}\Psi_n = E_n\Psi$$

where Ψ_n are eigenfunctions corresponding to the eigenvalues E_n
after solving above eigenvalue equation we get the ground state given by following wavefunction:

$$\Psi_1(x,t) = \frac{(cm)^{\frac{1}{8}}}{(\pi\hbar)^{\frac{1}{4}}}e^{-\left(\frac{\sqrt{cm}}{\hbar}\right)x^2}e^{\frac{-i}{2}\sqrt{\frac{c}{m}}t}$$

with the energy

$$E_1 = \frac{\hbar\omega}{2}$$

The corresponding probability distribution[4] is given by :

$$|\Psi(x)|^2 = \frac{(cm)^{\frac{1}{4}}}{(\pi\hbar)^{\frac{1}{2}}}e^{-\left(\frac{\sqrt{cm}}{\hbar}\right)x^2}$$

2.2 Classical Harmonic Oscillator

Consider a particle of mass m in one dimension under the harmonic potential $V(x) = \frac{1}{2}cx^2$ with the total energy E less than V

The probability of finding the particle on a given coordinate x is proportional to time spent by particle on that position which is further inversely proportional to its velocity at that instant. Therefore we have probability of obataining the particle at position x :

$$P(x) = \frac{B^2}{v(x)}$$

where B^2 is a normalization constant
By conservation of energy we have :

$$E = \frac{1}{2}mv^2 + \frac{1}{2}cx^2$$

substituting the value of $v(x)$ in above equation we get :

$$P(x) = \frac{B^2}{\sqrt{\frac{2}{m}}\sqrt{E - \frac{cx^2}{2}}}$$

Normalizing this equation we get

---

[4]we can see that probability distribution is independent of time because the system is in a stationary state.

$$B^2 = \frac{1}{\pi}\sqrt{\frac{c}{m}}$$

Therefore classical probability distribution is

$$P(x) = \frac{1}{\pi}\sqrt{\frac{c}{m}}\frac{1}{\sqrt{\frac{2}{m}}\sqrt{E - \frac{cx^2}{2}}}$$

AIM: To plot the probability density function of quantum harmonic oscillator in ground state and also for the classical harmonic oscillator

```
                        SCILAB CODE FOR PROBABILITY DENSITY OF QHO AND CHO

clc
clear
clf
disp(" ENTER 1 FOR QUANTUM HARMONIC OSCILLATOR AND
                       2 FOR CLASSICAL HARMONIC OSCILLATOR ")
p=input(" ENTER VALUE =  ")

c=10^(3)
m=10^(-26)
h_bar=6.626*10^(-34)/(2*%pi)
E=(h_bar*c)/(2*m)
A=((c*m)^(1/8))/((%pi*h_bar)^(1/4))
b_sq=0.5*sqrt(c/m)*(2/%pi)
function psi=f(x)
    psi=A^(2)*exp(-(sqrt(c*m)/h_bar)*x^2)
endfunction
function P=pr(x)


    P=b_sq/(sqrt(2/m)*sqrt(E-c*x^(2)/2))
endfunction

select p
case 1 then

xo=-2*(10)^(-11)
h=(10)^(-13)
for i=1:400
    x=xo+i*h
    plot(x,f(x),"*")
end
xtitle("$\huge probability \medspace density \medspace for \medspace
          quantum \medspace harmonic \medspace oscilator \medspace in
                                        \medspace ground \medspace state $")
xlabel("$\huge x$")
ylabel("$\huge |\Psi|^{2}$")
xstring(1e-11,8e10,["$\huge |\Psi(x)|^{2} = \frac{(cm)^{\frac{1}{8}}}
{(\pi\hbar)^{\frac{1}{4}}}e^{- \left(\frac{\sqrt{cm}}{\hbar}\right) x^{2}}$"])
```

```
case 2 then

xo=-1.05*(10)^(-4)
h=10^(-6)
for i=1:210
    x=xo+i*h
    plot(x,pr(x),'o')
end
xtitle("$\huge probability \medspace density \medspace for \medspace
               classical \medspace harmonic \medspace oscilator $")
xstring(-2*(10)^(-5),20000,["$\huge |\Psi(x)|^{2} = \frac{b^{2}}
               {\sqrt{\frac{2}{m}} \sqrt{E - \frac{cx^{2}}{2}}}$"])
xstring(-2*(10)^(-5),16000,
                    ["$\huge b^{2} = \frac{1}{\pi}\sqrt{\frac{c}{m}}$"])
xlabel("$\huge x$")
ylabel("$\huge |\Psi|^{2}$")

end
```


probability density for quantum harmonic oscilator in ground state

$$|\Psi(x)|^2 = \frac{(cm)^{\frac{1}{4}}}{(\pi\hbar)^{\frac{1}{2}}} \, e^{-\left(\frac{\sqrt{cm}}{\hbar}\right)x^2}$$
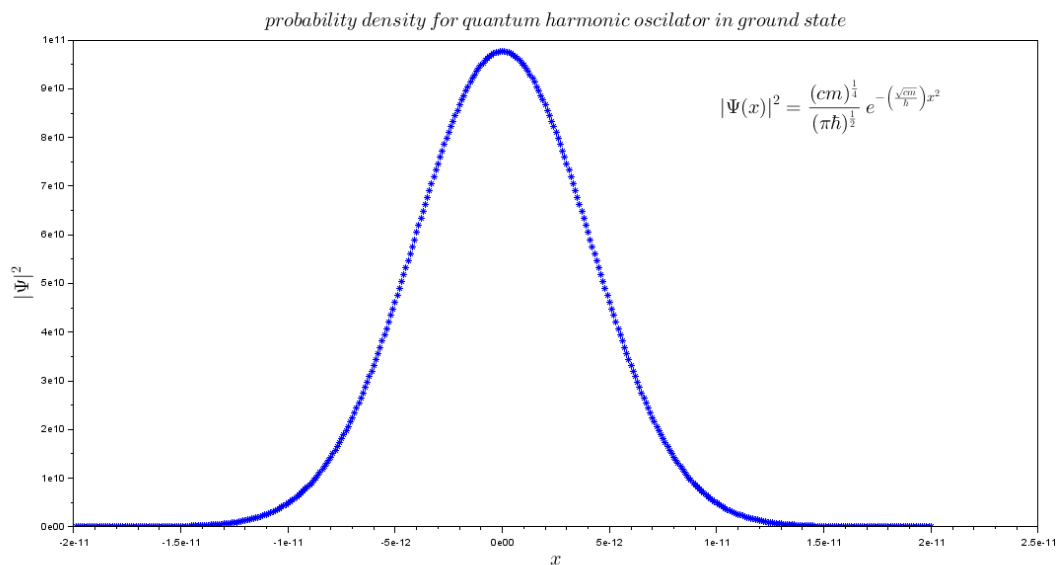
Figure 3: *Probabillty distribution for Quantum Harmonic Oscilator in ground state*

probability density for classical harmonic oscilator

$$|\Psi(x)|^2 = \frac{b^2}{\sqrt{\frac{2}{m}}\sqrt{E - \frac{cx^2}{2}}}$$

$$b^2 = \frac{1}{\pi}\sqrt{\frac{c}{m}}$$
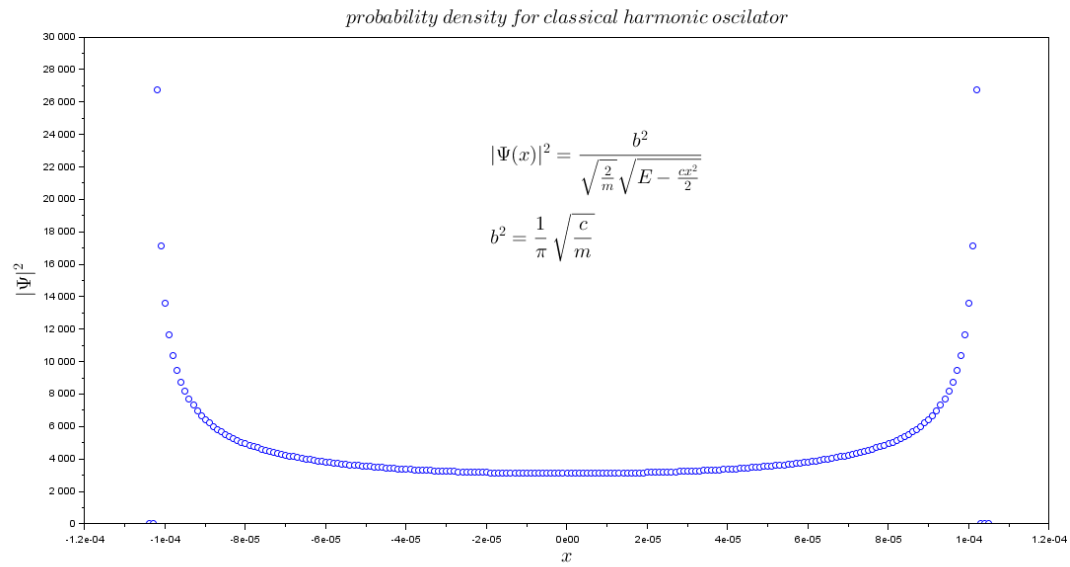
Figure 4: *Probability Distribution for Classical Harmonic Oscillator*

