

Scilab Manual for
CC-XI: Quantum Mechanics & Applications
(32221501)
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Experiment: 1

Solve the s-wave Schrodinger equation for the ground state and the first excited state of the hydrogen atom.

Scilab code Solution 1.01 Hydrogen atom problem

```
1 // Submitted by Dr. Neetu Agrawal. Assistant  
  Professor , Physics Dept., Daulat Ram College ,  
  Univ. of Delhi  
2  
3 // Aim: Solve the s-wave Schrodinger equation for  
  the ground state and the first excited  
4 //state of the hydrogen atom.
```

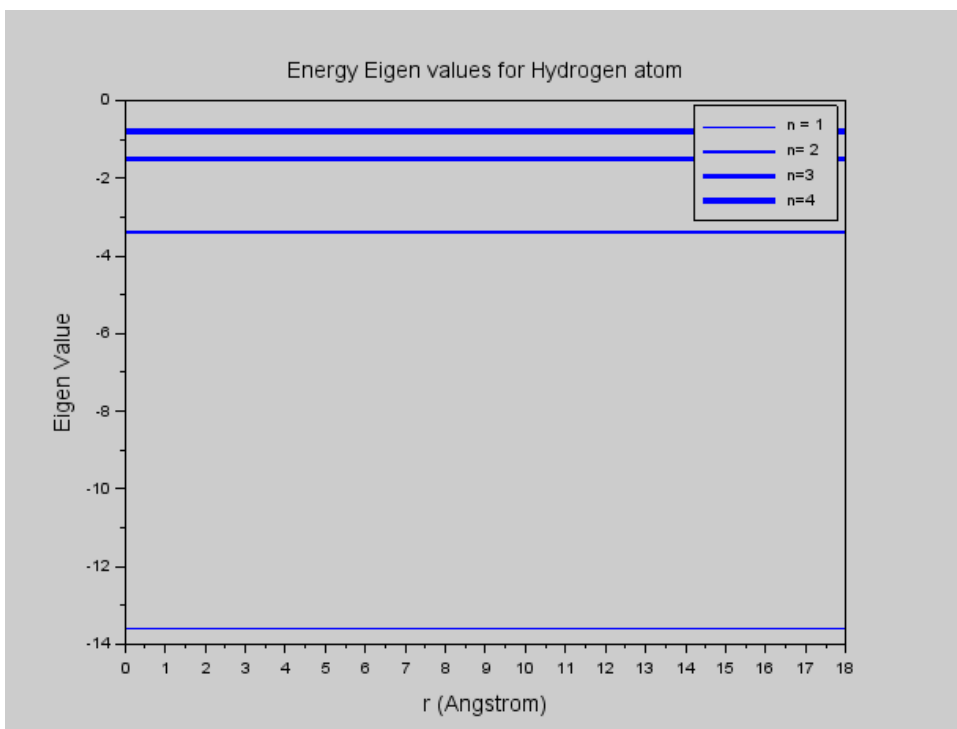


Figure 1.1: Hydrogen atom problem

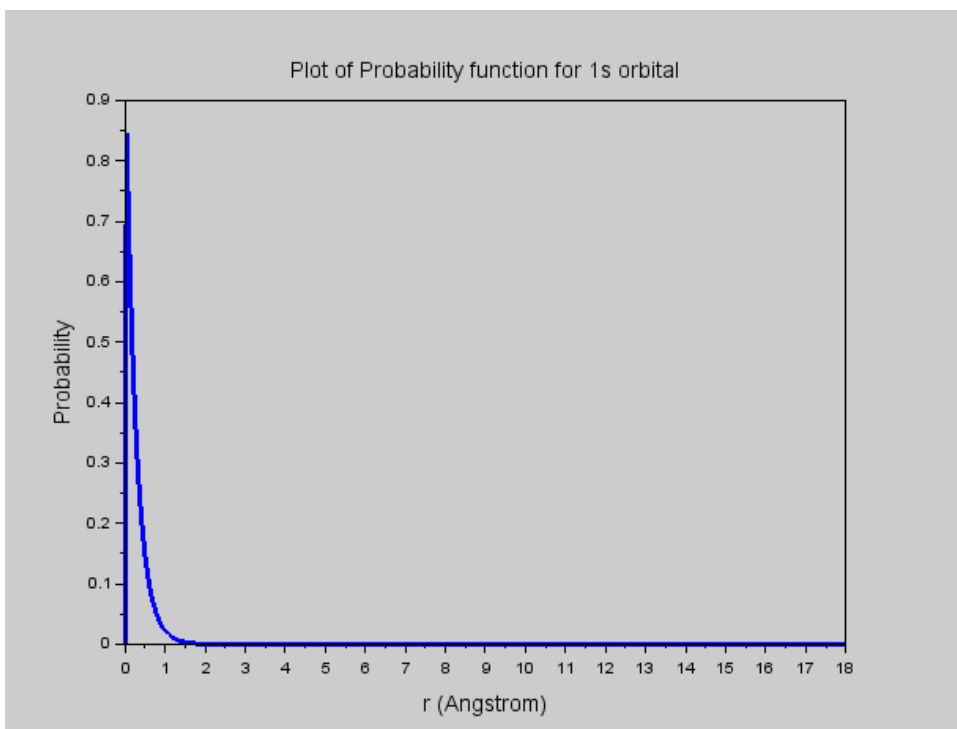


Figure 1.2: Hydrogen atom problem

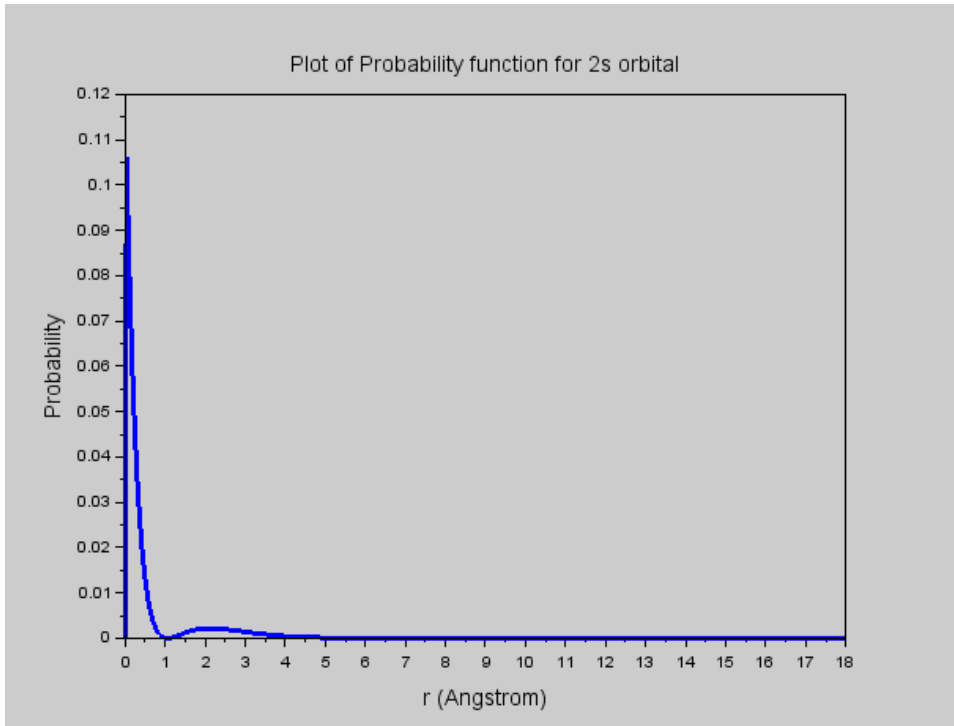


Figure 1.3: Hydrogen atom problem

```

Input the number of intervals (should be around 500 to 750 for good computation)500

Ground state energy (1S orbital) for hydrogen atom is (in eV) :

- 13.598212

First excited state (2S orbital) energy for hydrogen atom is (in eV):

- 3.4025004

Second excited state (3S orbital) energy for hydrogen atom is (in eV):

- 1.5118515

Third excited state (4S orbital) energy for hydrogen atom is (in eV):

- 0.7744925

--\

```

Figure 1.4: Hydrogen atom problem

