Quantum mechanics
Practical file

Submitted by :-

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Experiment-1

Time independent Schrodinger wave equation for a free particle (consider an electron) trapped inside a well of infinite potential can be written as

$$\frac{d^2\Psi}{dx^2} + \frac{2mE}{h^2}\Psi = 0$$

(I) Write Scilab codes to solve the above time independent Schrodinger wave equation using ODE module of Scilab.
Given to Use
L=1 angstrom
e=3.795 $(eVangstorm)^{1/2}$
hc=1973(eVA)
m=0.511*10^6 eV/c^6

(II) Plot eigen functions Ψ_1, Ψ_2. Write the corresponding energy values.
(III) Plot probability density $\Psi_1^*\Psi_1$, and $\Psi_2^*\Psi_2$.

Code for experiment 1

```
clc;
L=1 // unit of L is in angstrom
n=input("enter the size of matrix")
h=(L-0)/(n-1)
m=0.51*10^6 // mass of electron in (ev)/c^2
```

```
yc=1973 // ev in angstrom
k=(yc)^2/(2*m)
A=zeros(n,n)
for i=1:n
    A(i,i)=-2
end
for i=1:n-1
    A(i,i+1)=1
end
for i=2:n
    A(i,i-1)=1
end
B=A/h^2
H=-k*B
disp(H)
[p,q]=spec(H)
disp('eigenvector of H is',p)
disp('eigenvalues of H is ',diag(q))
subplot(2,2,1)
x= linspace(0,1,n) //for first order
plot(x,p(:,1),"red","linewidth",4)
xlabel('Length of the Box (angstrom)')
ylabel('Wavefunction')
title('Plot of ground-State')
[p,q]=spec(H)
r=diag(q)
disp('energy of ground state',r(1))

subplot(2,2,2)
x=linspace(0,1,n) //for second-order
plot (x,p(:,2), 'green', 'linewidth',2)
xlabel('Length of the Box (angstrom)')
ylabel('Wavefunction')
title('Plot of Excited State')
[P,q]=spec(H)
r=diag (q)
disp('energy of first excited state',r(2))
```

```
subplot(2,2,3)
x=linspace(0,1,n) //for-third order
plot (x,p(:,3), 'blue', 'linewidth',2)
xlabel('Length of the Box (angstrom)')
ylabel('Wavefunction')
title('Plot of Second Excited State')
[p,q]=spec (H)
r=diag(q)
disp('energy-of-second excited state',r(3))

subplot(2,2,4)
x=linspace(0,1,n) //for-fourth order
plot (x,p(:,4), 'black', 'linewidth',2)
xlabel('Length of the Box (angatrom)')
ylabel('Wavefunction')
title('Plot of Third Excited State')
[P,q]=spec (H)
r=diag(q)
disp('energy of third excited state',r(4))
```

or

```
clc;
L=1 // unit of L is in angstrom
n=input("enter the size of matrix")
h=(L-0)/(n-1)
m=0.51*10^6 // mass of electron in (ev)/c^2
yc=1973 // ev in angstrom
k=(yc)^2/(2*m)
A=zeros(n,n)
for i=1:n
    A(i,i)=-2
end
for i=1:n-1
    A(i,i+1)=1
end
```

```
for i=2:n
    A(i,i-1)=1
end
B=A/h^2
H=-k*B
disp(H)
[p,q]=spec(H)
disp('eigenvector of H is',p)
disp('eigenvalues of H is ',diag(q))
subplot(2,2,1)
x= linspace(0,1,n) //for first order
plot(x,p(:,1),"red","linewidth",4)
xlabel('Length of the Box (angstrom)')
ylabel('Wavefunction')
title('Plot of ground-State')
[p,q]=spec(H)
r=diag(q)
disp('energy of ground state',r(1))

subplot(2,2,2)
x=linspace(0,1,n) //for second-order
plot (x,p(:,2), 'green', 'linewidth',2)
xlabel('Length of the Box (angstrom)')
ylabel('Wavefunction')
title('Plot of Excited State')
[P,q]=spec(H)
r=diag (q)
disp('energy of first excited state',r(2))

subplot(2,2,3)
plot(x,p(:,1).*conj(p(:,1)),'red','linewidth',2) // probability density for
first order
xlabel('Length of the Box (angstrom)')
ylabel('Probability density')
title('Plot of probability density for first order')

subplot(2,2,4)
```

```
plot(x,p(:,2).*conj(p(:,2)),'green','linewidth',2) // probability density for second order
xlabel('Length of the Box (angstrom)')
ylabel('Probability density')
title('Plot of probability density for second order')
```

[NOTE : Here two codes are written where 1st part is only defined for the schrodinger wave equation whereas 2nd part defines the complete overall solution of the experiment I]

Image for the eigenfunction or energy

```
"energy of ground state"

 36.186483

"energy of first excited state"

 144.71092

"energy-of-second excited state"

 325.46833

"energy of third excited state"

 578.28383
```