Note : the probability distribution of QHO [5] and CHO [6] are opposite of each other in their behaviour at $x = 0$

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[5] Quantum Harmonic Oscillator
[6] Classical Harmonic Oscillator

3   Linear Boundary Value Problem by Finite Difference Method

Consider a steady state concentration profile $C(x)$ in the following reaction-diffusion problem in the domain $x \in [0,1]$

$$\frac{d^2C}{dx^2} - C(x) = 0$$

with boundary values $C(x = 0) = 0$ and $\frac{dC}{dx}(x = 1) = 0$

The above equation can be solved analytically and the solution obtained is :

$$C(x) = \frac{\exp(2 - x) + \exp(x)}{1 + e^2}$$

Now , Let us apply the finite difference method to the above B.V.P. We first approximate the second order derivative in given differential equation by centered difference formula [7] therfore,

$$\left(\frac{d^{(}2)C}{dx^2}\right)_i = \frac{C_{i+1} - 2C_i + C_{i-1}}{h^2}$$

for first order derivative we can have a similar approximation given by ,

$$\left(\frac{dC}{dx}\right)_i = \frac{C_{i+1} - C_{i-1}}{2h}$$

The local truncation error [8] for the above approximated derivatives is $O(h^2)$ Let us partition the interval $[0,1]$ into n subinterval each of width h so that $nh = 1$, therefore $x_1 = 0$ ... and $x_i = (i - 1)h$
Implimenting the given conditions we have ,

$$C_1 = C(x_1) = C(x = 0) = 0$$

and

$$\frac{C_{n+2} - C_n}{2h} = 0 \implies C_{n+2} - C_n = 0$$

So we have $C_{1,2,3,4,\ldots,n+1,n+2}$ values but C_{n+2} have to be discarded after obtaining the solution so we have the following matrix encompassing all the equations :

$$A = \begin{pmatrix} 1 & 0 & 0 & 0 & \ldots & 0 & 0 & 0 \\ 1 & -(2+h^2) & 1 & 0 & \ldots & 0 & 0 & 0 \\ 0 & 1 & -(2+h^2) & 1 & \ldots & 0 & 0 & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & 0 & 0 & \ldots & -1 & 0 & 1 \end{pmatrix}$$

where on the right hand side we have :

$$B = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 & 0 & 0 \end{pmatrix}^T$$

---

[7]the formula can easily br derived from taylor series expansion of the given function at x_{i+1} and x_{i-1} , then adding the two expansion upto $O(h^2)$.

[8]local truncation error is the error associated with each iteration

AIM: To solve the reaction-diffusion BVP using finite difference method and plot the numerical and analytical solution in scilab

```
clc
clear

// solving boundary value problem using finite difference method
//REACTION DIFFUSION PROBLEM
h=input("enter the step size = ")
n=1/h
A=zeros(n+2,n+2)

for i=2:n+1
    A(i,i)=-(2+h*h)
    if(i<n+1)
        A(i+1,i)=1
        A(i,i+1)=1
    end

end
A(1,1)=1
A(2,1)=1
A(n+2,n+2)=1
A(n+1,n+2)=1
A(n+2,n)=-1

B=zeros(n+2,1)
B(1,1)=1
[y,kerA]=linsolve(A,-B)

x=[0:h:1]
 i=[1:n+1]
plot(x(i),y(i),'*')
P=legend(["$\large h=0.1$";"$\huge analytical \medspace solution$"])
//ANALYTICAL SOLUTION

C=[(exp(2-x) + exp(x) )/ (1+%e^(2))]

plot(x',C,'r')
xtitle("$\huge Concentration \medspace profile \medspace in
            \medspace domain \medspace x \in [0,1] $")
xlabel("$\huge value \medspace of \medspace x $")
ylabel("$\huge C(x)\medspace - \medspace concentration$")
xstring(0.8,0.9,["$\huge \frac{d^{2}C}{dx^{2}} \medspace -
                           \medspace C \medspace = \medspace 0$"])
```
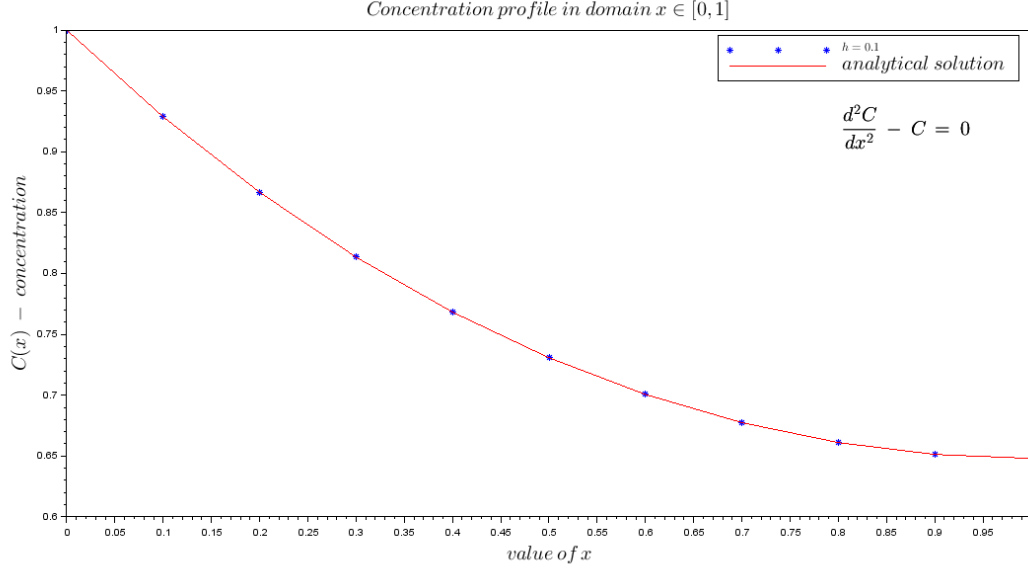
Figure 5: *analytical and numerical solution to BVP using FDM*

4 Solving the radial part of the Schrödinger equation for hydrogen atom

The hamiltonian for this quantum system can be written as ,

$$\hat{\mathcal{H}} = \left(\frac{-\hbar^2}{2m} \nabla^2 + V(r) \right)$$

where ∇^2 in spherical polar coordinates can be written as ,

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\left(\frac{\partial^2}{\partial \theta^2} + \frac{1}{tan(\theta)}\frac{\partial}{\partial \theta} + \frac{1}{sin^2\theta}\frac{\partial^2}{\partial \phi^2} \right)$$

the term in the parenthesis is equal to $-\frac{\mathcal{L}^2}{\hbar^2}$, therefore

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{1}{r^2}\frac{\mathcal{L}^2}{\hbar^2}$$

therefore the time-independent schrodinger equation become

$$\left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{1}{r^2}\frac{\mathcal{L}^2}{\hbar^2} \right) + V \right] \Psi(r,\theta,\phi) = E\Psi(r,\theta,\phi)$$

Now using the fact that $[(\hat{H}), \mathcal{L}^2] = 0$ and $[\hat{\mathcal{H}}, \mathcal{L}_z] = 0$ we have the following eigenvalue equation

$$\hat{\mathcal{H}}\Psi = E_n\Psi$$

$$\mathcal{L}^2\Psi = l(l+1)\Psi$$

$$\mathcal{L}_z\Psi = m\hbar\Psi$$

using seperation of variable technique we have $\Psi(r,\theta,\phi) = R(r)Y(\theta,\phi)$ and seperation constant l(l+1), therefore seperating out the radial part we get ,

$$\frac{1}{R(r)}\frac{d}{dr}\left(r^2\frac{d}{dr} \right)R(r) - \frac{2mr^2}{\hbar^2}\left[V(r) - E \right] = l(l+1)$$

substituting $R(r) = \frac{U(r)}{r}$ and m is replaced by reduced mass μ of the electron-proton system we get a solvable eigenvalue equation,

$$\frac{d^2U}{dr^2} + \left[\frac{2\mu e^2}{r\hbar^2} + \frac{2\mu E}{\hbar^2} - \frac{l(l+1)}{r^2} \right] U = 0$$

first four solution to the above equation can be written as follows

$$\mathcal{R}_{1,0} = 2a_o^{-\frac{3}{2}} e^{-\frac{r}{a_o}}$$

$$\mathcal{R}_{2,0} = \frac{1}{\sqrt{2}} a_o^{\frac{-3}{2}} \left(1 - \frac{r}{2a_o} \right) e^{\frac{-r}{2a_o}}$$

$$\mathcal{R}_{2,1} = \frac{1}{\sqrt{24}} a_o^{\frac{-3}{2}} \frac{r}{a_o} e^{\frac{-r}{2a_o}}$$

$$\mathcal{R}_{3,0} = \frac{2}{\sqrt{27}} a_o^{\frac{-3}{2}} \left(1 - \frac{2r}{3a_o} + \frac{2r^2}{27a_o^2} \right) e^{\frac{-r}{3a_o}}$$

where $a_o = 0.53\text{Å}$ is called the Bohr Radius.
AIM: To solve the s-wave radial equation for hydrogen atom using finite difference method and plot the probability density $|\Psi|^2$ and $\mathcal{U}(r)$, and also calculate their corresponding eigenvalues

