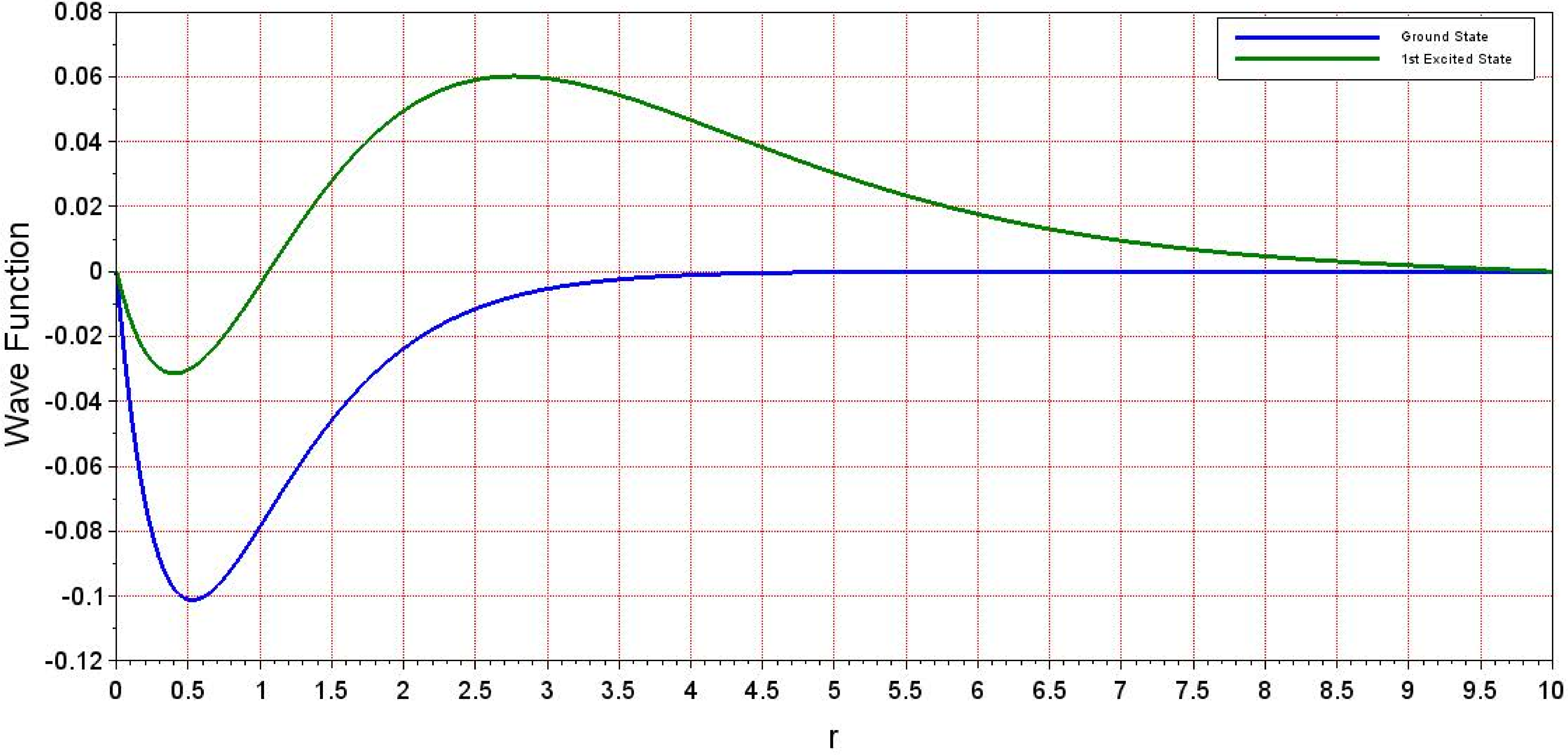
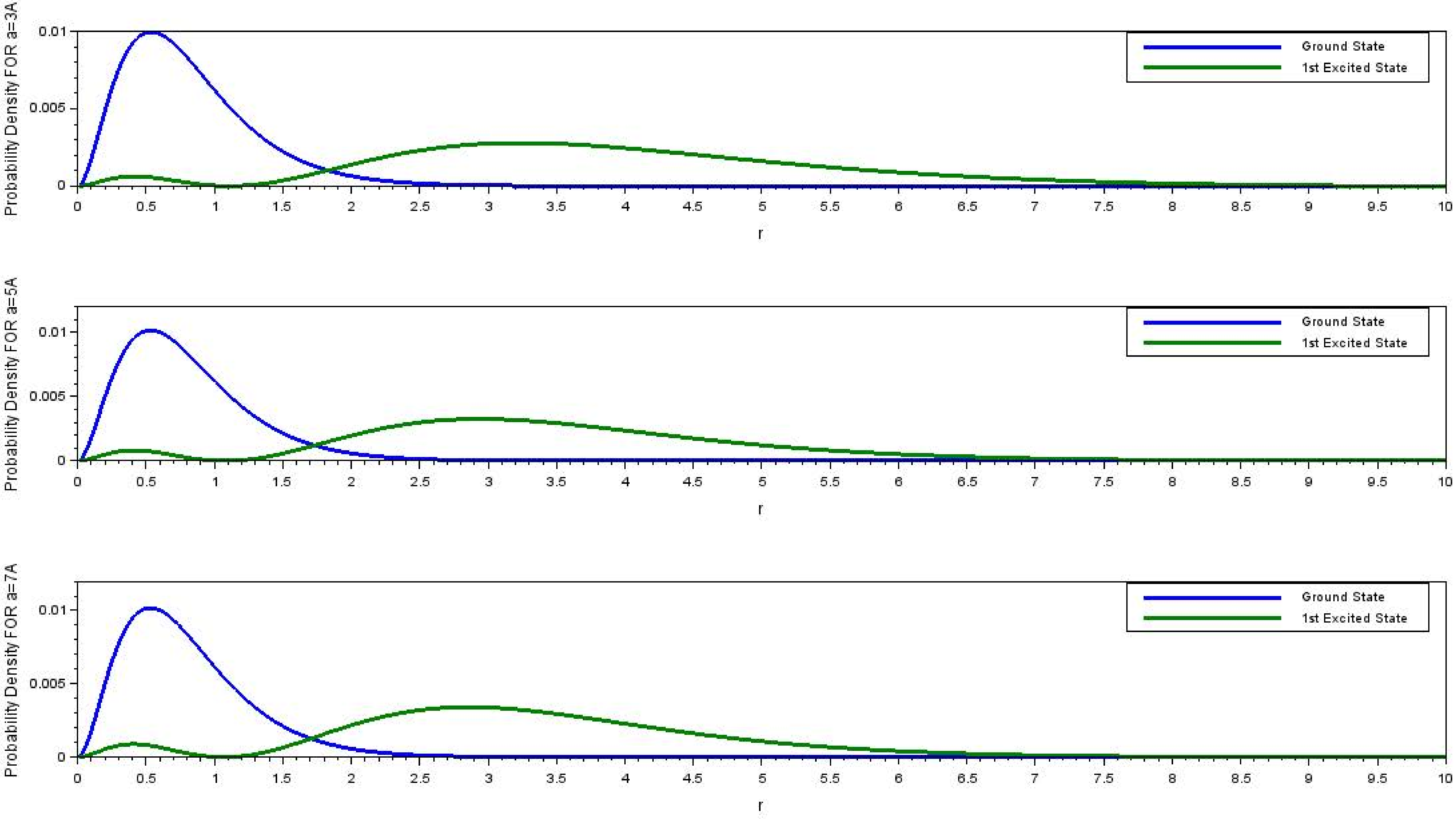
```
//SOLVE Schrodinger equation for H-atom in Coulomb's potential (using Finite Difference Method)

clc; clear; clf;    //Clearing console, variables and fig

//Describing Constants : h, e & m
h=1973; e=3.795; m=0.511e6;

rmin=1e-10; rmax=10; n=1000;
r=linspace(rmin,rmax,n);    //linspace = linearly spaced vector
d=r(2)-r(1);    //Incremental Step Size

//Defining Coulomb Potential using given formula
V=zeros(n,n);
for i=1:n
    V(i,i)=(-(e^2)/r(i));
end

//Defining Kinetic Energy using given formula
K=eye(n,n)*(-2);
for i=1:(n-1)
    K(i,i+1)=1;
    K(i+1,i)=1;
end

//Defining Hamiltonian Matrix using given formula
H=(-(h^2)/(2*m*d^2))*K+V;

//Evaluating Eigenvalues & Eigenvectors of H matrix using "spec" function
[U,EV]=spec(H); //U=Eigenvectors(used to plot Wavefunction) & EV=Eigenvalues(used to find Energies)
E=diag(EV) //Extracting diagonal elements of EV matrix using "diag" function
format(6)   //changing number format

//Since 1st eigenvalue is absurd, hence we took n=2 as GS and n=3 as 1st Excited state
disp("Grounded State Energy (in eV)",E(2),"1st Excited State Energy (in eV)",E(3))

//Plotting Probability Densities at GS State & 1st Excited State
```

```
plot(r',[U(:,2)**2,U(:,3)**2],"linewidth",3)
legend("Ground State","1st Excited State",1)