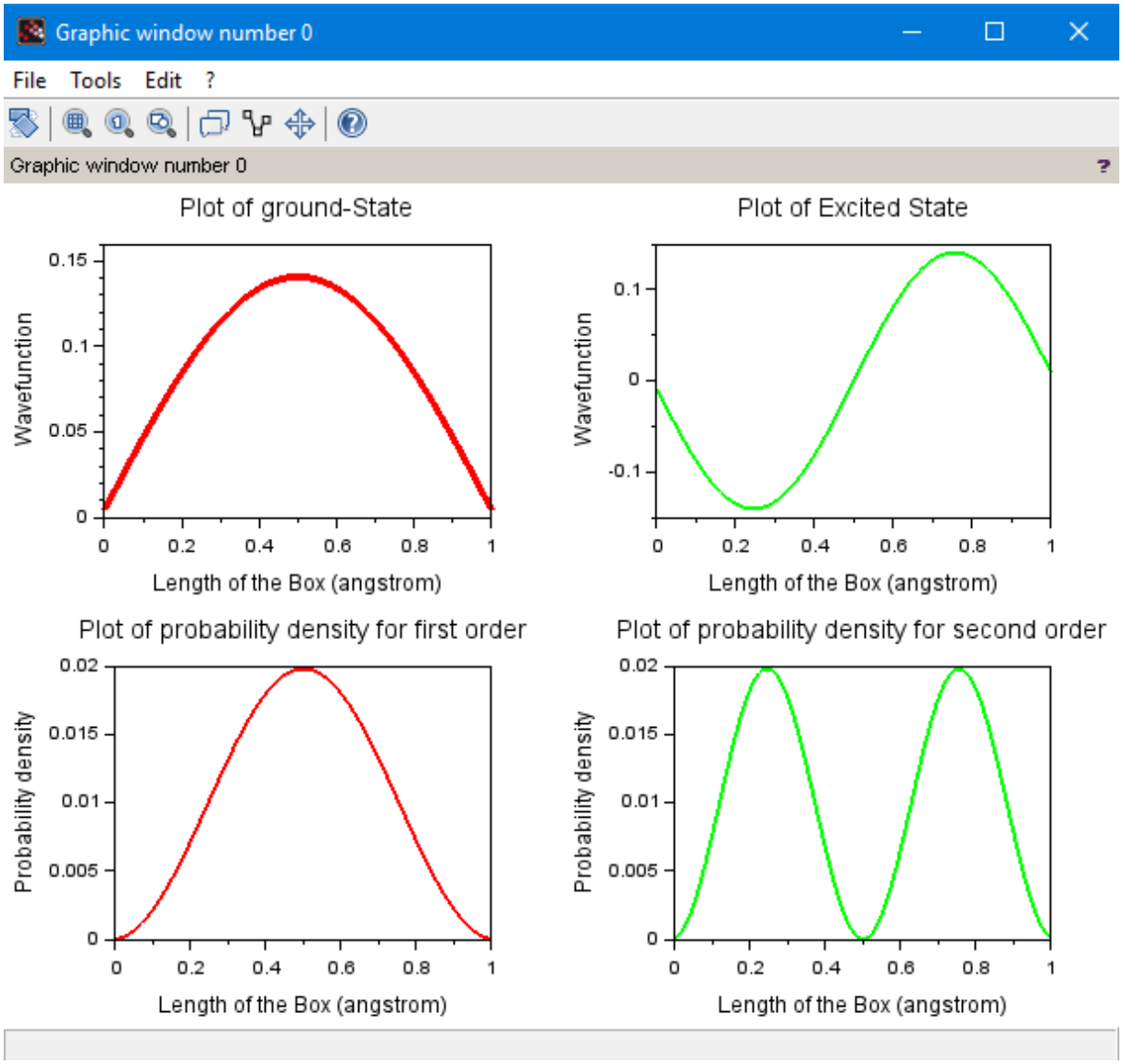
"eigenvalues of H is "

36.186483
144.71092
325.46833
578.28383
902.91284
1299.0413

1766.2860
2304.1949
2912.2476
3589.8559
16842.735
18341.473
19894.840
21501.333
23159.397
24867.429
26623.777
28426.741
30274.576
32165.496
34097.671
36069.232
38078.271
40122.844
42200.974
44310.651
46449.833
48616.450
50808.407
53023.584
55259.836
57515.001
59786.897
62073.326
64372.076
66680.923
68997.634
71319.967
73645.675
75972.509
78298.217
80620.550
82937.261
85246.108
87544.858
89831.287
92103.183
94358.348
96594.600
98809.777
101001.73
103168.35
105307.53
107417.21
109495.34
111539.91
113548.95
115520.51
117452.69
119343.61
121191.44
122994.41
124750.75
126458.79
128116.85

129723.34
131276.71
132775.45
134218.11
135603.29
136929.66
138195.94
139400.89
140543.35
141622.22
142636.45
143585.06
144467.13
145281.82
146028.33
146705.94
147313.99
147851.90
148319.14
148715.27
149039.90
149292.72
149473.47
149582.00

Graphical representation of all the defined/stated function



Experiment-2

Time independen

1.Write Scilab codes to solve the time independent Schrodinger wave equation for hydrogen atom in which electron follows the Coulomb potential.

2. Find the ground state and first excited state energy eigenvalue.

3. Plot the Ground state and first excited state eigenfunction.
4. Plot the probability density for the ground and the first excites state.
5. Find the most probable position for electron to be observed in Hydrogen atom.

Range of r = (1 × 10_10Å *to* 10Å)
Charge of electron = 3.795 (eVÅ)^1/2
Mass of particle m =0.511×106eV/c2
ħc = 1973 (eVÅ).

Code for experiment 2

```
clc // to clear the Console
L=10// Unit of L in angstrom
n= input (' Enter the dimension of the Matrix')
a=1e-16
h=(L-a)/(n-1)
e= 3.795
m= 0.51*10^6//Mass of electron in ev/c^2
oc= 1973 // ev angstrom
k=((oc)^2)/(2*m)
x=linspace(1e-16,10,n)
v=zeros(n,n)
for i= 1:n
   v(i,i)=-(e*e)/(x(i));
end
a=zeros(n,n) //creat a triogonal matrix of (1,-2,1)
for i= 1:n
   a(i,i)=-2
end
for i= 1:n-1
   a(i,i+1)=1
end
for i= 2:n
   a(i,i-1)=1
end
```

```
b=a/(h^2)
H=-k*b+v
disp(H)
[v,e]= spec(H)
disp('eigenvector of H is',v)
disp('eigenvalues of H is',diag(e))

subplot(2,2,1) //for first order
plot (x,v(:,2),'red','linewidth',3)
xlabel('Length of the Box (angstrom)')
ylabel('Wavefunction')
title('Plot of Ground State')

r=diag(e)
disp('energy of ground state',r(2))

subplot(2,2,2)
x=linspace(0,1,n) //for second order
plot (x,v(:,3),'green','linewidth',2)
xlabel('Length of the Box (angstrom)')
ylabel('Wavefunction')
title('Plot of Excited State')

disp('energy of second excited state',r(3))

subplot(2,2,3)

plot(x,v(:,2).*conj(v(:,2)),'red','linewidth',2) // probability density for
first order
xlabel('Length of the Box (angstrom)')
ylabel('Probability density')
title('Plot of probability density for ground order')
subplot(2,2,4)
plot(x,v(:,3).*conj(v(:,3)),'green','linewidth',2) // probability density
for second order
xlabel('Length of the Box (angstrom)')
ylabel('Probability density')
```

```
title('Plot of probability density for first order')
```