UNITS TO BE USED:

$$\hbar c = 1973 eV \text{Å}$$
$$m = 0.511 10^6 eV c^{-2}$$
$$step\ size\ h\ = 0.03\ \text{Å}$$
$$r_o = 0.000001 \text{Å}$$
$$e = 3.795 \sqrt{eV \text{Å}}$$

```scilab
// To solve the radial part of schrodinger equation for hydrogen atom
//constants used
clc
clear

h_bar=1973 // electron volt *angstrom / c
m = 0.511*10^(6)  // ev/c2
h = 0.03 //angstrom
A= -(h_bar)^(2)/(2*m*h^(2))
ro=0.000001
e=3.795  //(electron volt * angstrom)^(1/2)
n=input("enter the order of matrix = ")
M=zeros(n:n)

for i=1:n
    r(i,1)=ro + i*h
    B(i,1)=(h_bar)^(2)/(m*h^(2)) - e^(2)/r(i,1)
    M(i,i)=B(i,1)
    if(i<n)
        M(i,i+1)=A
        M(i+1,i)=A
    end

  end
[V,E]=spec(M)
[a,b]=max(V(:,1))
L=[8,12,25,35]
for j=1:4

for i=1:n
    if(r(i,1)<L(1,j)) then
        x(i,1)=r(i,1)
        v(i,j)=V(i,j)
    end
end
   subplot(2,2,j)
   plot(x,v(:,j),'r')
   plot(x,diag(zeros(length(x),length(x))),'b')

   xlabel('$\huge radial \medspace distance \medspace r(\AA) $')
   ylabel('$\huge \mathcal{U}(r) $')

end

/*  OUTPUT FOR ENERGY EIGENVALUES AND BOHR RADIUS

--> disp(r(b,1))

   0.540001
--> disp(E(1,1))

  -13.602913
--> disp(E(2,2))

  -3.402789
--> disp(E(3,3))

  -1.5125213
--> disp(E(4,4))

  -0.850827

  */
```
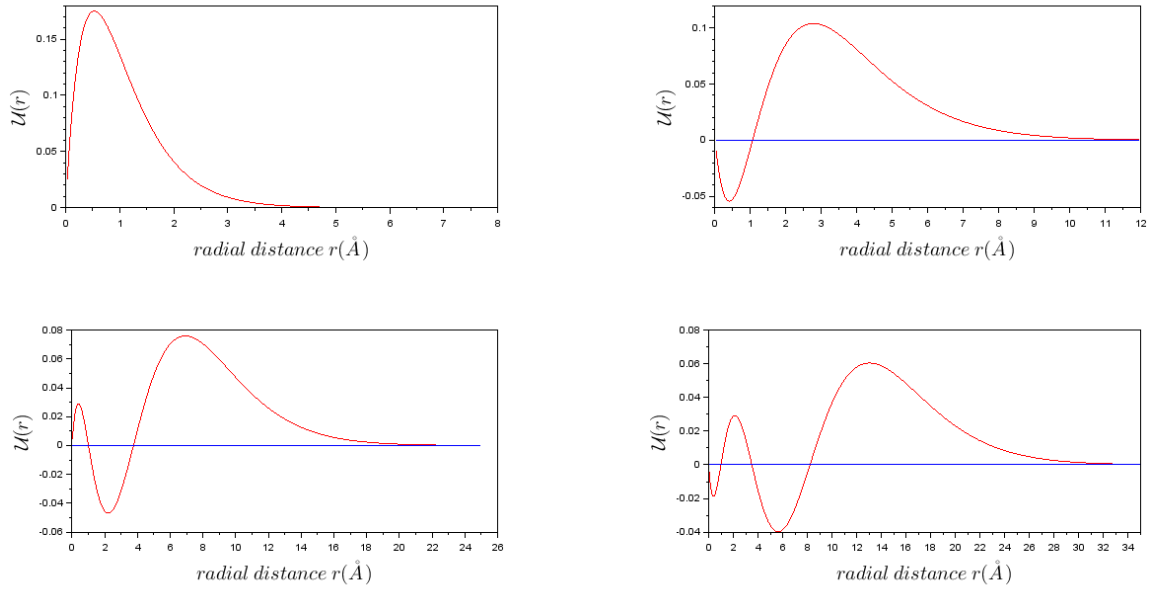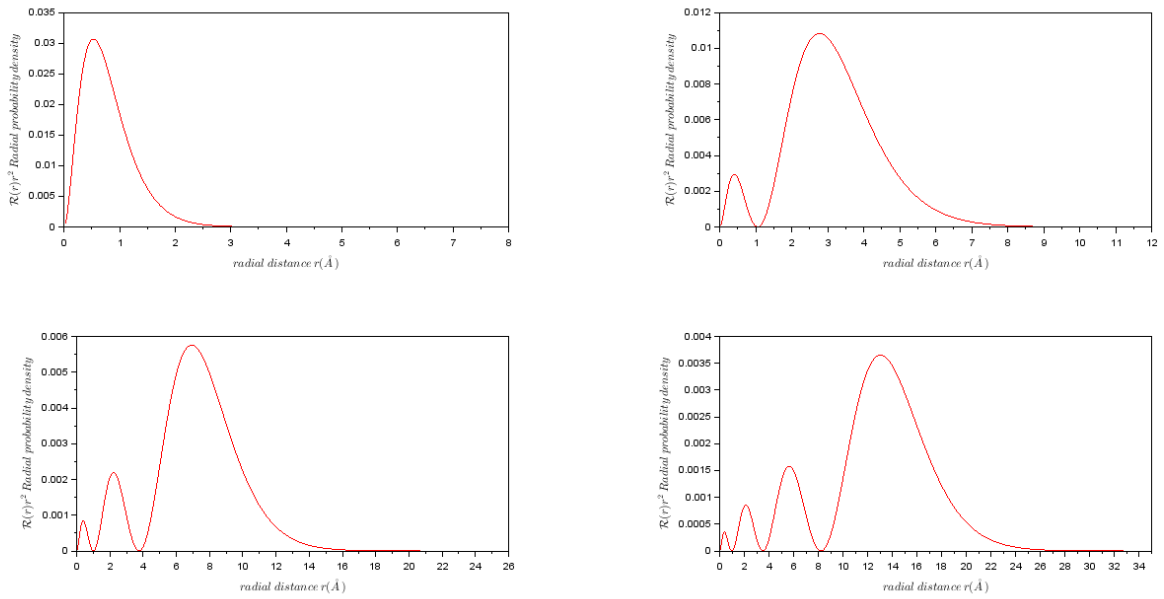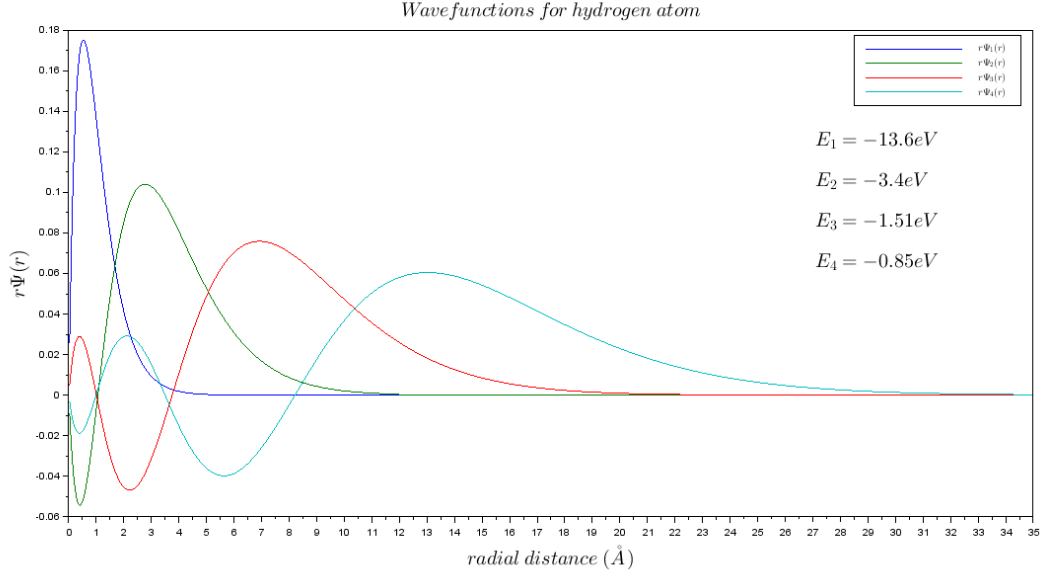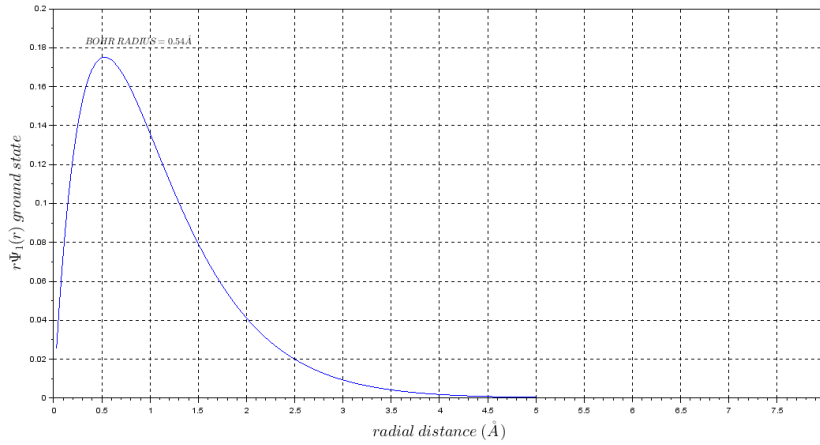
Figure 6: *Numerical solution to first four radial wavefunctions*