xset("font size",4);
xlabel("r","fontsize",5);
ylabel("Probability Density","fontsize",5);
xgrid(5);

b= h^2/(e^2*m)
disp("The Bohr radius is (in angstrom) :",b)

scf(2)
for i=1:5:n
        subplot(2,2,1)


        plot(r(i),U(i,2),"r*","linewidth",2,"markersize",2)
        plot(r(i),U(i,3),"b-","linewidth",2,"markersize",2)
        xgrid()
        legend("Ground State","First Excited State")
        ylabel("Wave Function u(r)")
        xlabel("r")
        title('Numerical')

        subplot(2,2,2)


        plot(r(i),U(i,2)**2,"r*","linewidth",2,"markersize",2)
        plot(r(i),U(i,3)**2,"b-","linewidth",2,"markersize",2)
        xgrid()
        legend("Ground State","First Excited State")
        ylabel("Probability Density u(r)*u(r)")
        xlabel("r")
        title('Numerical')

        subplot(2,2,3)

        x = [0:0.1:10]
        plot((2/b^(3/2))*x.*exp(-x/b),'r')
        plot( 1/b^(3/2)*(x.*exp(-x/(2*b)) - 1/(2*b)*x^2.*exp(-x/(2*b))))
        xgrid()
        legend("Ground State","First Excited State")
        ylabel("Wavefunction u(r)")
        xlabel("r")
        title('Theoretical')

        subplot(2,2,4)

        plot(((2/b^(3/2))*x.*exp(-x/b))^2,'r')
        plot((1/b^(3/2)*(x.*exp(-x/(2*b)) - 1/(2*b)*x^2.*exp(-x/(2*b))))^2)
        xgrid()
        legend("Ground State","First Excited State")