Graphical representation of all the defined/stated function

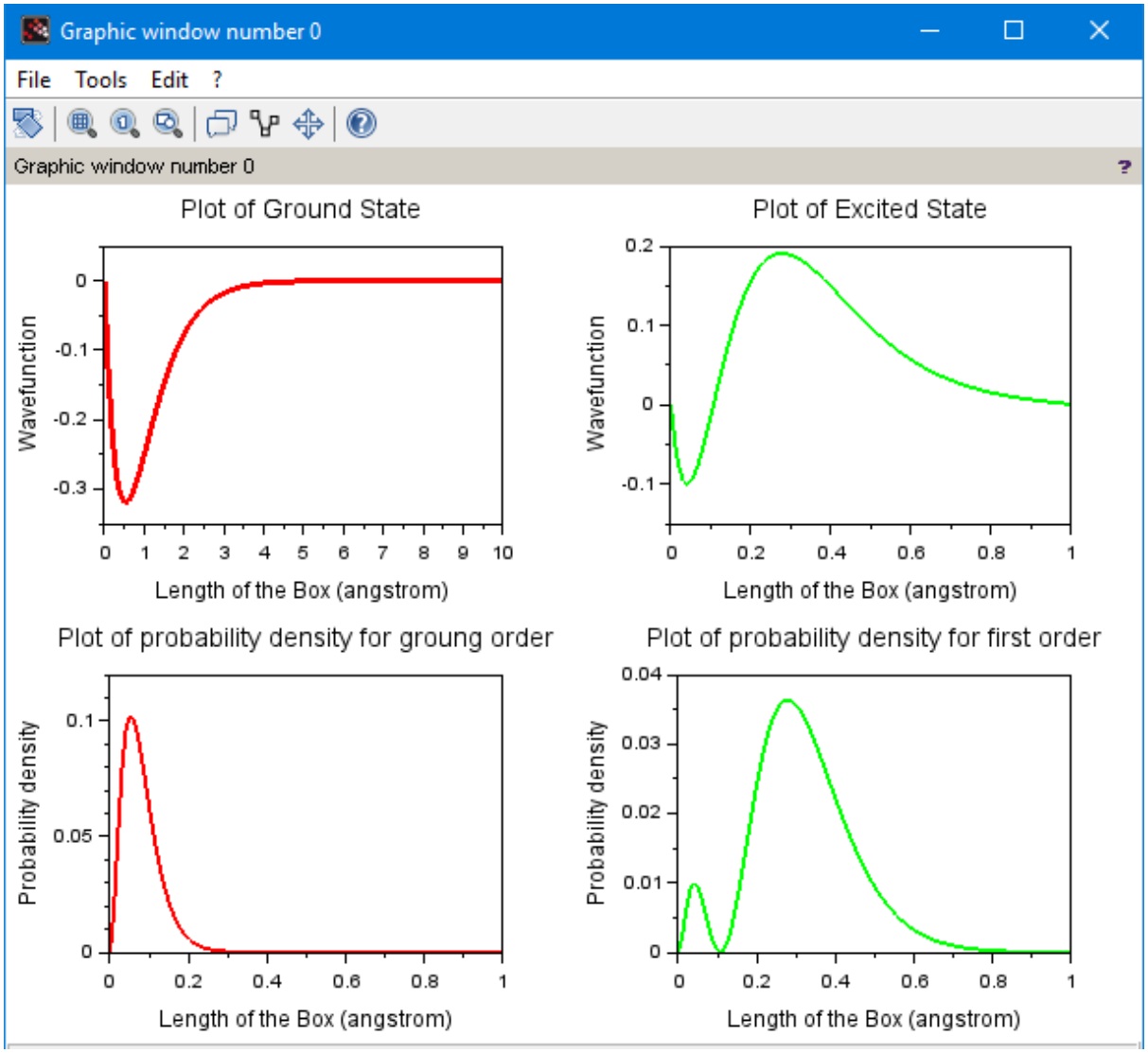


Image for the eigenfunction or energy

```
"energy of ground state"

-13.466100

"energy of second excited state"

-3.3884124
```

[NOTE: Here two part of code is defined one depicts the energy eigen values and other depicts the probablilty density]

Experiment-3

1. Write radial part of time independent Schrodinger wave equation for an electron orbiting around proton and follows the screened coulomb potential

$$v(r) = -\frac{e^2}{r} e^{-\frac{r}{a}}$$

2.Write Scilab codes to solve the above Schrodinger equation using finite difference method.

3. Complete the following table

Range of r = (1 × 10_10Å *to* 10Å)
Charge of electron = 3.795 (*eV*Å)61/2
Mass of particle m =0.511×106eV/c2
ħc = 1973 (eVÅ)