Figure 7: *Probability density plot for first four radial wavefunction obtained numerically*

Figure 8: *Wavefunction with respective energies*

Figure 9: *ground state solution with bohr radius*

5 Atom under Screened-Coulombic Potential

Now, We consider the atom under Screened Coulombic potential given by,

$$\mathcal{V}(r) = \frac{-e^2}{r} exp\left(\frac{-r}{a}\right)$$

where $a = \{3, 5, 7\}$

we now solve the TISE $\boxed{\hat{\mathcal{H}}\Psi_n = E_n\Psi_n}$ for the given values of a in the ground state .

AIM: To solve the above TISE for screened coulombic potential for various values of a and plot the solution and their respective eigen-energies UNITS USED: same as previous scilab program
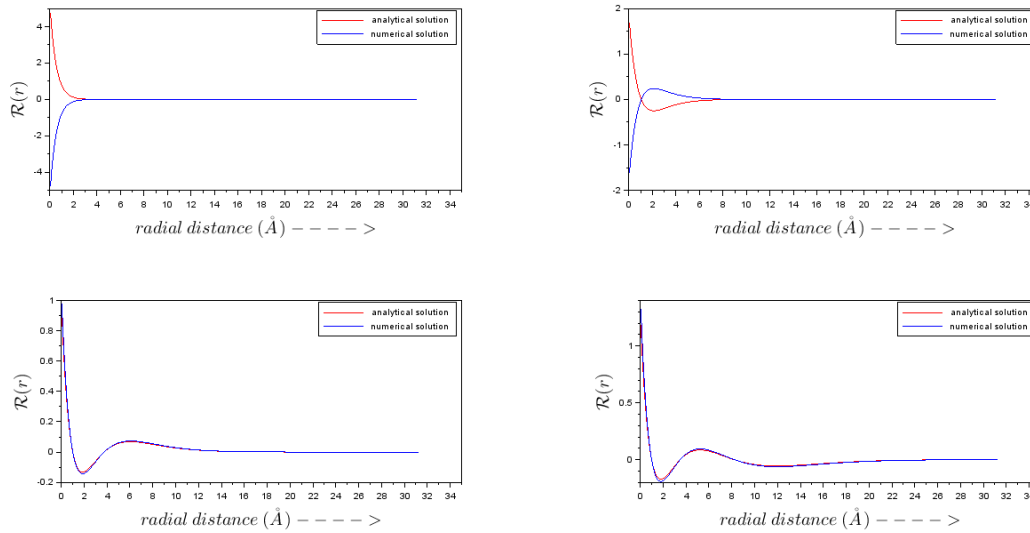
Figure 10: *plot of* $\mathcal{R}_{1,0}, \mathcal{R}_{2,0}, \mathcal{R}_{3,0}, \mathcal{R}_{4,0}$ *versus r*

```
             SCILAB CODE For SCREENED COULOMBIC POTENTIAL

// To solve the radial part of schrodinger equation for an atom with screened coulomb potential
//constants used
clc
clear

h_bar=1973 // electron volt *angstrom / c
m = 0.511*10^(6)  // ev/c2
h = 0.008 //angstrom
A= -(h_bar)^(2)/(2*m*h^(2))
ro=0.000001
e=3.795  //(electron volt * angstrom)^(1/2)
n=input("enter the order of matrix = ")
for p=1:3
M=zeros(n:n)
 ao= [3,5,7]
for i=1:n
    r(i,1)=ro + i*h
    B(i,1)=(h_bar)^(2)/(m*h^(2)) - (e^(2)*exp(-r(i,1)/ao(p)))/r(i,1)
    M(i,i)=B(i,1)
    if(i<n)
        M(i,i+1)=A
        M(i+1,i)=A
    end

    end

[V,E]=spec(M)
// numerical solution plot
    subplot(2,2,p)
    xlabel('$\huge radial \medspace distance \medspace (\AA) $')
    ylabel('$\huge U(r)  $')
    xstring(2.5,max(V(:,1))/2,["$\huge E_{ground} = \medspace \medspace \medspace
    \medspace \medspace \medspace \medspace \medspace \medspace \medspace eV$"])
    xnumb(3.5,max(V(:,1))/2,E(1,1))
for i=1:n
    plot(r(i,1),V(i,1),'o')
end
end
```
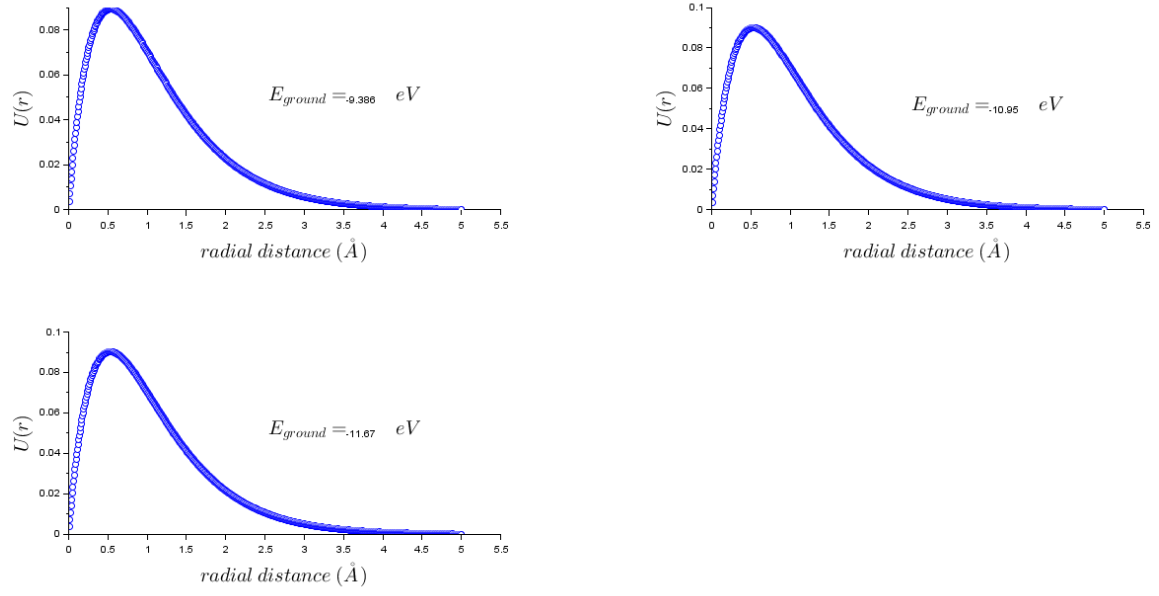
Figure 11: *Solution of TISE for given values a under anharmonic potential*