        ylabel("Probability Density u(r)*u(r)")
        xlabel("r")
        title('Theoretical')
end
```


Ground State
1st Excited State
Wave Function
0.08
0.06
0.04
0.02
0
-0.02
-0.04
-0.06
-0.08
-0.1
-0.12
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
5.5
6
6.5
7
7.5
8
8.5
9
9.5
10
r

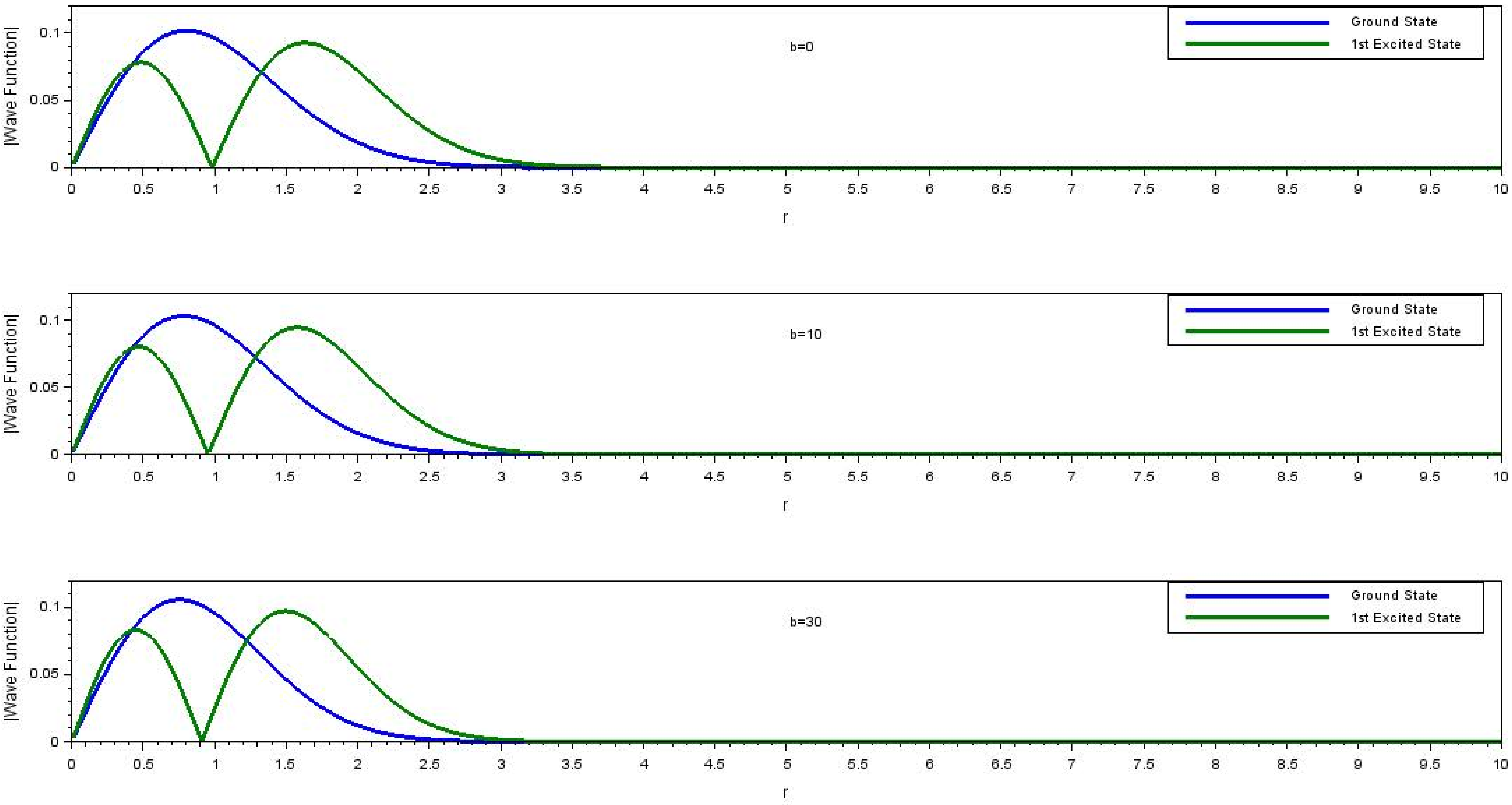
```
//SOLVE Schrodinger equation for H-atom in Screened Coulomb potential (using Finite Difference Method)

clc; clear; clf;    //Clearing console, variables and fig

//Describing Constants : h, e, m, a1, a2, a3
h=1973; e=3.795; m=0.511e6; a1=3; a2=5; a3=7;

rmin=0.01; rmax=10; n=1000;
r=linspace(rmin,rmax,n);    //linspace = linearly spaced vector
d=r(2)-r(1);    //Incremental Step Size

//Defining Potential Energy Matrix
V1=zeros(n,n);
for i=1:n
    V1(i,i)=-(e^2)*exp(-r(i)/a1)/r(i);
end
V2=zeros(n,n);
for i=1:n
    V2(i,i)=-(e^2)*exp(-r(i)/a2)/r(i);
end
V3=zeros(n,n);
for i=1:n
    V3(i,i)=-(e^2)*exp(-r(i)/a3)/r(i);
end

//Defining Kinetic Energy using given formula
K=eye(n,n)*(-2);
for i=1:(n-1)
    K(i,i+1)=1;
    K(i+1,i)=1;
end

//Defining Hamiltonian Matrix using given formula
H1=(-(h^2)/(2*m*d^2))*K+V1;
H2=(-(h^2)/(2*m*d^2))*K+V2;
H3=(-(h^2)/(2*m*d^2))*K+V3;

//Evaluating Eigenvalues & Eigenvectors of H matrix using "spec" function
[U1,EV1]=spec(H1);
[U2,EV2]=spec(H2);
