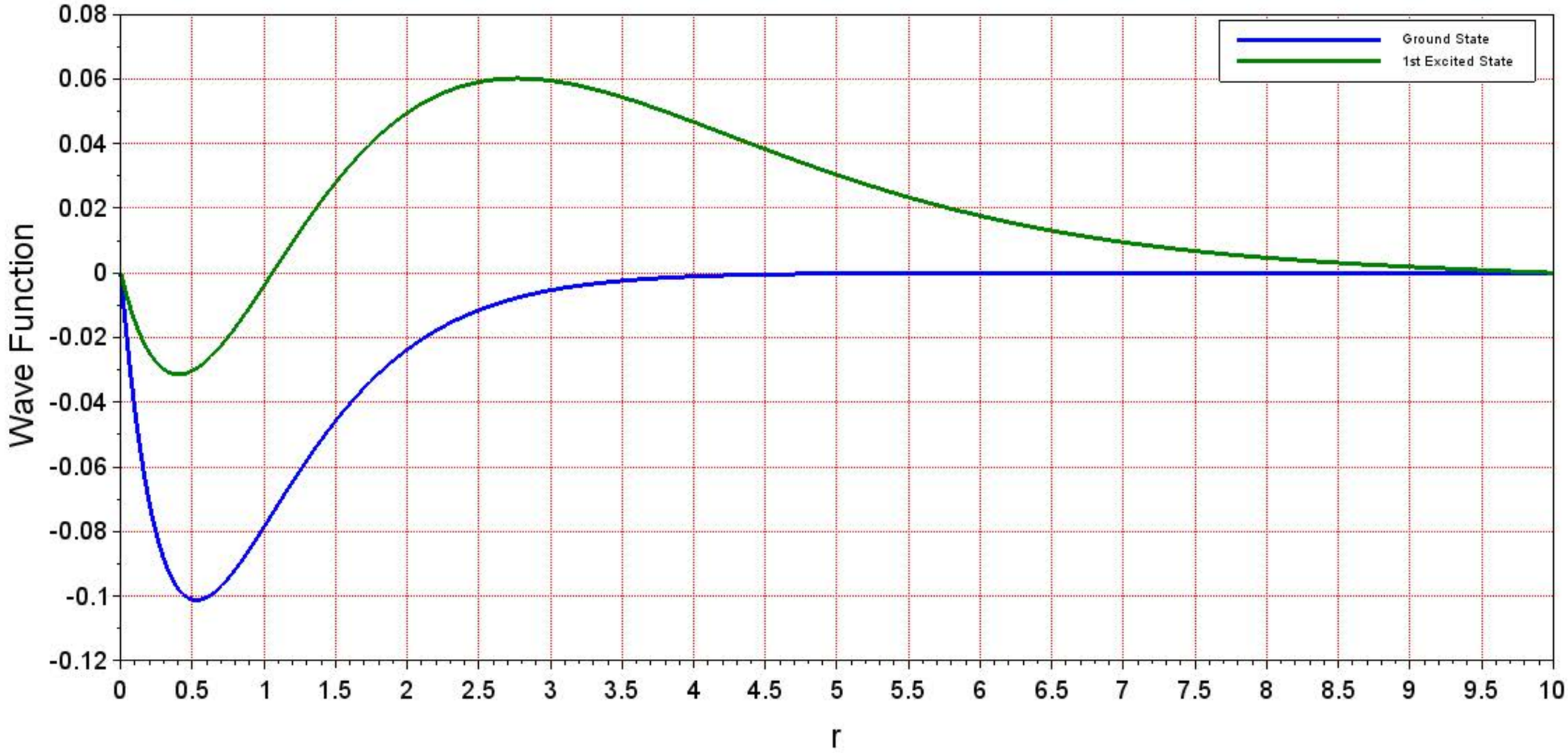
```
0001  //SOLVE Schrodinger equation for H-atom in Coulomb's
 potential (using Finite Difference Method)
0002
0003  clc; clear; clf;    //Clearing console, variables and fig
0004
0005  //Describing Constants : h, e & m
0006  h=1973; e=3.795; m=0.511e6;
0007
0008  rmin=1e-10; rmax=10; n=1000;
0009  r=linspace(rmin,rmax,n);    //linspace = linearly spaced
 vector
0010  d=r(2)-r(1);    //Incremental Step Size
0011
0012  //Defining Coulomb Potential using given formula
0013  V=zeros(n,n);
0014  for i=1:n
0015      V(i,i)=(-(e^2)/r(i));
0016  end
0017
0018  //Defining Kinetic Energy using given formula
0019  K=eye(n,n)*(-2);
0020  for i=1:(n-1)
0021      K(i,i+1)=1;
0022      K(i+1,i)=1;
0023  end
0024
0025  //Defining Hamiltonian Matrix using given formula
0026  H=(-(h^2)/(2*m*d^2))*K+V;
0027
0028  //Evaluating Eigenvalues & Eigenvectors of H matrix
 using "spec" function
0029  [U,EV]=spec(H); //U=Eigenvectors(used to plot
 Wavefunction) & EV=Eigenvalues(used to find Energies)
0030  E=diag(EV) //Extracting diagonal elements of EV matrix
 using "diag" function
0031  format(6)   //changing number format
0032
0033  //Since 1st eigenvalue is absurd, hence we took n=2 as GS
 and n=3 as 1st Excited state
0034  disp("Grounded State Energy (in eV)",E(2),"1st Excited
 State Energy (in eV)",E(3))
0035
0036  //Plotting Probability Densities at GS State & 1st Excited
 State
```