```

5 //Here, m is the reduced mass of the electron.
   Obtain the energy eigenvalues and plot
6 // the corresponding wavefunctions. Remember that
   the ground state energy of the
7 //hydrogen atom is  $-13.6$  eV. Take  $e = 3.795$  (eV )
    $^{1/2}$ ,  $c = 1973$  (eV ) and  $m = 0.511 \times 10^6$  eV/c2.
8
9 close;
10 clear;
11 clc;
12
13 // declaring constant values
14
15 hbarc=1973;//Plancks constant h divided by 2*(pi)
   called as hbar=(h/2*pi). This factor when
   multiplied by speed of light c then hbar*c in the
   units of (eV ) comes out to be 1973;
16 mcsq=0.511*10^(6);//This is mass of electron*c ^2 we
   call it mcsq in units of (eV);
17 e = 3.795; // (eV ) ^1/2
18
19 // We hereby input the 'r' values so as to obtain
   the potential V(r) as a function of 'r')
20 r_min=0 // in units of angstrom
21 r_max=18 // in units of angstrom
22 N = input("Input the number of intervals (should be
   around 500 to 750 for good computation)")
23 s = (r_max-r_min)/N; //step size
24 factor1=-((hbarc^2)/(2*mcsq*s^2)); // this factor is
   ((hbar^2*c^2/2m*c^2) divided by s^2 //k=(hbar_c*
   hbar_c)/(2*m)
25
26 // Kinetic energy matrix (Using central difference
   formula)
27
28 T=zeros(N-1,N-1)
29 for i=1:N-1
30     T(i,i)=-2