[U3,EV3]=spec(H3);
```

```
E1=diag(EV1);
E2=diag(EV2);
E3=diag(EV3);
format(6)   //changing number format

disp("Grounded State Energy (in eV) for a=3A, 5A and 7A",[E1(1) E2(1) E3(1)],"1st Excited State Energy (in eV)for a=3A, 5A and 7A",[E1(2) E2(2) E3(2)])

//Plotting Probability Densities at GS State & 1st Excited State
subplot(3,1,1)
plot(r',[U1(:,1)**2,U1(:,2)**2],"linewidth",3)
legend("Ground State","1st Excited State",1)
xlabel("r","fontsize",2);
ylabel("Probability Density","fontsize",2);
title("a=3A")

subplot(3,1,2)
plot(r',[U2(:,1)**2,U2(:,2)**2],"linewidth",3)
legend("Ground State","1st Excited State",1)
xlabel("r","fontsize",2);
ylabel("Probability Density","fontsize",2);
title("a=5A")

subplot(3,1,3)
plot(r',[U3(:,1)**2,U3(:,2)**2],"linewidth",3)
legend("Ground State","1st Excited State",1)
xlabel("r","fontsize",2);
ylabel("Probability Density","fontsize",2);
title("a=7A")

//OUTPUT :
//"Grounded State Energy (in eV) for a=3A, 5A and 7A"
//
//-9.386  -10.95  -11.67
//
//"1st Excited State Energy (in eV)for a=3A, 5A and 7A"
//
//-0.483  -1.272  -1.747
```


Probability Density FOR a=3A
0.01
0.005
0
Ground State
1st Excited State
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
5.5
6
6.5
7
7.5
8
8.5
9
9.5
10
r
Probability Density FOR a=5A
0.01
0.005
0
Ground State
1st Excited State