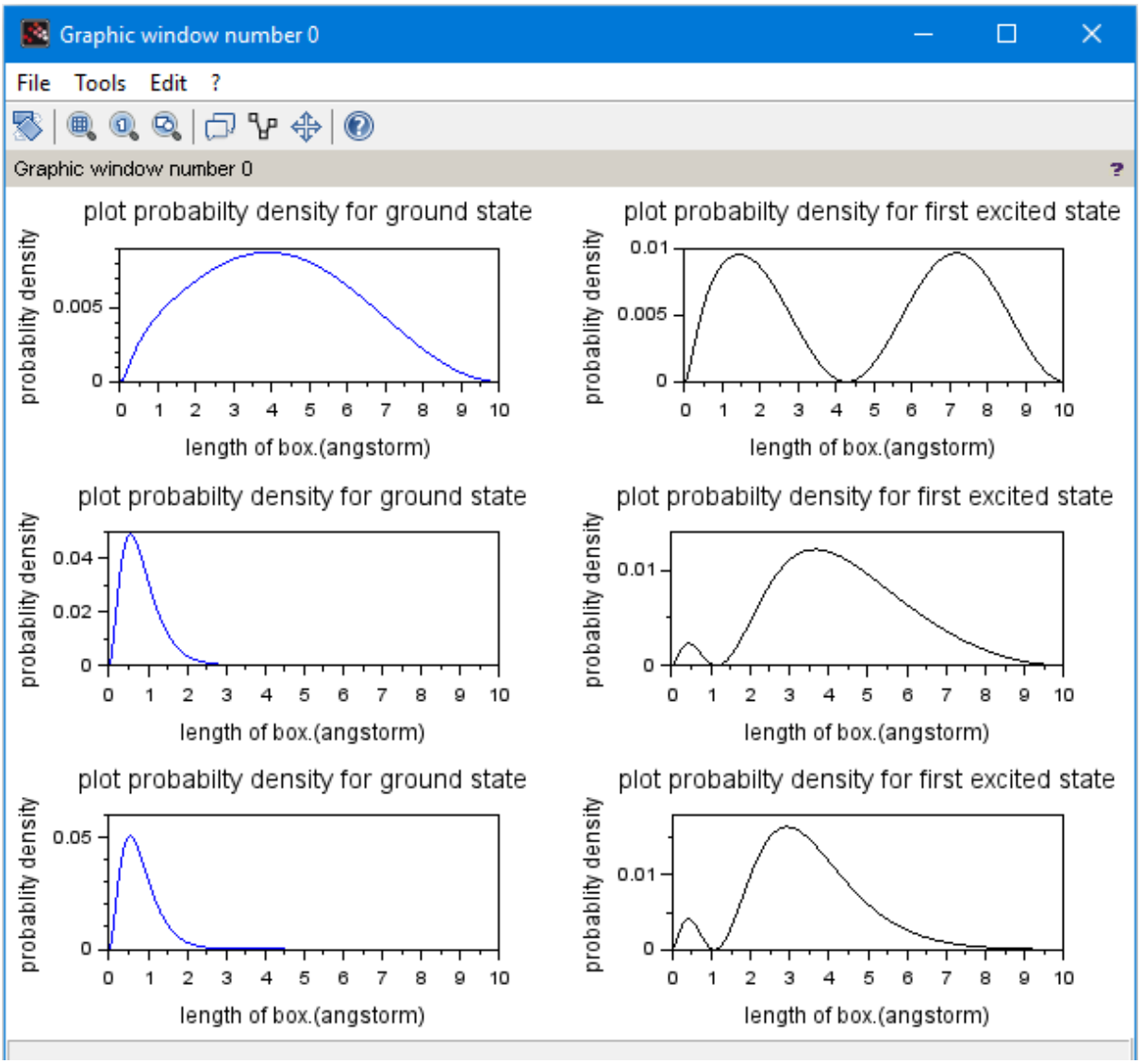
Code for experiment 3

```
clc // to clear the Console
L=10// Unit of L in angstrom
n= input (' Enter the dimension of the Matrix')
a=1e-16
h=(L-a)/(n-1)
e= 3.795
m= 0.51*10^6//Mass of electron in ev/c^2
oc= 1973 // ev angstrom
 // p = screening factor
k=((oc)^2)/(2*m)
x=linspace(1e-16,10,n)

a=zeros(n,n) //creat a triogonal matrix of (1,-2,1)
for i= 1:n
```

```
    a(i,i)=-2
end
for i= 1:n-1
    a(i,i+1)=1
end
for i= 2:n
    a(i,i-1)=1
end

v1=zeros(n,n)
for i= 1:n
    v1(i,i)=(-(e*e)*(e^(-x(i)/0.5)))/x(i);
end
v2=zeros(n,n)
for i= 1:n
    v2(i,i)=(-(e*e)*(e^(-x(i)/3)))/x(i);
end
v3=zeros(n,n)
for i= 1:n
    v3(i,i)=(-(e*e)*(e^(-x(i)/7)))/x(i);
end
b=a/(h^2)
H1=-k*b+v1;
H2=-k*b+v2;
H3=-k*b+v3;
disp(H)
[v1,e1]= spec(H1)
disp('eigenvector of H is',v1)
disp('eigenvalues of H is',diag(e1))
[v3,e3]= spec(H3)
disp('eigenvector of H is',v3)
disp('eigenvalues of H is',diag(e3))
[v2,e2]= spec(H2)
disp('eigenvector of H is',v2)
disp('eigenvalues of H is',diag(e2))
```

```
subplot(3,2,1)
plot(x,v1(:,2).*conj(v1(:,2)),"blue")//probablity density
title("plot probabilty density for ground state")
xlabel("length of box.(angstorm)")
ylabel("probablity density")

subplot(3,2,2)
plot(x,v1(:,3).*conj(v1(:,3)),"black")//probablity density
title("plot probabilty density for first excited state")
xlabel("length of box.(angstorm)")
ylabel("probablity density")

subplot(3,2,3)
plot(x,v2(:,2).*conj(v2(:,2)),"blue")//probablity density
title("plot probabilty density for ground state")
xlabel("length of box.(angstorm)")
ylabel("probablity density")

subplot(3,2,4)
plot(x,v2(:,3).*conj(v2(:,3)),"black")//probablity density
title("plot probabilty density for first excited state")
xlabel("length of box.(angstorm)")
ylabel("probablity density")

subplot(3,2,5)
plot(x,v3(:,2).*conj(v3(:,2)),"blue")//probablity density
title("plot probabilty density for ground state")
xlabel("length of box.(angstorm)")
ylabel("probablity density")

subplot(3,2,6)
plot(x,v3(:,3).*conj(v3(:,3)),"black")//probablity density
title("plot probabilty density for first excited state")
xlabel("length of box.(angstorm)")
ylabel("probablity density")
```

Graphical representation of all the defined/stated function(probability density)




```
subplot(3,2,1) //for ground state
plot (x,v1(:,2),'red','linewidth',3)
xlabel('Length of the Box (angstrom)')
ylabel('Wavefunction')
title('Plot of Ground State')
r=diag(e1)
disp('energy of ground state',r(2))

subplot(3,2,2)
x=linspace(0,1,n) //for first state
plot (x,v1(:,3),'green','linewidth',2)
xlabel('Length of the Box (angstrom)')
ylabel('Wavefunction')
title('Plot of Excited State')
disp('energy of first excited state',r(3))
```

```
subplot(3,2,3) //for ground state
plot (x,v2(:,2),'red','linewidth',3)
xlabel('Length of the Box (angstrom)')
ylabel('Wavefunction')
title('Plot of Ground State')
r=diag(e2)
disp('energy of ground state',r(2))

subplot(3,2,4)
x=linspace(0,1,n) //for first state
plot (x,v2(:,3),'green','linewidth',2)
xlabel('Length of the Box (angstrom)')
ylabel('Wavefunction')
title('Plot of Excited State')
disp('energy of first excited state',r(3))

subplot(3,2,5) //for ground state
plot (x,v3(:,2),'red','linewidth',3)
xlabel('Length of the Box (angstrom)')
ylabel('Wavefunction')
title('Plot of Ground State')
r=diag(e3)
disp('energy of ground state',r(2))

subplot(3,2,6)
x=linspace(0,1,n) //for first state
plot (x,v3(:,3),'green','linewidth',2)
xlabel('Length of the Box (angstrom)')
ylabel('Wavefunction')
title('Plot of Excited State')
disp('energy of first excited state',r(3))
```