```

```

31     if i<N-1 then
32         T(i,i+1)=1
33         T(i+1,i)=1
34     end
35 end
36
37 T_matrix = factor1*T;    // Kinetic Energy Matrix
    final (scaling done)
38
39 //Potential energy matrix
40 V_matrix=zeros(N-1,N-1)
41 for i=1:N-1
42     r(i)=r_min+i*s
43     V_matrix(i,i)=-(e*e)/r(i);
44 end
45
46 // Hamiltonian matrix
47 H_matrix=T_matrix+V_matrix
48
49 // energy eigenvalue and eigenstates
50 [u,eigen]=spec(H_matrix);
51
52 // displaying of the ground and first excited state
    energies
53 disp("Ground state energy (1S orbital) for hydrogen
    atom is (in eV) : ")
54 disp(eigen(1,1))
55 disp("First excited state (2S orbital) energy for
    hydrogen atom is (in eV): ")
56 disp(eigen(2,2))
57 disp("Second excited state (3S orbital) energy for
    hydrogen atom is (in eV): ")
58 disp(eigen(3,3))
59 disp("Third excited state (4S orbital) energy for
    hydrogen atom is (in eV): ")
60 disp(eigen(4,4))
61
62 rmatrix = [0;r;15]; //including the first and last

```

```

        point at which wavefunction is zero.
63
64 //Displaying the first four energy eigen values
65 figure(1);
66 //scf()
67 for n = 1:1:4
68 plot(rmatrix, eigen(n,n)*ones(N+1,1), 'linewidth',n)
69 hl=legend(['n = 1'; 'n= 2'; 'n=3'; 'n=4']);
70 title('Energy Eigen values for Hydrogen atom', '
        fontsize',3)
71 xlabel('r (Angstrom)', 'fontsize',3)
72 ylabel('Eigen Value', 'fontsize',3)
73 end
74
75 //Plotting the Probability |Psi^2| as a function of
        r
76 figure(2);
77 //scf()
78 R_wave_1s=u(:,1)./r; //Radial wavefunction
79 R_wave_1s_final=[0;R_wave_1s;0]; //including the
        first and last point at which wavefunction is
        zero.
80 // plot of probability function
81 P_wave_1s= R_wave_1s_final.*R_wave_1s_final;
82 plot(rmatrix,P_wave_1s, 'linewidth',3)
83 title('Plot of Probability function for 1s orbital',
        'fontsize',3)
84 xlabel('r (Angstrom)', 'fontsize',3)
85 ylabel('Probability', 'fontsize',3)
86
87 figure(3);
88 //scf()
89 R_wave_2s=u(:,2)./r;
90 R_wave_2s_final=[0;R_wave_2s;0]; //including the
        first and last point at which wavefunction is
        zero.
91 // plot of probability function
92 P_wave_2s= R_wave_2s_final.*R_wave_2s_final;

```

```
93 plot(rmatrix,P_wave_2s, 'linewidth',3)
94 title('Plot of Probability function for 2s orbital',
        'fontsize',3)
95 xlabel('r (Angstrom)', 'fontsize',3)
96 ylabel('Probability', 'fontsize',3)
```

Experiment: 2

Solve the s-wave radial Schrodinger equation for an atom for the screened coulomb potential.