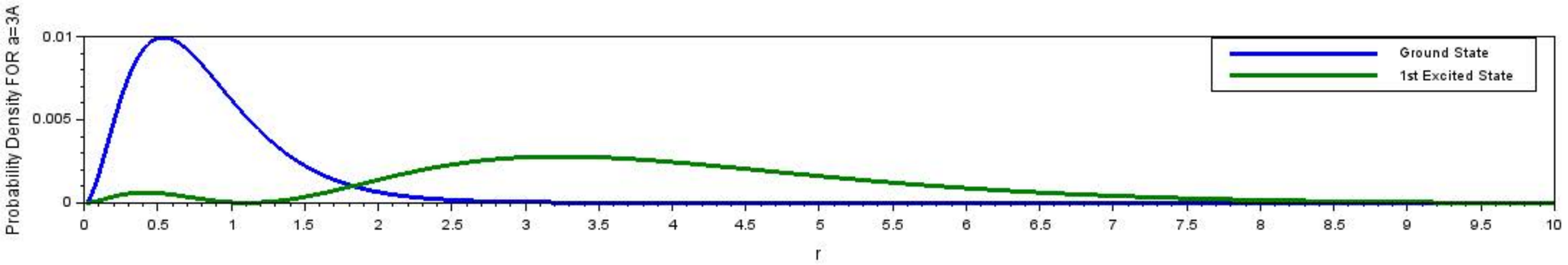
```
0037  plot(r',[U(:,2)**2,U(:,3)**2],"linewidth",3)
0038  legend("Ground State","1st Excited State",1)
0039  xset("font size",4);
0040  xlabel("r","fontsize",5);
0041  ylabel("Probability Density","fontsize",5);
0042  xgrid(5);
0043
0044  b= h^2/(e^2*m)
0045  disp("The Bohr radius is (in angstrom) :",b)
0046
0047  scf(2)
0048  for i=1:5:n
0049          subplot(2,2,1)
0050
0051
  plot(r(i),U(i,2),"r*","linewidth",2,"markersize",2)
0052
  plot(r(i),U(i,3),"b-","linewidth",2,"markersize",2)
0053          xgrid()
0054          legend("Ground State","First Excited State")
0055          ylabel("Wave Function u(r)")
0056          xlabel("r")
0057          title('Numerical')
0058
0059          subplot(2,2,2)
0060
0061
  plot(r(i),U(i,2)**2,"r*","linewidth",2,"markersize",2)
0062
  plot(r(i),U(i,3)**2,"b-","linewidth",2,"markersize",2)
0063          xgrid()
0064          legend("Ground State","First Excited State")
0065          ylabel("Probability Density u(r)*u(r)")
0066          xlabel("r")
0067          title('Numerical')
0068
0069          subplot(2,2,3)
0070
0071          x = [0:0.1:10]
0072          plot((2/b^(3/2))*x.*exp(-x/b),'r')
0073
  plot( 1/b^(3/2)*(x.*exp(-x/(2*b)) - 1/(2*b)*x^2.*exp(-x/(2*b))))
0074          xgrid()
0075          legend("Ground State","First Excited State")
```