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
5.5
6
6.5
7
7.5
8
8.5
9
9.5
10
r
Probability Density FOR a=7A
0.01
0.005
0
Ground State
1st Excited State
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
5.5
6
6.5
7
7.5
8
8.5
9
9.5
10
r

```
//SOLVE Schrodinger equation for H-atom in Screened Anharmonic Oscillator potential (using Finite Difference Method)

clc; clear; clf;    //Clearing console, variables and fig

//Describing Constants : h, k, m, b1, b2, b3
h=197.3; k=100; m=940; b1=0; b2=10; b3=30;

rmin=0.01; rmax=10; n=1000;
r=linspace(rmin,rmax,n);    //linspace = linearly spaced vector
d=r(2)-r(1);    //Incremental Step Size

//Defining Potential Energy Matrix
V1=zeros(n,n);
for i=1:n
    V1(i,i)=(k*(r(i)^2))/2 + (b1*(r(i)^3))/3;
end
V2=zeros(n,n);
for i=1:n
    V2(i,i)=(k*(r(i)^2))/2 + (b2*(r(i)^3))/3;
end
V3=zeros(n,n);
for i=1:n
    V3(i,i)=(k*(r(i)^2))/2 + (b3*(r(i)^3))/3;
end

//Defining Kinetic Energy using given formula
K=eye(n,n)*(-2);
for i=1:(n-1)
    K(i,i+1)=1;
    K(i+1,i)=1;
end

//Defining Hamiltonian Matrix using given formula
H1=(-(h^2)/(2*m*d^2))*K+V1;
H2=(-(h^2)/(2*m*d^2))*K+V2;
H3=(-(h^2)/(2*m*d^2))*K+V3;

//Evaluating Eigenvalues & Eigenvectors of H matrix using "spec" function
[U1,EV1]=spec(H1);
[U2,EV2]=spec(H2);
```

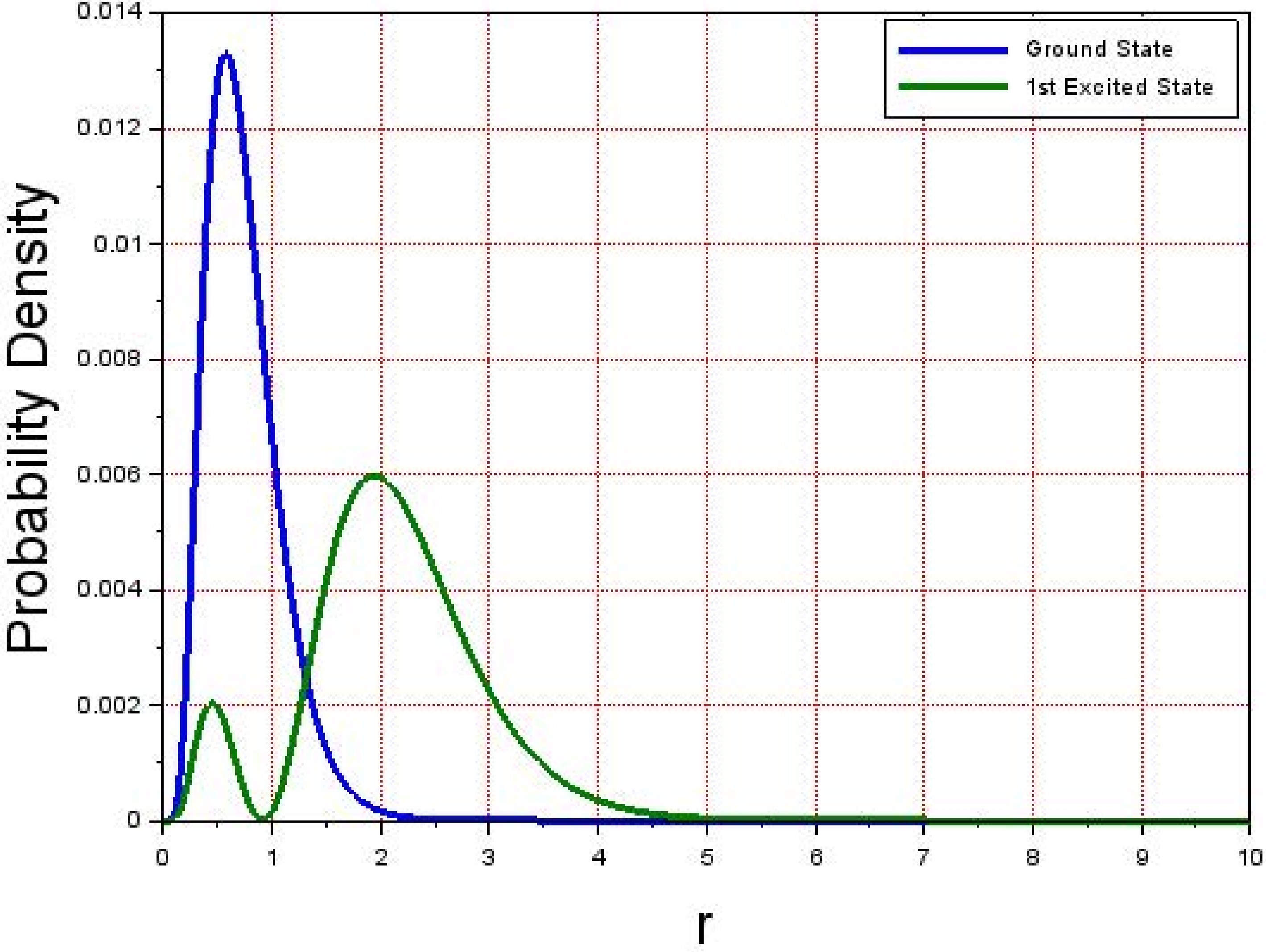
```
[U3,EV3]=spec(H3);
E1=diag(EV1);
E2=diag(EV2);