Graphical representation of all the defined/stated function

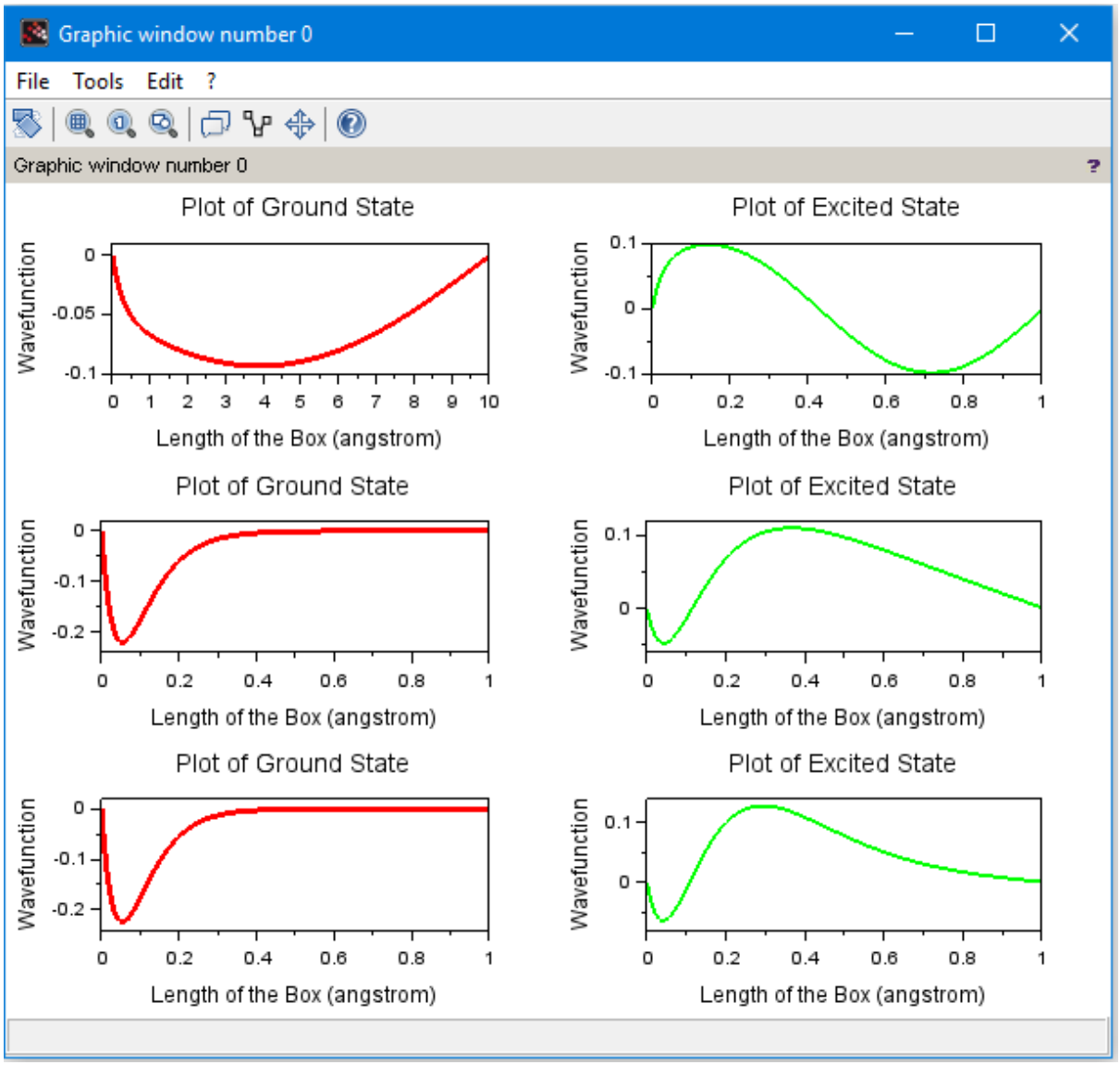


Image for the eigenfunction or energy

```
"energy of ground state"
 0.2488582
"energy of first excited state"
 1.1268910
"energy of ground state"
-8.1498551
"energy of first excited state"
-0.0833000
"energy of ground state"
-11.008664
"energy of first excited state"
-1.3375138
```

[NOTE: Here two part of code is defined one depicts the energy eigen values and other depicts the probablilty density]

Experiment-4

1.write scilab codes to solve time independent s-wave radial part of Schrodinger wave equation for a particle follows potential

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

2. Plot the potential as a function of r for different value of b.

Range of r = ($-5\ fm\ to\ 5\ fm$)
K = 100 MeV fm-2
b = 0,10,30 MeV fm^{-3}
Mass of particle m =940 M eV/c2
ħc = 197.3 (MeV fm)

Code for experiment 4

```
clc // to clear the Console
L=5// Unit of L in angstrom
n= input (' Enter the dimension of the Matrix')
a=-5
h=(L-a)/(n-1)
e= 3.795
m=940//Mass of electron in ev/c^2
oc= 197.3 // ev angstrom
 // p = screening factor
k=((oc)^2)/(2*m)
x=linspace(-5,5,n)

A=zeros(n,n) //creat a triogonal matrix of (1,-2,1)
for i= 1:n
    A(i,i)=-2
end
for i= 1:n-1
    A(i,i+1)=1
end
for i= 2:n
    A(i,i-1)=1
end

v1=zeros(n,n)
for i= 1:n
    v1(i,i)=1/2*(100*x(i)^2)+1/3*(0*x(i)^3);
end
v2=zeros(n,n)
for i= 1:n
    v2(i,i)=1/2*(100*x(i)^2)+1/3*(10*x(i)^3);
end
v3=zeros(n,n)
for i= 1:n
    v3(i,i)=1/2*(100*x(i)^2)+1/3*(30*x(i)^3);
```

```
end
b=A/(h^2)
H1=-k*b+v1;
H2=-k*b+v2;
H3=-k*b+v3;
[T1,e1]= spec(H1)
disp('eigenvector of H is',T1)
disp('eigenvalues of H is',diag(e1))
[T3,e3]= spec(H3)
disp('eigenvector of H is',T3)
disp('eigenvalues of H is',diag(e3))
[T2,e2]= spec(H2)
disp('eigenvector of H is',T2)
disp('eigenvalues of H is',diag(e2))

subplot(3,2,1) //for ground state
plot (x,T1(:,1),'red','linewidth',3)
xlabel('Length of the Box (angstrom)')
ylabel('Wavefunction')
title('Plot of Ground State with B=0')
r=diag(e1)
disp('energy of ground state',r(1))

subplot(3,2,2)
plot (x,T1(:,2),'green','linewidth',2)
xlabel('Length of the Box (angstrom)')
ylabel('Wavefunction')
title('Plot of  firstExcited State with B=0')
disp('energy of first excited state',r(2))

subplot(3,2,3) //for ground state
plot (x,T2(:,1),'red','linewidth',3)
xlabel('Length of the Box (angstrom)')
ylabel('Wavefunction')
title('Plot of Ground State with B=10')
r=diag(e2)
disp('energy of ground state',r(1))
```