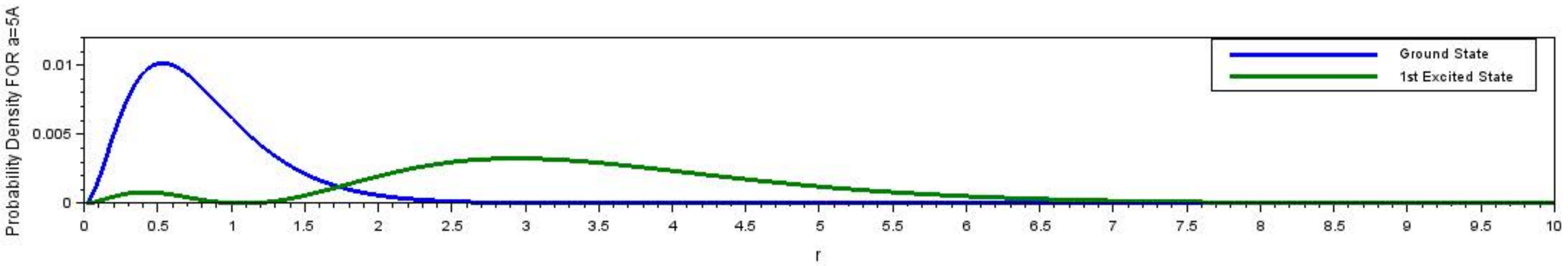
```
0076          ylabel("Wavefunction u(r)")
0077          xlabel("r")
0078          title('Theoretical')
0079
0080          subplot(2,2,4)
0081
0082          plot(((2/b^(3/2))*x.*exp(-x/b))^2,'r')
0083
  plot((1/b^(3/2)*(x.*exp(-x/(2*b)) - 1/(2*b)*x^2.*exp(-x/(2*b))))^2)
0084          xgrid()
0085          legend("Ground State","First Excited State")
0086          ylabel("Probability Density u(r)*u(r)")
0087          xlabel("r")
0088          title('Theoretical')
0089   end
```