value of a	$E_{ground}(eV)$
3	-9.386
5	-10.95
7	-11.67

6 Atom under Anharmonic Potential

Now , Consider the atom under the anharmonic potential given by

$$\mathcal{V}(r) = \frac{1}{2}kr^{2c} + \frac{1}{3}br^3$$

where b = $\{0, 10, 30\}$ MeV respectively
UNITS USED:

$$\hbar c = 197.3 MeV\ fm$$

$$m = 940 MeV c^{-2}$$

$$step\ size\ h = 0.008 fm$$

$$r_o = 0.000001 fm$$

$$e = 3.795\sqrt{0.1}\sqrt{MeV fm}$$

```
                 SCILAB CODE FOR ATOM UNDER AN ANHARMONIC OSCILLATOR

// To solve the s wave radial equation for an atom with anharmonic potential
//constants used
clc
clear

h_bar=197.3 // Melectron volt *fm / c
m = 940  // Mev/c2
h = 0.008 //fm
A= -(h_bar)^(2)/(2*m*h^(2))
ro=0.000001
e=3.795*sqrt(0.1)  //(Melectron volt * angstrom)^(1/2)
n=input("enter the order of matrix = ")
for p=1:3

M=zeros(n:n)
// potential constants
k=100 , b= [0,10,30]
for i=1:n
    r(i,1)=ro + i*h
    B(i,1)=(h_bar)^(2)/(m*h^(2)) + ( (0.5)*k*r(i,1)^(2)  +  (1/3)*b(p)*r(i,1)^(3))
    M(i,i)=B(i,1)
    if(i<n)
        M(i,i+1)=A
        M(i+1,i)=A
    end

    end

[V,E]=spec(M)
// analytical solution plot
subplot(2,2,p)
xlabel('$\huge radial \medspace distance \medspace  (fm) $')
ylabel('$\huge U(r)^{2}  $')
xstring(3.5,max(V(:,1).*V(:,1))/2,["$\huge E_{ground}= $"])
xnumb(4.5,max(V(:,1).*V(:,1))/2,E(1,1))
for i=1:n
    plot(r(i,1),(V(i,1))^(2),'o')

end
end
```
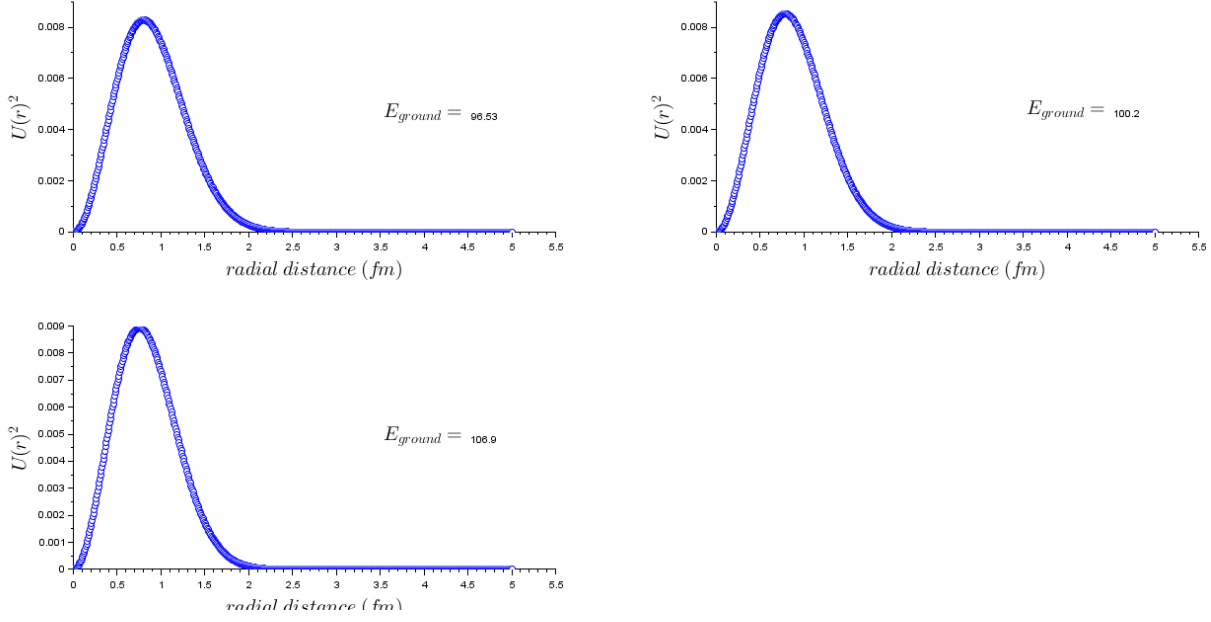
value of b	$E_{ground}(eV)$
0	96.53
10	100.2
30	106.9

Figure 12: $U^2(r) \, VS \, r \, - \, solved \, numerically \, for \, various \, values \, of \, b$

7 Molecules under Morse Potential

Morse potential is a convenient model for interatomic potential energy of a diatomic molecule , it includes the effects of bond breaking and justifies the existence of bound states. the potential energy function is given by the following expression

$$V(r) = D_e \left(1 - e^{-\alpha(r-r_o)^2}\right)^2$$

where

$$\alpha = \sqrt{\frac{k_e}{2D_e}}$$

where k_e is the force constant at the minimum of potential V . therefore

$$k_e = \left(\frac{d^2V}{dr^2}\right)_{r=r_o}$$

and D_e is the potential depth from v=0.
here is the given data for three molecules

molecule	α	D_e	r_o	$\mu_{reducedmass}$
Nacl	2.448	4.62 eV	2.36	12877.09MeV
H_2	1.92	4.75eV	0.75	469.4MeV
HCl	1.8594	4.62eV	1.28	913.9MeV