Scilab code Solution 2.0 Screened coulomb potential

```
1 //Solve the s-wave Schrodinger equation for the
   ground state and the first excited
2 //state of the hydrogen atom.
3
4 close;
5 clear;
6 clc;
7
8 // declaring constant values
9 hbarc=1973;// Plancks constant = h , hbar*c=(h/2*pi)
   ^c.
10 mcsq=0.511*10^(6); // (mass of electron)*c ^2 in
   units of (eV);
11 e = 3.795; // (eV )^1/2
12 //a = input("Input the vaue of a in units of
```

```

        angstrom: ") ;
13 a=3 ; // in units of Angstrom
14 // we can check it for 3, 5, 7 angstrom etc..
15
16 r_min=0 // in units of angstrom
17 r_max=5 // in units of angstrom
18 N = input("Input the number of intervals (should be
        around 500 to 1000 for good computation): ")
19 s = (r_max-r_min)/N; //step size
20 factor1=-(hbar*c^2)/(2*mcsq*s^2);
21 // this factor is (hbar^2*c^2/2m*c^2) divided by s^2
        //k=(hbar_c*hbar_c)/(2*m)
22
23 // Kinetic energy matrix (Using central difference
        formula)
24 T=zeros(N-1,N-1)
25 for i=1:N-1
26     T(i,i)=-2
27     if i<N-1 then
28         T(i,i+1)=1
29         T(i+1,i)=1
30     end
31 end
32 // Kinetic Energy Matrix final (scaling factor
        included)
33 T_matrix = factor1*T;
34
35 //Potential energy matrix
36 V_matrix=zeros(N-1,N-1)
37 for i=1:N-1
38     r(i)=r_min+i*s
39     V_vector(i,1) = -((e*e)/r(i))*exp(-r(i)/a);
40     V_matrix(i,i)=-((e*e)/r(i))*exp(-r(i)/a);
41 end
42
43 // This is to plot the potential V(r)as a function
        of r
44 figure;

```

```

45 plot(r,V_vector, '-.', 'linewidth',3)
46 xlabel('r (in Angstrom units)', 'fontsize',2)
47 ylabel('V(r)', 'fontsize',2)
48 legend(['Screened coloumb potential'])
49
50 // Hamiltonian matrix
51 H_matrix=T_matrix+V_matrix
52
53 // energy eigenvalue and eigenstates
54 [u,eigen]=spec(H_matrix);
55
56 // displaying of the groundstate energies
57 disp("Ground state energy in the presence of
      screened coloumb potential is : ")
58 disp(eigen(1,1))
59
60 //Radial wavefuction
61 figure();
62 Psi=u(:,1)./r;
63 plot(r,Psi, 'm', 'linewidth',3)
64 title('Eign function plot in presence of screened
      coloumb potential', 'fontsize',2)
65 xlabel('r (in Angstrom units)', 'fontsize',2)
66 ylabel('Eigen Function', 'fontsize',2)
67 legend(['Ground state wavefunction'])

```

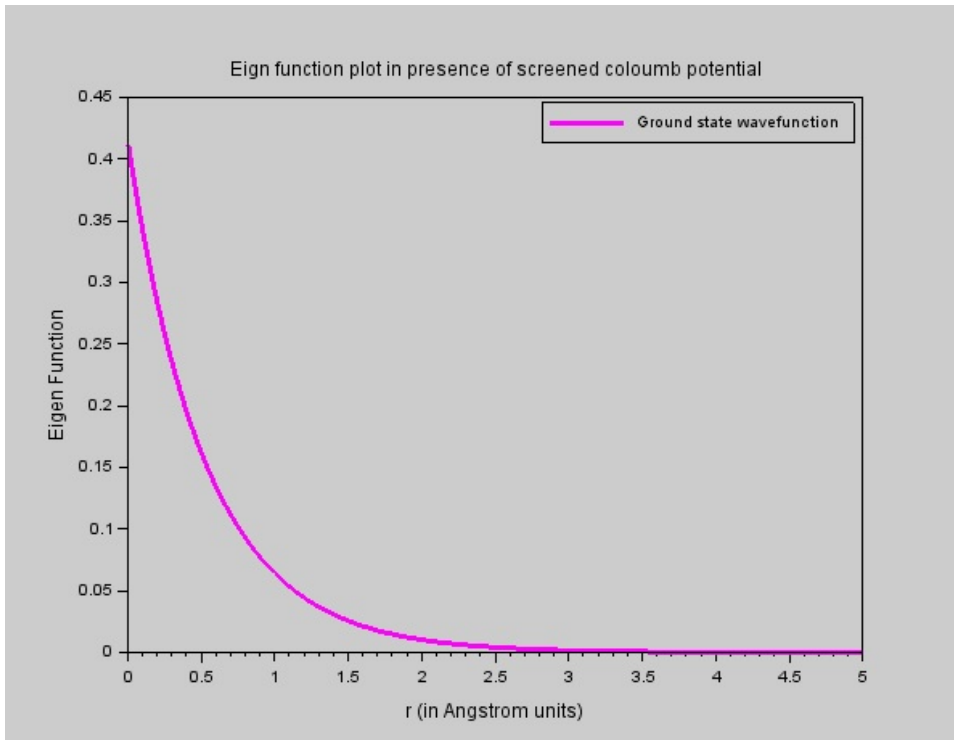


Figure 2.1: Screened coulomb potential

```

Scilab 6.1.0 Console
Input the number of intervals (should be around 500 to 1000 for good computation): 750

"Ground state energy in the presence of screened coloumb potential is : "
-9.3865350
-->