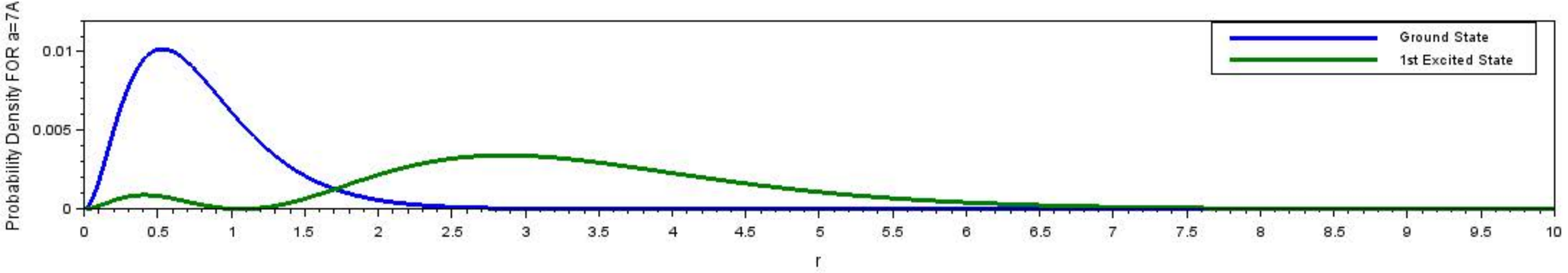

Ground State
1st Excited State
Wave Function
r
0.08
0.06
0.04
0.02
0
-0.02
-0.04
-0.06
-0.08
-0.1
-0.12
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
5.5
6
6.5
7
7.5
8
8.5
9
9.5
10

```
0001  //SOLVE Schrodinger equation for H-atom in Screened
 Coulomb potential (using Finite Difference Method)
0002
0003  clc; clear; clf;    //Clearing console, variables and fig
0004
0005  //Describing Constants : h, e, m, a1, a2, a3
0006  h=1973; e=3.795; m=0.511e6; a1=3; a2=5; a3=7;
0007
0008  rmin=0.01; rmax=10; n=1000;
0009  r=linspace(rmin,rmax,n);    //linspace = linearly spaced
 vector
0010  d=r(2)-r(1);    //Incremental Step Size
0011
0012  //Defining Potential Energy Matrix
0013  V1=zeros(n,n);
0014  for i=1:n
0015      V1(i,i)=-(e^2)*exp(-r(i)/a1)/r(i);
0016  end
0017  V2=zeros(n,n);
0018  for i=1:n
0019      V2(i,i)=-(e^2)*exp(-r(i)/a2)/r(i);
0020  end
0021  V3=zeros(n,n);
0022  for i=1:n
0023      V3(i,i)=-(e^2)*exp(-r(i)/a3)/r(i);
0024  end
0025
0026  //Defining Kinetic Energy using given formula
0027  K=eye(n,n)*(-2);
0028  for i=1:(n-1)
0029      K(i,i+1)=1;
0030      K(i+1,i)=1;
0031  end
0032
0033  //Defining Hamiltonian Matrix using given formula
0034  H1=(-(h^2)/(2*m*d^2))*K+V1;
0035  H2=(-(h^2)/(2*m*d^2))*K+V2;
0036  H3=(-(h^2)/(2*m*d^2))*K+V3;
0037
0038  //Evaluating Eigenvalues & Eigenvectors of H matrix
 using "spec" function
0039  [U1,EV1]=spec(H1);
0040  [U2,EV2]=spec(H2);
0041  [U3,EV3]=spec(H3);
```

```
0042  E1=diag(EV1);
0043  E2=diag(EV2);
0044  E3=diag(EV3);
0045  format(6)   //changing number format
0046
0047  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)])
0048
0049  //Plotting Probability Densities at GS State & 1st Excited
 State
0050  subplot(3,1,1)
0051  plot(r',[U1(:,1)**2,U1(:,2)**2],"linewidth",3)
0052  legend("Ground State","1st Excited State",1)
0053  xlabel("r","fontsize",2);
0054  ylabel("Probability Density","fontsize",2);
0055  title("a=3A")
0056
0057  subplot(3,1,2)
0058  plot(r',[U2(:,1)**2,U2(:,2)**2],"linewidth",3)
0059  legend("Ground State","1st Excited State",1)
0060  xlabel("r","fontsize",2);
0061  ylabel("Probability Density","fontsize",2);
0062  title("a=5A")
0063
0064  subplot(3,1,3)
0065  plot(r',[U3(:,1)**2,U3(:,2)**2],"linewidth",3)
0066  legend("Ground State","1st Excited State",1)
0067  xlabel("r","fontsize",2);
0068  ylabel("Probability Density","fontsize",2);
0069  title("a=7A")
0070
0071  //OUTPUT :
0072  //"Grounded State Energy (in eV) for a=3A, 5A and 7A"
0073  //
0074  //-9.386  -10.95  -11.67
0075  //
0076  //"1st Excited State Energy (in eV)for a=3A, 5A and 7A"
0077  //
0078  //-0.483  -1.272  -1.747
```

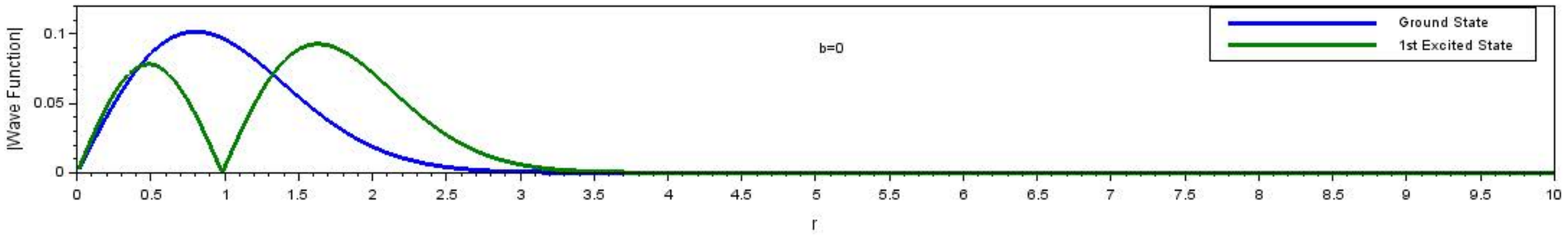

Probability Density FOR a=3A
0.01
0.005
0
0 0.5 1 1.5 2 2.5 3 3.5 4 4.5 5 5.5 6 6.5 7 7.5 8 8.5 9 9.5 10
r
Ground State
1st Excited State