7.1 Solving Schrodinger equation for H_2 ,Nacl amd HCl molecule using FDM

AIM: solve the TISE for above specified molecules and solve for the energy eigenvalues of molecules using the above specified parameters and potential

```
                        SCILAB CODE FOR MORSE POTENTIAL
 // To solve the shrodinger equation of a molecule under morse potential
//constants used
clc
clear

// UNIVERSAL CONSTANTS
h_bar=1973
h = 0.008
ro=0.000001
e=3.795

n=input("enter the order of matrix = ")
M=zeros(n:n)

// DATA FOR A PARTICULAR MOLECULE
disp("  ENTER 1 FOR Hcl    ")
disp("  ENTER 2 FOR H2     ")
disp("  ENTER 3 FOR NaCl  ")
p=input("enter the choice of molecule =  ")
select p

case 1 then
D=4.62
alpha=1.859375
Ro=1.28
m = 913.9*10^(6)

case 2  then
D=4.75
alpha=1.92
Ro=0.75
m=463.687*(10)^(6)

case 3 then
D=4.62
alpha=2.448
Ro=2.36
m=12877.09*(10)^(6)
end

//solving the schrodinger equation
A= -(h_bar)^(2)/(2*m*h^(2))
for i=1:n
    r(i,1)=ro + i*h
    x(i,1)= (r(i,1) - Ro)
B(i,1)=(h_bar)^(2)/(m*h^(2)) + D*(1 - exp(- alpha*x(i,1)))^(2)
    M(i,i)=B(i,1)
    if(i<n)
        M(i,i+1)=A
        M(i+1,i)=A
    end
    end
```

```
[V,E]=spec(M)

//plotting the solution

select p

case 1  then
xtitle("$\huge MORSE \medspace POTENTIAL  \medspace (MOLECULE) \medspace WITH
          \medspace RESPECTIVE \medspace ENERGY \medspace EIGENVALUES$")
xlabel('$\huge internuclear \medspace distance \medspace (\AA)\medspace  ---- >$')
ylabel('$\huge U(r) \medspace morse \medspace potential(eV) \medspace ---- > $')
xstring(3.6,9.5,["$\huge constants \medspace used :$"])
xstring(3.6,9,["$\huge \alpha = 1.8594$"])
xstring(3.6,8.5,["$\huge \mu_{HCL} = 913.9 MeV$"])
xstring(3.6,8,["$\huge M_{H} = 940 MeV \medspace and \medspace M_{Cl} = 33.02 GeV$"])
xstring(3.6,7.5,["$\huge r_{o} = 1.28\AA : equilibrium \medspace bond \medspace length$"])
xstring(3.6,7,["$\huge  D_{e} = 4.62 eV \medspace: potential \medspace well-depth  $"])
xstring(3.6,6.5,["$\huge D_{o} = 4.4375eV \medspace : \medspace calculated \medspace
                    dissociation \medspace energy$"])
k=1


for i=1:500

    R(i,1)=0.8 +i*h
    plot(R(i,1),D*(1 - exp(- 1.859375*(R(i,1)-1.28)))^(2),'.')



end
for i=1:n
for j=1:500
if(D*(1 - exp(- 1.859375*(R(j,1)-1.28)))^(2)<E(i,i)) then

e(k,1)=R(j,1)
k=k+1
end

end

plot(e,diag(E(i,i)*ones(k-1,k-1)),'r')
if(i<8) then

xnumb(e(1,1)-0.3,E(i,i)-0.2,E(i,i))
xstring(e(1,1)-0.15,E(i,i)-0.2,["eV"])
end
k=1
if(E(i,i)>D) break
    end
end

case 2    then


xtitle("$\huge MORSE \medspace POTENTIAL \medspace (H_{2} \medspace MOLECULE)
        \medspace WITH \medspace RESPECTIVE \medspace ENERGY \medspace EIGENVALUES$")
xlabel('$\huge internuclear \medspace distance \medspace (\AA)\medspace  ---- >$')
ylabel('$\huge U(r) \medspace morse \medspace potential(eV) \medspace ---- > $')
xstring(2.6,8.5,["$\huge constants \medspace used :$"])
xstring(2.6,8,["$\huge \alpha = 1.92 \AA^{-1}$"])
xstring(2.6,7.5,["$\huge \mu_{H_{2}} = 469.4 MeV$"])
xstring(2.6,7,["$\huge M_{H} = 938.8 MeV $"])
```

```
xstring(2.6,6.5,["$\huge r_{o} = 0.75\AA : equilibrium \medspace bond \medspace length$"])
xstring(2.6,6,["$\huge  D_{e} = 4.75 eV \medspace: potential \medspace well-depth  $"])
xstring(2.6,5.5,["$\huge D_{o} = 4.48eV \medspace : \medspace calculated \medspace
            dissociation  \medspace energy$"])
k=1


for i=1:350


    R(i,1)=0.3 +i*h
    plot(R(i,1),D*(1 - exp(- 1.92*(R(i,1)-0.75)))^(2),'.')




end
for i=1:n
for j=1:350
if(D*(1 - exp(- 1.92*(R(j,1)-0.75)))^(2)<E(i,i)) then

e(k,1)=R(j,1)
k=k+1
end

end

plot(e,diag(E(i,i)*ones(k-1,k-1)),'r')
if(i<8) then

xnumb(e(1,1)-0.3,E(i,i)-0.2,E(i,i))
xstring(e(1,1)-0.15,E(i,i)-0.2,["eV"])
end
k=1
if(E(i,i)>D) break
    end
end

xlabel('$\huge Internuclear \medspace Distance \medspace r(\AA) ------>$')
ylabel('$\huge Potential \medspace energy \medspace  function \medspace U(r)
                \medspace -----> $')

xtitle("$\huge morse \medspace potential \medspace with \medspace eigenfunctions
        \medspace for  \medspace H_{2} $")

case 3 then

xtitle("$\huge MORSE \medspace POTENTIAL \medspace (NaCl \medspace MOLECULE)
            \medspace WITH \medspace RESPECTIVE \medspace ENERGY
             \medspace EIGENVALUES$")
xlabel('$\huge internuclear \medspace distance \medspace (\AA)\medspace  ---- >$')
ylabel('$\huge U(r) \medspace morse \medspace potential(eV) \medspace ---- > $')
xstring(4.6,7.8,["$\huge constants \medspace used :$"])
xstring(4.6,7.5,["$\huge \alpha = 2.448\AA$"])
xstring(4.6,7,["$\huge \mu_{NaCl} = 12877.09 MeV$"])
xstring(4.6,6.5,["$\huge M_{Na} = 940 MeV \medspace and \medspace M_{Cl} = 33.02 GeV$"])
xstring(4.6,6,["$\huge r_{o} = 2.36\AA : equilibrium \medspace bond \medspace length$"])
xstring(4.6,5.5,["$\huge  D_{e} = 4.62 eV \medspace: potential \medspace well-depth  $"])
xstring(4.6,5,["$\huge D_{o} = 4.558eV \medspace : \medspace calculated \medspace
                    dissociation \medspace energy$"])
k=1
for i=1:500
    R(i,1)=2 +i*h
    plot(R(i,1),D*(1 - exp(- 2.448*(R(i,1)-2.36)))^(2),'.')
end
```

```
for i=1:n
for j=1:500
if(D*(1 - exp(- 2.448*(R(j,1)-2.36)))^(2)<E(i,i)) then

e(k,1)=R(j,1)
k=k+1
end

end

plot(e,diag(E(i,i)*ones(k-1,k-1)),'r')
if(i<8) then

xnumb(4,0.5*i,E(i,i))
xstring(4.2,0.5*i,["$eV$"])
end
k=1
if(E(i,i)>D) break
    end
end

xlabel('$\huge Internuclear \medspace Distance \medspace r(\AA) ------>$')
ylabel('$\huge Potential \medspace energy \medspace  function  \medspace U(r) \medspace -----> $')

xtitle("$\huge morse \medspace potential \medspace with \medspace eigenfunctions $")

end
```
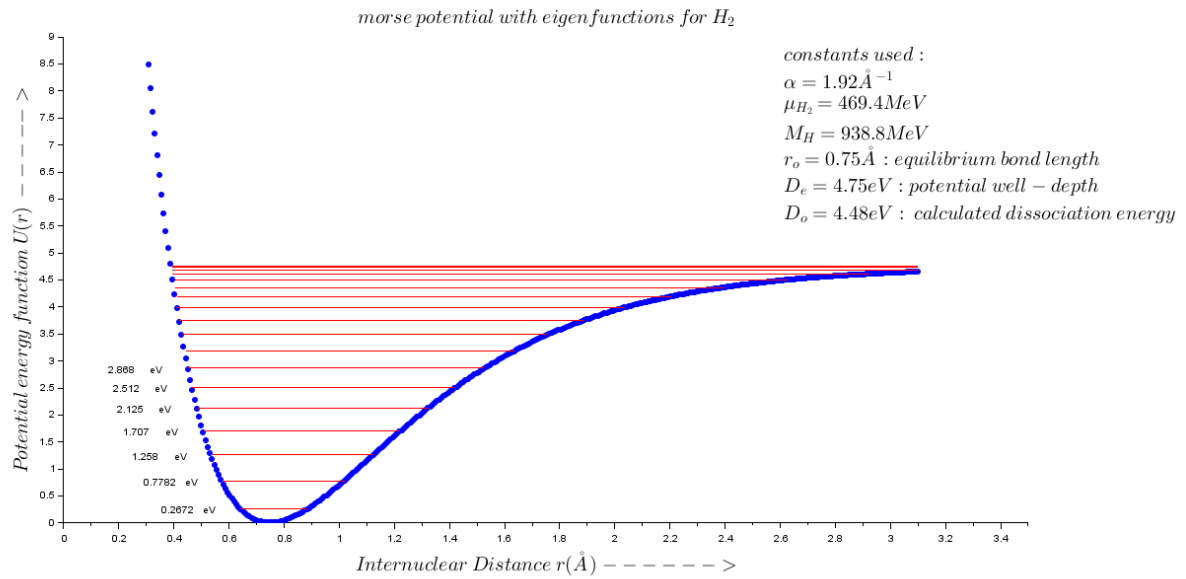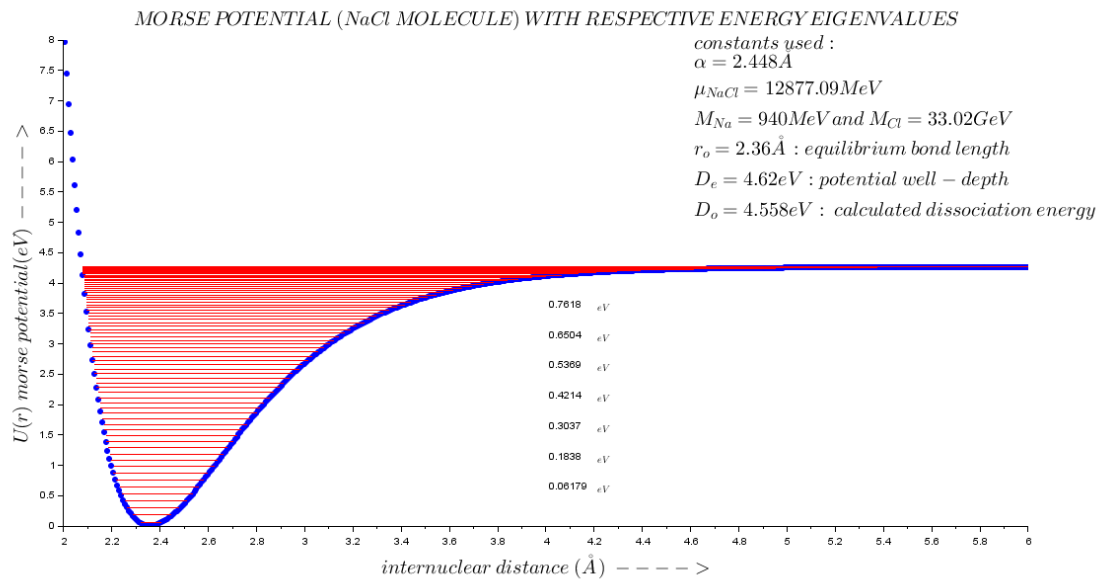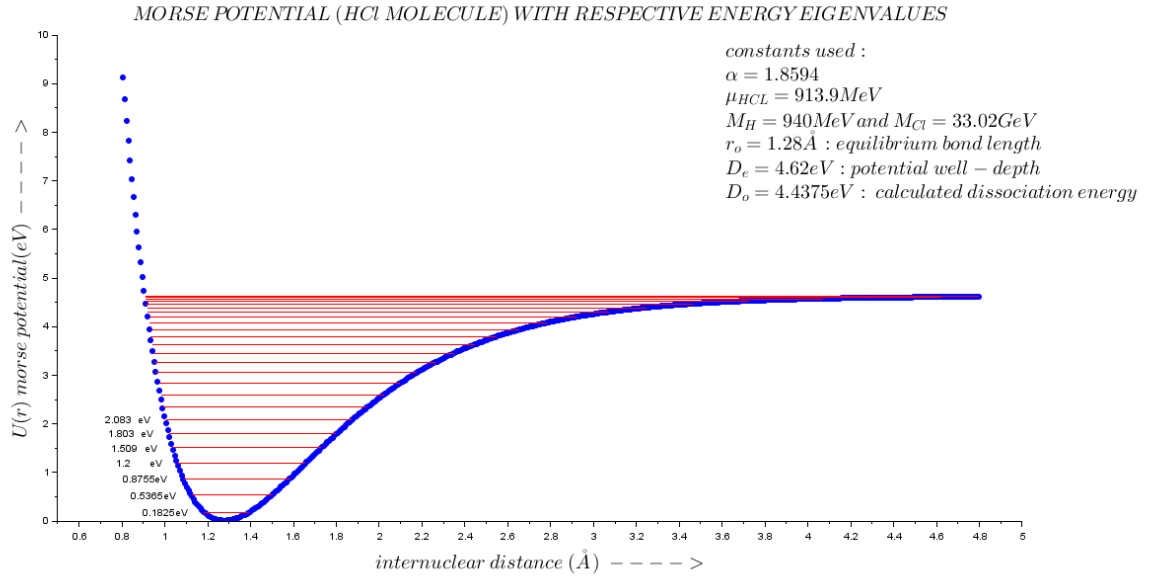
7.1.1 ENERGY EIGENVALUES OBTAINED FOR THE GIVEN MOLECULES