E3=diag(EV3);
format(6)   //changing number format

disp("Grounded State Energy (in eV) for b=0, 10 and 30",[E1(1) E2(1) E3(1)],"1st Excited State Energy (in eV)for b=0, 10 and 30",[E1(2) E2(2) E3(2)])

//Plotting Wavefunctions at GS State & 1st Excited State
subplot(3,1,1)
plot(r',[abs(U1(:,1))**2,abs(U1(:,2))**2],"linewidth",3)
legend("Ground State","1st Excited State",1)
xlabel("r","fontsize",2);
ylabel("Probability Density","fontsize",2);
title("b=0","position",[5 0.08])

subplot(3,1,2)
plot(r',[abs(U2(:,1))**2,abs(U2(:,2))**2],"linewidth",3)
legend("Ground State","1st Excited State",1)
xlabel("r","fontsize",2);
ylabel("Probability Density","fontsize",2);
title("b=10","position",[5 0.08])

subplot(3,1,3)
plot(r',[abs(U3(:,1))**2,abs(U3(:,2))**2],"linewidth",3)
legend("Ground State","1st Excited State",1)
xlabel("r","fontsize",2);
ylabel("Probability Density","fontsize",2);
title("b=30","position",[5 0.08])
```

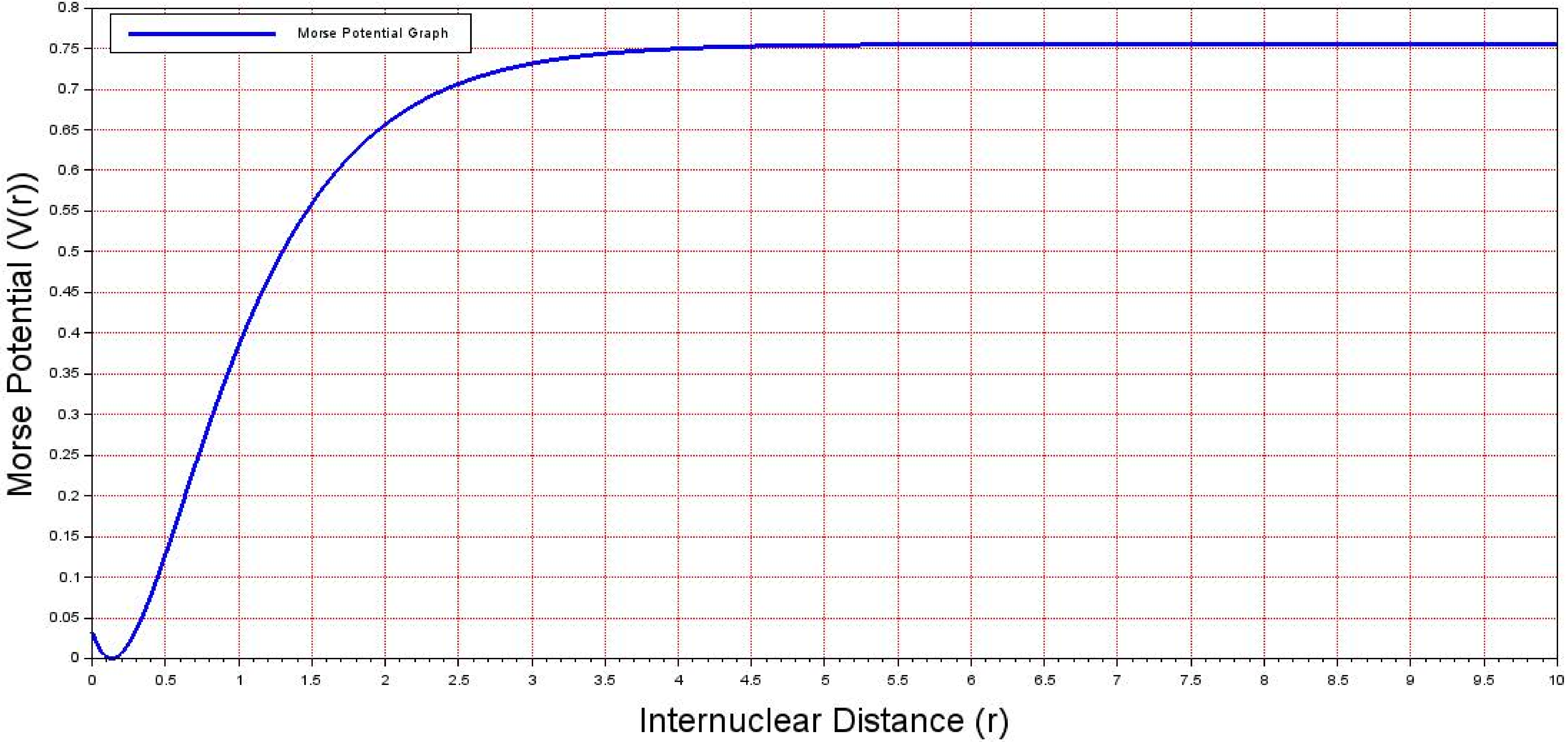

|Wave Function|
0.1
0.05
0
b=0
Ground State
1st Excited State
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
5.5
6
6.5
7
7.5
8
8.5
9
9.5
10
r
b=10
b=30

```
//SOLVE Schrodinger equation for H-atom in Morse potential (using Finite Difference Method)

clc; clear; clf;    //Clearing console, variables and fig

//Describing Constants