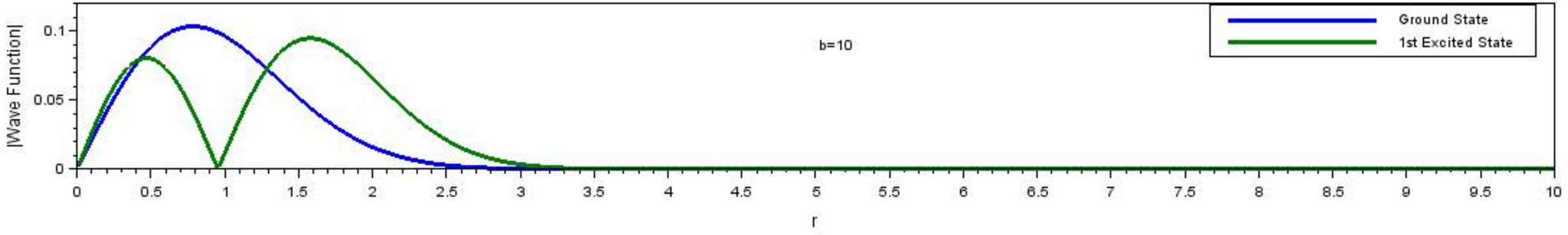

Probability Density FOR a=5A
0.01
0.005
0
0 0.5 1 1.5 2 2.5 3 3.5 4 4.5 5 5.5 6 6.5 7 7.5 8 8.5 9 9.5 10
r
Ground State
1st Excited State

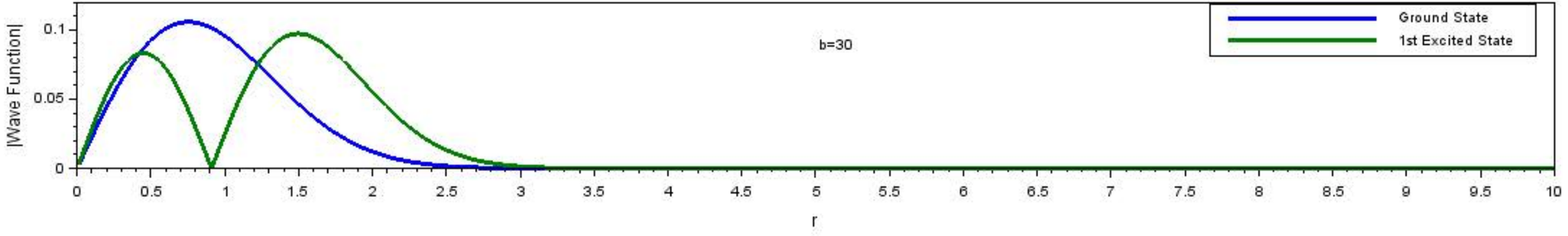

Probability Density FOR a=7A
0.01
0.005
0
0 0.5 1 1.5 2 2.5 3 3.5 4 4.5 5 5.5 6 6.5 7 7.5 8 8.5 9 9.5 10
r
Ground State
1st Excited State

```
0001  //SOLVE Schrodinger equation for H-atom in Screened
 Anharmonic Oscillator potential (using Finite Difference
 Method)
0002
0003  clc; clear; clf;    //Clearing console, variables and fig
0004
0005  //Describing Constants : h, k, m, b1, b2, b3
0006  h=197.3; k=100; m=940; b1=0; b2=10; b3=30;
0007
0008  rmin=0.01; rmax=10; n=1000;
0009  r=linspace(rmin,rmax,n);    //linspace = linearly spaced
 vector
0010  d=r(2)-r(1);    //Incremental Step Size
0011
0012  //Defining Potential Energy Matrix
0013  V1=zeros(n,n);
0014  for i=1:n
0015      V1(i,i)=(k*(r(i)^2))/2 + (b1*(r(i)^3))/3;
0016  end
0017  V2=zeros(n,n);
0018  for i=1:n
0019      V2(i,i)=(k*(r(i)^2))/2 + (b2*(r(i)^3))/3;
0020  end
0021  V3=zeros(n,n);
0022  for i=1:n
0023      V3(i,i)=(k*(r(i)^2))/2 + (b3*(r(i)^3))/3;
0024  end
0025
0026  //Defining Kinetic Energy using given formula
0027  K=eye(n,n)*(-2);
0028  for i=1:(n-1)
0029      K(i,i+1)=1;
0030      K(i+1,i)=1;
0031  end
0032
0033  //Defining Hamiltonian Matrix using given formula
0034  H1=(-(h^2)/(2*m*d^2))*K+V1;
0035  H2=(-(h^2)/(2*m*d^2))*K+V2;
0036  H3=(-(h^2)/(2*m*d^2))*K+V3;
0037
0038  //Evaluating Eigenvalues & Eigenvectors of H matrix
 using "spec" function
0039  [U1,EV1]=spec(H1);
0040  [U2,EV2]=spec(H2);
```

```
0041  [U3,EV3]=spec(H3);
0042  E1=diag(EV1);
0043  E2=diag(EV2);
0044  E3=diag(EV3);
0045  format(6)   //changing number format
0046
0047  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)])
0048
0049  //Plotting Wavefunctions at GS State & 1st Excited State
0050  subplot(3,1,1)
0051  plot(r',[abs(U1(:,1))**2,abs(U1(:,2))**2],"linewidth",3)
0052  legend("Ground State","1st Excited State",1)
0053  xlabel("r","fontsize",2);
0054  ylabel("Probability Density","fontsize",2);
0055  title("b=0","position",[5 0.08])
0056
0057  subplot(3,1,2)
0058  plot(r',[abs(U2(:,1))**2,abs(U2(:,2))**2],"linewidth",3)
0059  legend("Ground State","1st Excited State",1)
0060  xlabel("r","fontsize",2);
0061  ylabel("Probability Density","fontsize",2);
0062  title("b=10","position",[5 0.08])
0063
0064  subplot(3,1,3)
0065  plot(r',[abs(U3(:,1))**2,abs(U3(:,2))**2],"linewidth",3)
0066  legend("Ground State","1st Excited State",1)
0067  xlabel("r","fontsize",2);
0068  ylabel("Probability Density","fontsize",2);
0069  title("b=30","position",[5 0.08])
```