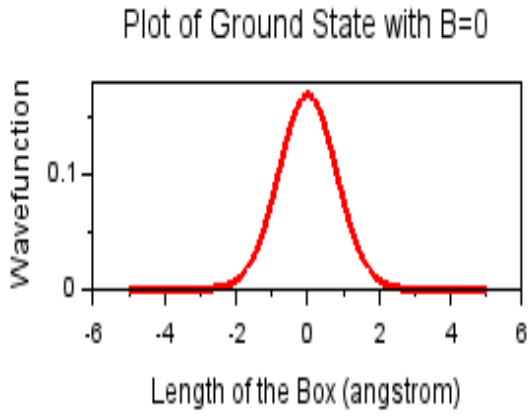
```
subplot(3,2,4)
plot (x,T2(:,2),'green','linewidth',2)
xlabel('Length of the Box (angstrom)')
ylabel('Wavefunction')
title('Plot of Excited State with B=10')
disp('energy of first excited state',r(2))

subplot(3,2,5) //for ground state
plot (x,T3(:,1),'red','linewidth',3)
xlabel('Length of the Box (angstrom)')
ylabel('Wavefunction')
title('Plot of Ground State with B=30')
r=diag(e3)
disp('energy of ground state',r(1))

subplot(3,2,6)
plot (x,T3(:,2),'green','linewidth',2)
xlabel('Length of the Box (angstrom)')
ylabel('Wavefunction')
title('Plot of Excited State with B=30')
disp('energy of first excited state',r(2))
```

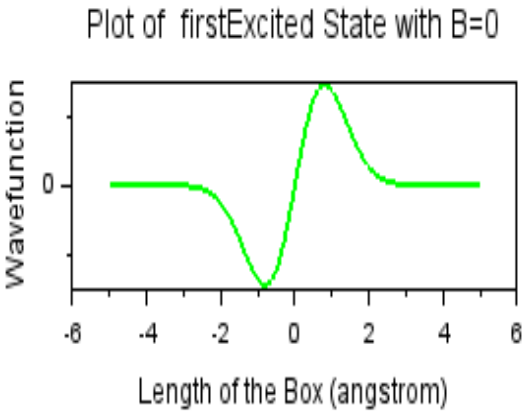
Graphical representation of all the defined/stated function with different values of B=0,10,30

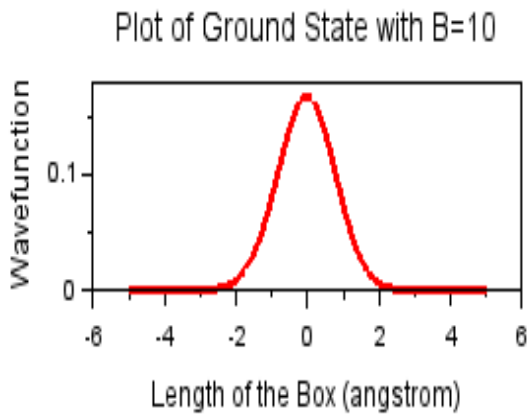
Graphic window number 0

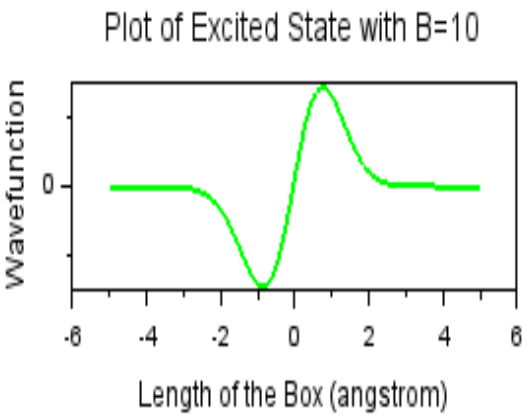
File Tools Edit ?

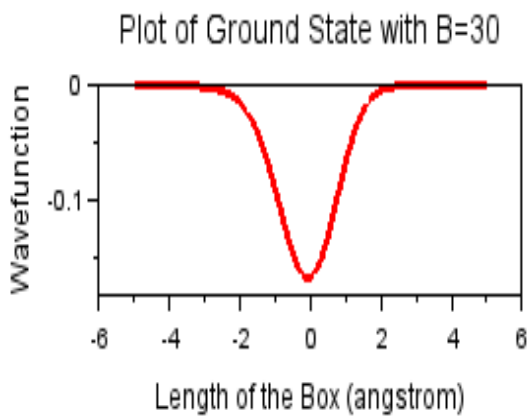
Graphic window number 0 ?