h=1973; D=0.755501; m=940*10^6; a=1.44; ro=0.131349;

rmin=0.01; rmax=10; n=1000;
r=linspace(rmin,rmax,n);    //linspace = linearly spaced vector
d=r(2)-r(1);    //Incremental Step Size

//Defining Morse Potential using given formula
V=zeros(n,n);
for i=1:n
    rp=(r(i)-ro)/r(i);
    V(i,i)=D*(exp(-2*a*rp)-exp(-a*rp));
end

//Defining Kinetic Energy using given formula
K=eye(n,n)*(-2);
for i=1:(n-1)
    K(i,i+1)=1;
    K(i+1,i)=1;
end

//Defining Hamiltonian Matrix using given formula
H=(-(h^2)/(2*m*d^2))*K+V;

//Evaluating Eigenvalues & Eigenvectors of H matrix using "spec" function
[U,EV]=spec(H); //U=Eigenvectors(used to plot Wavefunction) & EV=Eigenvalues(used to find Energies)
E=diag(EV); //Extracting diagonal elements of EV matrix using "diag" function
format(6);   //changing number format

disp("Grounded State Energy (in eV)",E(1),"1st Excited State Energy (in eV)",E(2));

//Plotting Wavefunctions at GS State & 1st Excited State
plot(r',[abs(U(:,1))**2,abs(U(:,2))**2],"linewidth",3);
legend("Ground State","1st Excited State",1);
```

```
xlabel("r","fontsize",5);
ylabel("Probability Density","fontsize",5);
xgrid(5);

//Finding Bohr Radius (using SI unit)
E= -13.6; //Energy required to separate electron and proton, eV
e= 1.6*(10^(-19)); //charge of an electron, C
E= E*e; //converting to J
Po= 8.85*(10^(-12)); //Permittivity of free space, F/m