b=0
Ground State
1st Excited State
|Wave Function|
r
0
0.05
0.1
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

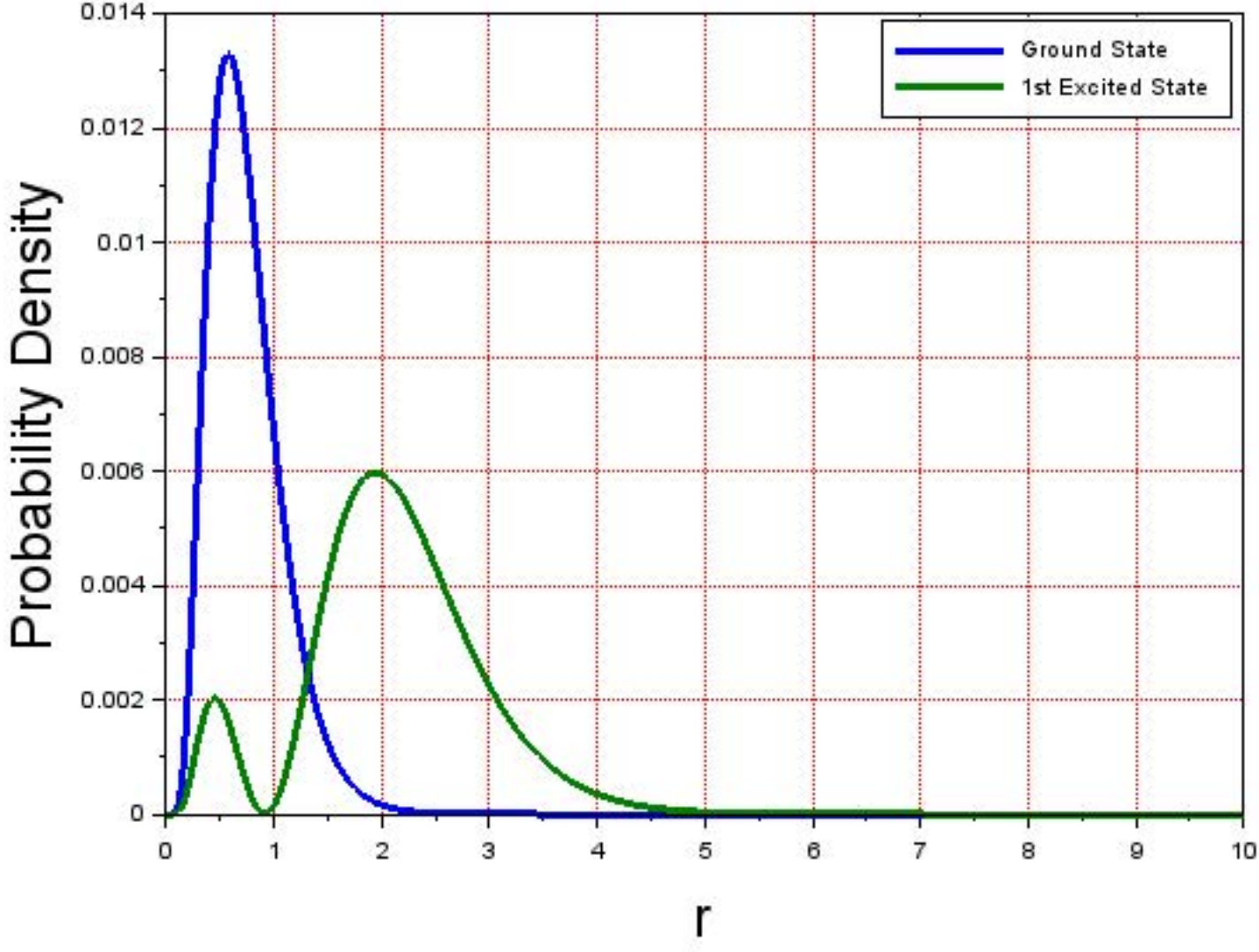

b=10
Ground State
1st Excited State
|Wave Function|
r
0
0.05
0.1
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
5.5
6
6.5
7
7.5
8
8.5
9
9.5
10