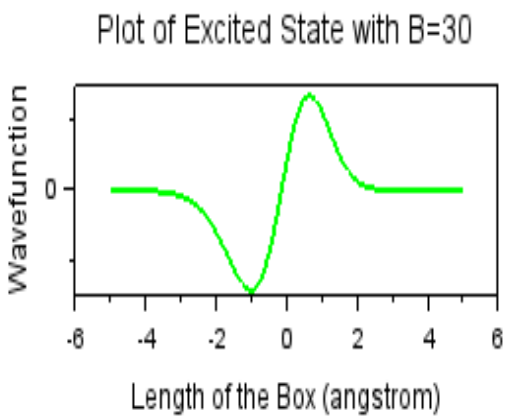


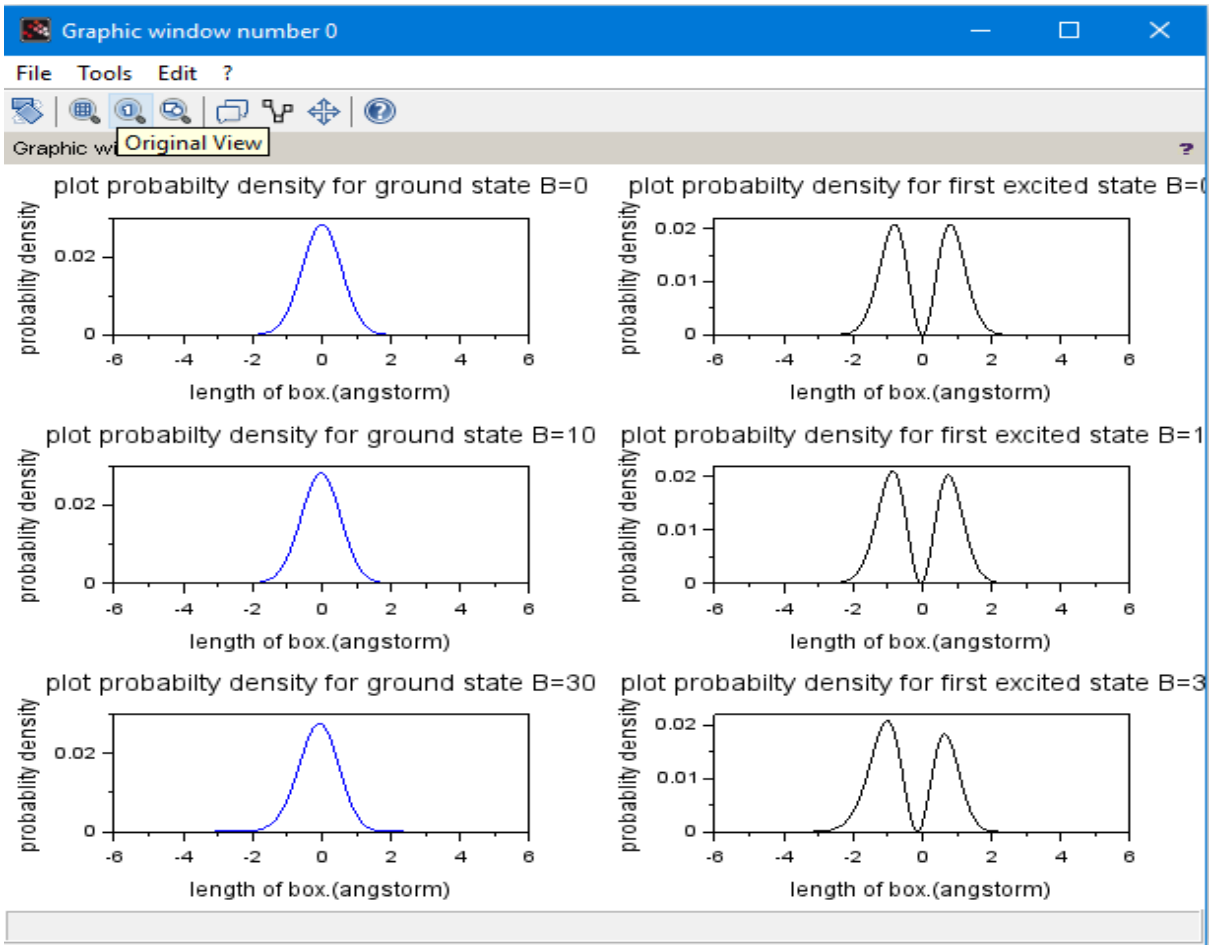
Image for the eigenfunction or energy

```
 "energy of ground state"
  32.171041
 "energy of first excited state"
  96.503038
 "energy of ground state"
  32.107318
 "energy of first excited state"
  96.089097
 "energy of ground state"
  31.556466
 "energy of first excited state"
  92.191950
```

```
//subplot(3,2,1)
//plot(x,T1(:,1).*conj(T1(:,1)),"blue")//probablity density
//title("plot probabilty density for ground state B=0")
//xlabel("length of box.(angstorm)")
//ylabel("probablity density")
//
//subplot(3,2,2)
//plot(x,T1(:,2).*conj(T1(:,2)),"black")//probablity density
//title("plot probabilty density for first excited state B=0")
//xlabel("length of box.(angstorm)")
//ylabel("probablity density")
//
//subplot(3,2,3)
//plot(x,T2(:,1).*conj(T2(:,1)),"blue")//probablity density
//title("plot probabilty density for ground state B=10")
//xlabel("length of box.(angstorm)")
//ylabel("probablity density")
```

```
//subplot(3,2,4)
//plot(x,T2(:,2).*conj(T2(:,2)),"black")//probablity density
//title("plot probabilty density for first excited state B=10")
//xlabel("length of box.(angstorm)")
//ylabel("probablity density")
//
//subplot(3,2,5)
//plot(x,T3(:,1).*conj(T3(:,1)),"blue")//probablity density
//title("plot probabilty density for ground state B=30")
//xlabel("length of box.(angstorm)")
//ylabel("probablity density")
//
//subplot(3,2,6)
//plot(x,T3(:,2).*conj(T3(:,2)),"black")//probablity density
//title("plot probabilty density for first excited state B=30")
//xlabel("length of box.(angstorm)")
//ylabel("probablity density")
```

Graphical representation of all the defined/stated function(probability density) with different value of B=0,10,30



[NOTE: Here two part of code is defined one depicts the energy eigen values and other depicts the probablilty density]NOTE: Here two part of code is defined one depicts the energy eigen values and other depicts the probablilty density]

Experiment-5

1.Write Scilab codes to solve the time independent radial wave equation for Molecule which follows Morse potential.

$$V(r) = D(e^{-2\alpha r'} - 2e^{-\alpha r'})$$

Where r'=$\frac{r-r_o}{r_o}$, r_o is the equilibrium separation α and D are constant dependent on
molecule.
2. Plot Morse potential as a function of r for different Molecules

Range of r = (1 × 10_10Å *to* 2 Å)
ħc = 1973 (eVÅ)
D (eV) =4.7446
ro (Å)= 0.7416
μ (amu)= 0.50391/c2
α =1.44055

Code for experiment 5

```
clc // to clear the Console
L=4// Unit of L in angstrom
n= input (' Enter the dimension of the Matrix')
a=0.01
h=(L-a)/(n-1)
D= 4.7446
m=940e6//Mass of electron in M ev/c^2
oc= 1973 // ev angstrom
k=((oc)^2)/(2*m)
R=0.7416
alpha=1.44056
R1=linspace(a,L,n)
R2=(R1-R)*R
A=zeros(n,n) //creat a triogonal matrix of (1,-2,1)
for i= 1:n
    A(i,i)=-2
end
for i= 1:n-1
    A(i,i+1)=1
end
```