r= e^2/(8*(%pi)*Po*E); //radius, m
r=-r;
disp("Bohr Radius(in m) = ",r);

//NOTE : U here is not the radial function. Instead U/r is the radial function

//SECOND PART OF PROGRAM to find Dissociation Energy & plot potential
//Defining Morse Potential using given formula
rmin=0.001; rmax=10; n=1000;
r=linspace(rmin,rmax,n);    //linspace = linearly spaced vector
V=zeros(n,1);
for i=1:n
    V(i)=D*( (1-exp(-a*(r(i)-ro))) **(2));
end
scf(2);
plot(r',V,"linewidth",3);
legend("Morse Potential Graph",2);
xlabel("Internuclear Distance (r)","fontsize",5);
ylabel("Morse Potential (V(r))","fontsize",5);
xgrid(5);

//D is the well depth (defined relative to the dissociated atoms)
Dissociation_Energy = V(n)-V(1)
disp("Dissociation Energy = ",Dissociation_Energy)

//OUTPUT
//
//  "Grounded State Energy (in eV)"
//
//  -0.155
```

```
//
//  "1st Excited State Energy (in eV)"
//
//  -0.143
//
//  "Bohr Radius(in m) = "
//
//   5.D-11
//
//  "Dissociation Energy = "
//
//   0.723
```


Probability Density
0.014
0.012
0.01
0.008
0.006
0.004
0.002
0
0
1
2
3
4
5
6
7
8
9
10
r
Ground State
1st Excited State


Morse Potential Graph
Morse Potential (V(r))
Internuclear Distance (r)
0
0.05
0.1
0.15
0.2
0.25
0.3
0.35
0.4
0.45
0.5
0.55
0.6
0.65
0.7
0.75
0.8
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
5.5
6
6.5
7
7.5
8
8.5
9
9.5
10