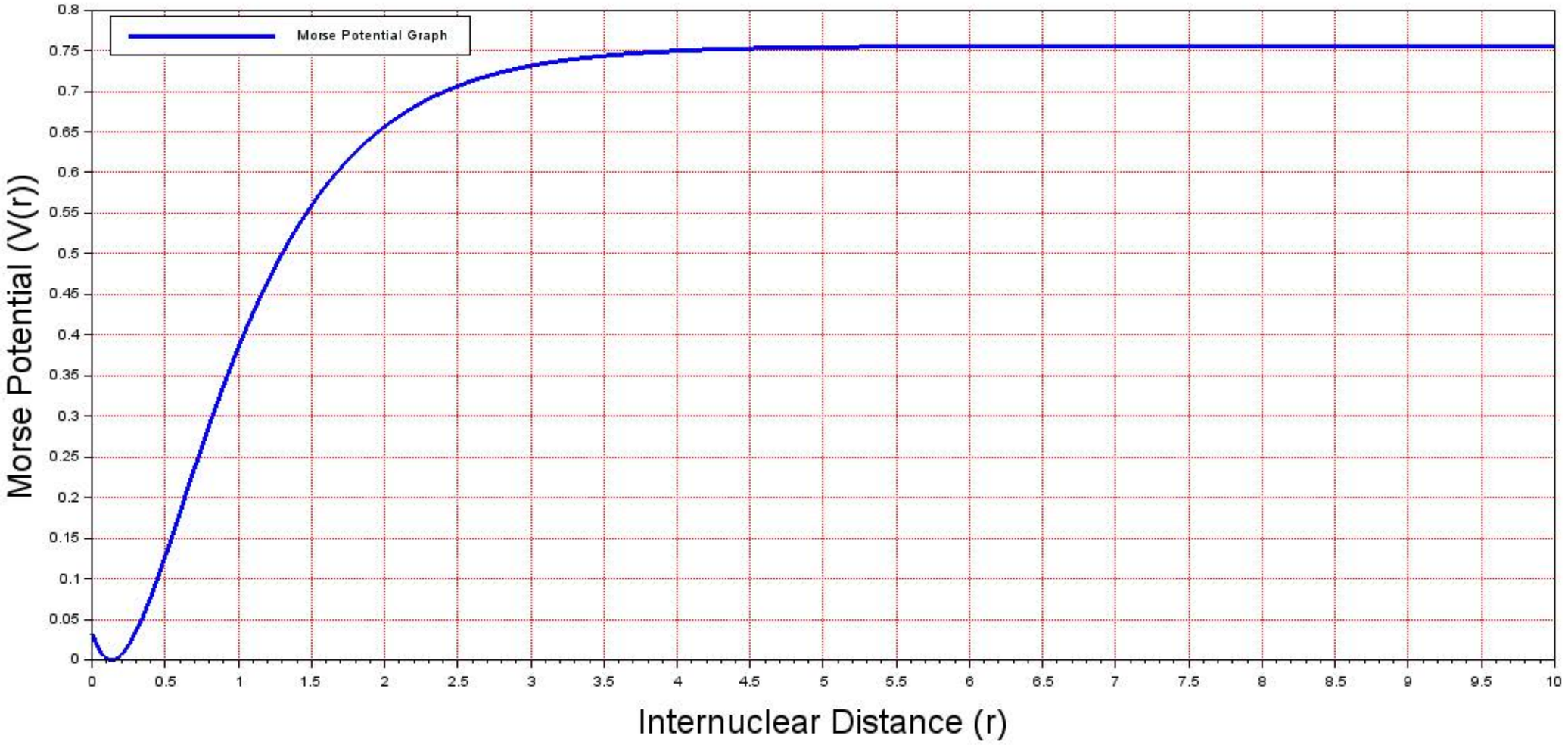

b=30
Ground State
1st Excited State
|Wave Function|
r
0
0.05
0.1
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
5.5
6
6.5
7
7.5
8
8.5
9
9.5
10

```
0001  //SOLVE Schrodinger equation for H-atom in Morse potential
 (using Finite Difference Method)
0002
0003  clc; clear; clf;    //Clearing console, variables and fig
0004
0005  //Describing Constants
0006  h=1973; D=0.755501; m=940*10^6; a=1.44; ro=0.131349;
0007
0008  rmin=0.01; rmax=10; n=1000;
0009  r=linspace(rmin,rmax,n);    //linspace = linearly spaced
 vector
0010  d=r(2)-r(1);    //Incremental Step Size
0011
0012  //Defining Morse Potential using given formula
0013  V=zeros(n,n);
0014  for i=1:n
0015      rp=(r(i)-ro)/r(i);
0016      V(i,i)=D*(exp(-2*a*rp)-exp(-a*rp));
0017  end
0018
0019  //Defining Kinetic Energy using given formula
0020  K=eye(n,n)*(-2);
0021  for i=1:(n-1)
0022      K(i,i+1)=1;
0023      K(i+1,i)=1;
0024  end
0025
0026  //Defining Hamiltonian Matrix using given formula
0027  H=(-(h^2)/(2*m*d^2))*K+V;
0028
0029  //Evaluating Eigenvalues & Eigenvectors of H matrix
 using "spec" function
0030  [U,EV]=spec(H); //U=Eigenvectors(used to plot
 Wavefunction) & EV=Eigenvalues(used to find Energies)
0031  E=diag(EV); //Extracting diagonal elements of EV matrix
 using "diag" function
0032  format(6);   //changing number format
0033
0034  disp("Grounded State Energy (in eV)",E(1),"1st Excited
 State Energy (in eV)",E(2));
0035
0036  //Plotting Wavefunctions at GS State & 1st Excited State
0037  plot(r',[abs(U(:,1))**2,abs(U(:,2))**2],"linewidth",3);
0038  legend("Ground State","1st Excited State",1);
```

```
0039  xlabel("r","fontsize",5);
0040  ylabel("Probability Density","fontsize",5);
0041  xgrid(5);
0042
0043  //Finding Bohr Radius (using SI unit)