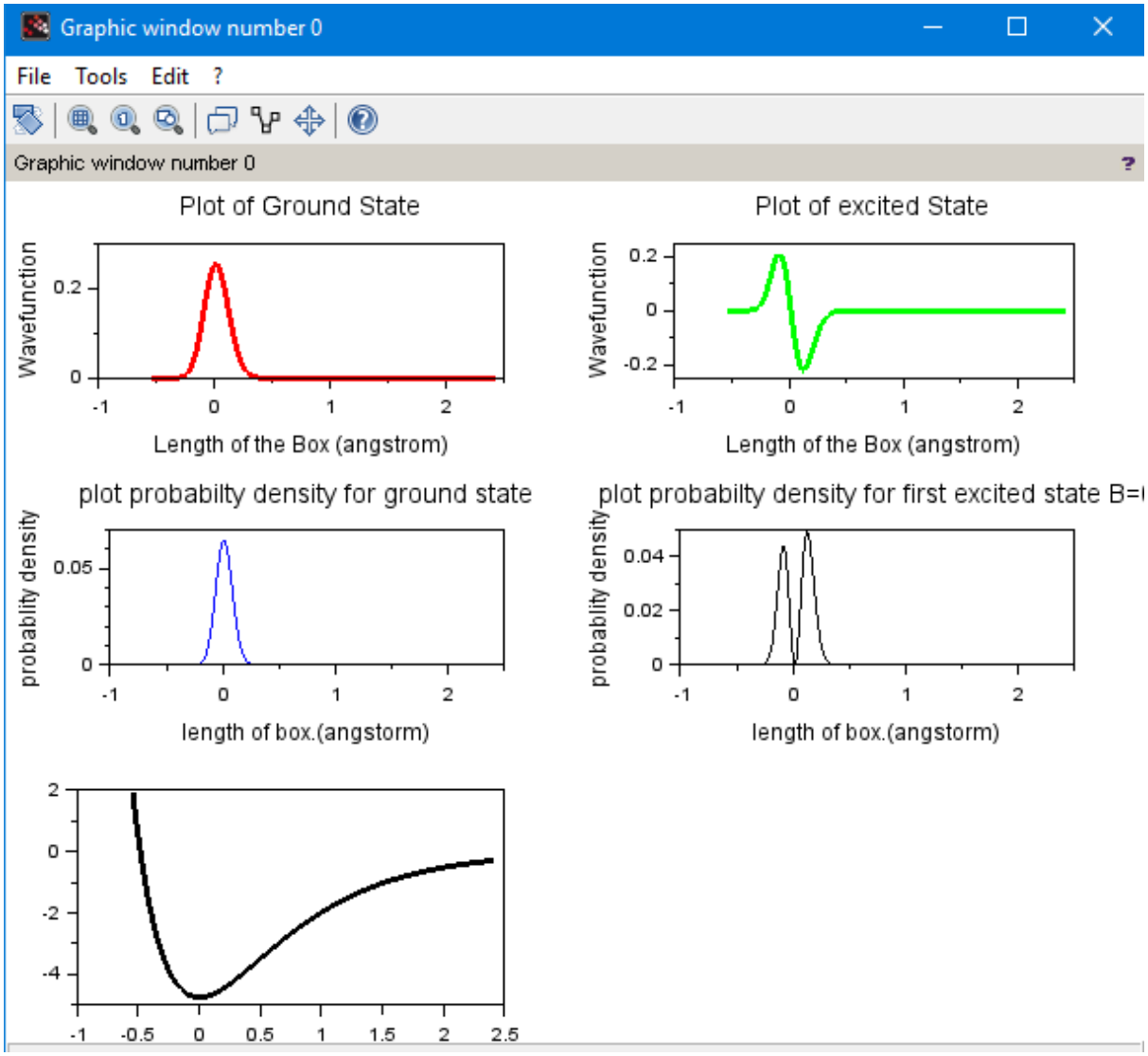
```
for i= 2:n
    A(i,i-1)=1
end
v=zeros(n,n)
for i=1:n
    v(i,i)=D*((exp(-2*alpha*R2(i)))-(2*(exp(-1*alpha*R2(i)))))
end
b=A/(h^2)
H=-k*b+v;
[p,q]= spec(H)
disp('eigenvector of H is',p)
disp('eigenvalues of H is',diag(q))

subplot(3,2,1) //for ground state
plot (R2,p(:,1),'red','linewidth',3)
xlabel('Length of the Box (angstrom)')
ylabel('Wavefunction')
title('Plot of Ground State ')
r=diag(q)
disp('energy of ground state',r(1))
subplot(3,2,2) //for first state
plot (R2,p(:,2),'green','linewidth',3)
xlabel('Length of the Box (angstrom)')
ylabel('Wavefunction')
title('Plot of excited State ')
disp('energy of ground state',r(2))
subplot(3,2,3)
plot(R2,p(:,1).*conj(p(:,1)),"blue")//probablity density
title("plot probabilty density for ground state ")
xlabel("length of box.(angstorm)")
ylabel("probablity density")
subplot(3,2,4)
plot(R2,p(:,2).*conj(p(:,2)),"black")//probablity density
title("plot probabilty density for first excited state B=0")
xlabel("length of box.(angstorm)")
ylabel("probablity density")
subplot(3,2,5)
```

```
plot(R2,diag(v),'black','linewidth',3)
```

Image for the eigenfunction or energy

```
"energy of ground state"

-4.6393879

"energy of excited state"

-4.4326637
```

Graphical representation of all the defined/stated function


Graphic window number 0
File Tools Edit ?
Graphic window number 0
Plot of Ground State
Wavefunction
0.2
0
-1 0 1 2
Length of the Box (angstrom)
Plot of excited State
Wavefunction
0.2
0
-0.2
-1 0 1 2
Length of the Box (angstrom)
plot probabilty density for ground state
probability density
0.05
0
-1 0 1 2
length of box.(angstorm)
plot probabilty density for first excited state B=
probability density
0.04
0.02
0
-1 0 1 2
length of box.(angstorm)
2
0
-2
-4
-1 -0.5 0 0.5 1 1.5 2 2.5