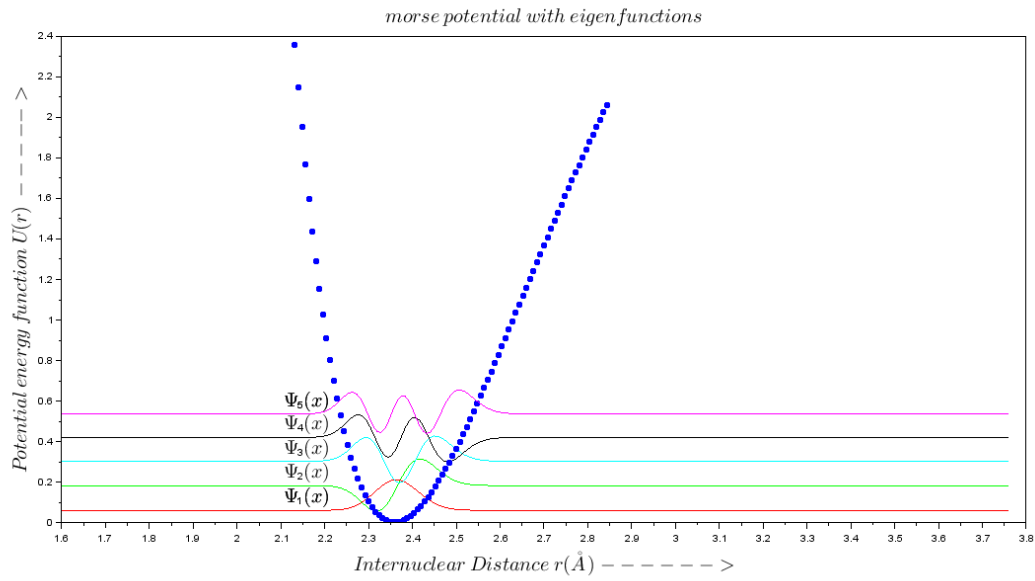**Figure 13:** *energy eigenvalues in H_2 molecule*

Figure 14: *energy eigenvalues in NaCl molecule*

Figure 15: *energy eigenvalues in HCl molecule*

7.1.2 wavefunctions for the corresponding eigenvalues of the 3 molecules

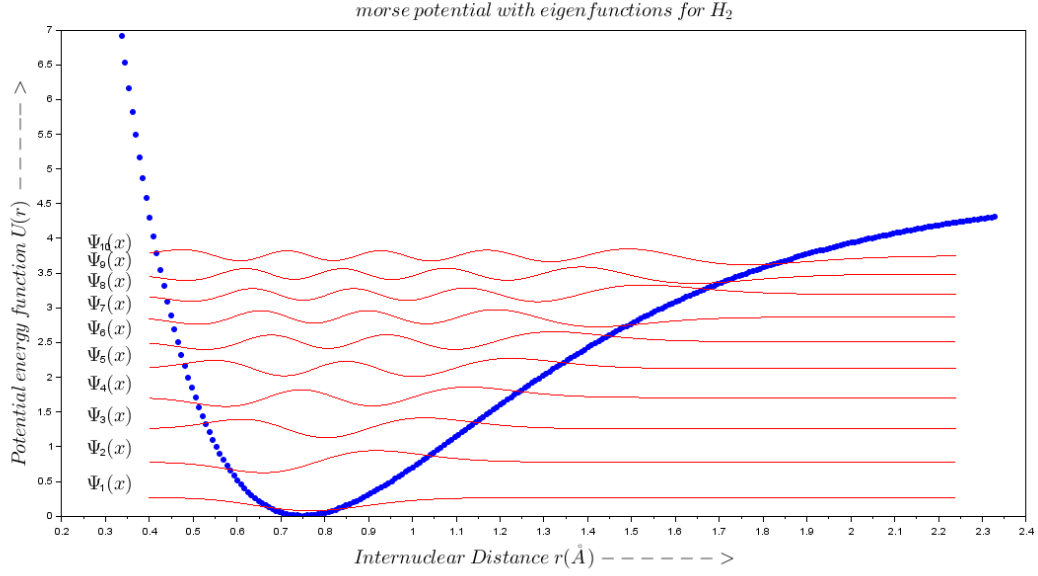**Figure 16:** *wavefunctions for H_2 molecule*

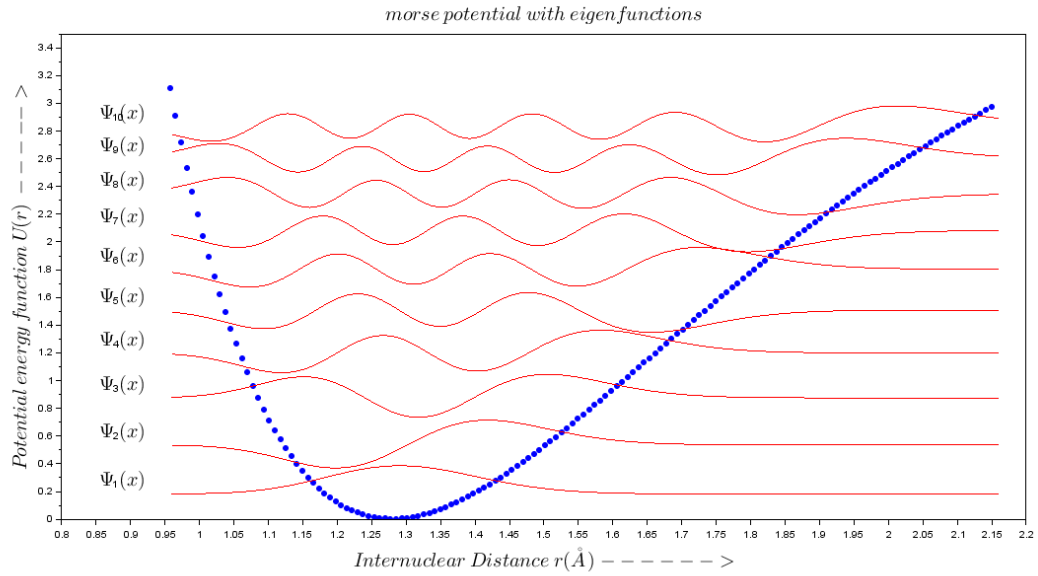**Figure 17:** *wavefunctions for HCl molecule*