0044  E= -13.6; //Energy required to separate electron and
 proton, eV
0045  e= 1.6*(10^(-19)); //charge of an electron, C
0046  E= E*e; //converting to J
0047  Po= 8.85*(10^(-12)); //Permittivity of free space, F/m
0048  r= e^2/(8*(%pi)*Po*E); //radius, m
0049  r=-r;
0050  disp("Bohr Radius(in m) = ",r);
0051
0052  //NOTE : U here is not the radial function. Instead U/r is
 the radial function
0053
0054  //SECOND PART OF PROGRAM to find Dissociation Energy &
 plot potential
0055  //Defining Morse Potential using given formula
0056  rmin=0.001; rmax=10; n=1000;
0057  r=linspace(rmin,rmax,n);    //linspace = linearly spaced
 vector
0058  V=zeros(n,1);
0059  for i=1:n
0060      V(i)=D*( (1-exp(-a*(r(i)-ro))) **(2));
0061  end
0062  scf(2);
0063  plot(r',V,"linewidth",3);
0064  legend("Morse Potential Graph",2);
0065  xlabel("Internuclear Distance (r)","fontsize",5);
0066  ylabel("Morse Potential (V(r))","fontsize",5);
0067  xgrid(5);
0068
0069  //D is the well depth (defined relative to the dissociated
 atoms)
0070  Dissociation_Energy = V(n)-V(1)
0071  disp("Dissociation Energy = ",Dissociation_Energy)
0072
0073  //OUTPUT
0074  //
0075  //  "Grounded State Energy (in eV)"
0076  //
0077  //  -0.155
```

```
0078  //
0079  //  "1st Excited State Energy (in eV)"
0080  //
0081  //  -0.143
0082  //
0083  //  "Bohr Radius(in m) = "
0084  //
0085  //   5.D-11
0086  //
0087  //  "Dissociation Energy = "
0088  //
0089  //   0.723
```


Ground State
1st Excited State
Probability Density
r
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


Morse Potential Graph
Morse Potential (V(r))
Internuclear Distance (r)
0.8
0.75
0.7
0.65
0.6
0.55
0.5
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
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