Figure 18: *wavefunction for NaCl molecule*

8 $\mathcal{R}_{(2,1)}$ solution to the Schrodinger equation for hydrogen atom

Refering to the below equation from previous program we have

$$\frac{d^2U}{dr^2} + \left[\frac{2\mu e^2}{r\hbar^2} + \frac{2\mu E}{\hbar^2} - \frac{l(l+1)}{r^2}\right] U = 0$$

So far we have numerically solved the equation for 1s , 2s , 3s , 4s orbital and obtained their radial wavefunctions and their respective energy values. Now for 2p orbital we $l = 1$ so our above becomes

$$\frac{d^2U}{dr^2} + \left[\frac{2\mu e^2}{r\hbar^2} + \frac{2\mu E}{\hbar^2} - \frac{2}{r^2}\right] U = 0$$

which only modifies the Hamiltonian slightly by adding a r-dependent term to it. this equation can again be solved easily using FDM.

AIM: To solve the radial schrodinger equation for hydrogen atom for $(l = 1)$ (2p-orbital).

UNITS USED : Same as previous s-wave program.
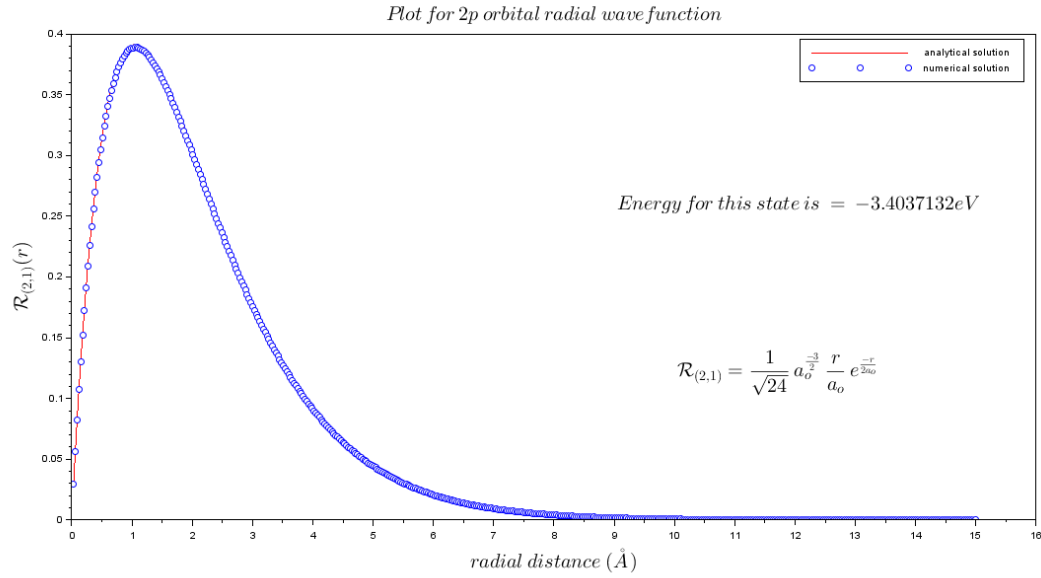
Figure 19: *Analytical and numerical solution plot for $\mathcal{R}_{(1,2)}$*

```
                        SCILAB CODE FOR THE PROGRAM

// To solve the radial part of schrodinger equation for hydrogen atom
//constants used
clc
clear
//value of n = 2000
l=1
h_bar=1973 // electron volt *angstrom / c
m = 0.511*10^(6)  // ev/c2
h = 0.03 //angstrom
A= -(h_bar)^(2)/(2*m*h^(2))
ro=0.000001
e=3.795  //(electron volt * angstrom)^(1/2)
n=input("enter the order of matrix = ")
M=zeros(n:n)
c=0
for i=1:n
    r(i,1)=ro + i*h
    B(i,1)=(h_bar)^(2)/(m*h^(2)) - e^(2)/r(i,1) + (l*(l+1))/(r(i,1)^(2))*(((h_bar)^(2))/(2*m))
    M(i,i)=B(i,1)
    if(i<n)
        M(i,i+1)=A
        M(i+1,i)=A
    end
    R(i,1)=(1/sqrt(24))*(0.528)^(-3/2)*(r(i,1)/0.528)*%e^(-r(i,1)/(2*0.528))

    end

[V,E]=spec(M)
plot(r,R(:,1),'r')
for i=1:n
plot(r(i,1),5.75*V(i,1)/r(i,1),'o')
end

xtitle("$\huge Plot \medspace for \medspace 2p \medspace orbital \medspace
                radial \medspace wavefunction $")
xstring(10,0.1,["$\huge\mathcal{R}_{(2,1)} = \frac{1}{\sqrt{24}}a_{o}^{\frac{-3}{2}}
                                \frac{r}{a_{o}}e^{\frac{-r}{2a_{o}}}$"])
xstring(9,0.25,["$\huge Energy \medspace for \medspace this \medspace state
            \medspace is \medspace = \medspace -3.4037132eV$"])
L=legend(["analytical solution";"numerical solution"])
xlabel('$\huge radial \medspace distance \medspace ( \AA) $')
ylabel('$\huge \mathcal{R}_{(2,1)}(r) $')
/*
//ploting numerical solution
S=[4.5,4.3,4.8,10]
// analytical solution plot
for k=1:4

    subplot(2,2,k)
    plot(r,R(:,k),'r')
for i=1:n

    psi(i,k)=S(1,k)*V(i,k)/r(i,1)
end
  plot(r,psi(:,k),'b')
xlabel('$\huge radial \medspace distance \medspace (\AA)  ---- >$')
ylabel('$\huge \mathcal{R}(r) $')
L=legend(["analytical solution"; "numerical solution"])
end
```

Appendix

Consider a second order linear differential equation given by :

$$\frac{d^2y}{dx^2} + \mathcal{P}(x)\frac{dy}{dx} + \mathcal{Q}(x)y = \mathcal{R}(x)$$

for $y \in \Omega^9$

where $\mathcal{P}(x)$, $\mathcal{Q}(r)$ and $\mathcal{R}(x)$ are assumed to be nice function in the domain of solution of the differential equation.

For the solution to exist we assume the solution $y(x)$ is atleast twice differentiable function.

Therefore we can have a taylor expansion of the assumed solution $y(x)$ at x_{i+1} and $x_{i-1} \in \Omega$

$$y(x_i) = y(x_{i-1}) - \left(\frac{dy}{dx}\right)_{x_{i-1}} h + \frac{1}{2}\left(\frac{d^2y}{dx^2}\right)_{x_{i-1}} h^2 + \mathcal{O}(h^3)$$

similarily

$$y(x_i) = y(x_{i+1}) + \left(\frac{dy}{dx}\right)_{x_{i+1}} h + \frac{1}{2}\left(\frac{d^2y}{dx^2}\right)_{x_{i+1}} h^2 + \mathcal{O}(h^3)$$

from the above two equations we have :

$$\left(\frac{dy}{dx}\right)_{x_i} = \frac{y(x_{i+1}) - y(x_{i-1})}{2h} + \mathcal{O}(h^2)$$

and

$$\left(\frac{d^2y}{dx^2}\right)_{x_i} = \frac{y(x_{i+1}) - 2y(x_i) + y(x_{i-1})}{h^2} + \mathcal{O}(h^2)$$

So the given differential equation can be written as :

$$\frac{y(x_{i+1}) - 2y(x_i) + y(x_{i-1})}{h^2} + \mathcal{P}(x_i)\frac{y(x_{i+1}) - y(x_{i-1})}{2h} + \mathcal{Q}(x_i)y(x_i) = \mathcal{R}(x_i)$$

therefore the equation becomes:

$$y(x_{i+1})\left(\frac{1}{h^2} + \frac{\mathcal{P}(x_i)}{2h}\right) + y(x_i)\left(\frac{-2}{h^2} + \mathcal{Q}(x_i)\right) + y(x_{i-1})\left(\frac{-\mathcal{P}(x_i)}{2h} + \frac{1}{h^2}\right) = \mathcal{R}(x_i)$$

Now i runs from 1 to n-1 to cover the whole domain of definition Ω.

For the boundary conditions $y(x_o)$ and $y(x_n)$ the above equation forms a linear set of n equation which can be solved by linear algebraic method like Gauss Seidel , Gauss Elimination etc.

---

[9] domain of solution