```

Figure 2.2: Screened coulomb potential

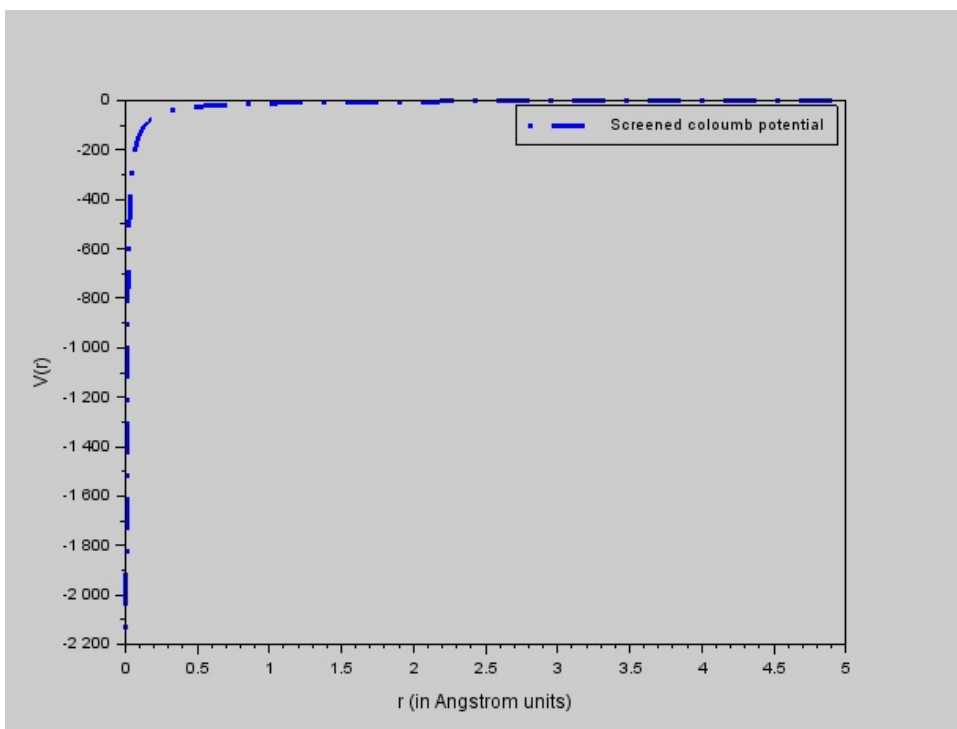


Figure 2.3: Screened coulomb potential

Experiment: 3

Solve the s-wave radial Schrodinger equation for a particle of mass m , for an harmonic oscillator potential. Plot wavefunctions.

Scilab code Solution 3.0 Harmonic Oscillator

```
1 //Solve the s-wave radial Schrodinger equation for a
   particle of mass m
2 //for an harmonic oscillator potential for ground
   state energy (in MeV).
3
4 close;
5 clear;
6 clc;
7
8 // declaring constant values
9 hbarc=197.3 //Plancks constant h divided by 2*(pi)
   called as hbarc=(h/2*pi)*c.
10 mcsq=940; // mass of electron*c^2 = mcsq in units
```

```

    of (MeV);
11 k = 100; // harmonic oscillator potential constant
    in units of MeV fm-2
12 b = 0;
13 disp("The value of b in the potential is chosen to
    be:");
14 disp(b)
15 //To obtain the plot the potential V(r) as a
    function of 'r'
16 r_min = 0;
17 r_max = 4;
18 N = input("Input the number of intervals (should be
    around 500 to 1000 for good computation: )")
19 s = (r_max-r_min)/N; //step size
20 factor1=-(hbarc^2)/(2*mcsq*s^2);
21
22 // making a row vector to input r values
23 for i=1:1:N
24     rmat(1,i)=r_min+(i-1)*s
25 end
26
27 for ir = 1:1:size(rmat,2)
28     r = rmat(ir);
29 V(1,ir) = 0.5*k*(r)^2 + 0.5*b*(r)^3;
30 end
31 figure;
32 plot(rmat,V,'-.','linewidth',3)
33
34 // Kinetic energy matrix (Using central difference
    formula)
35 T=zeros(N,N)
36 for i=1:1:N
37     T(i,i)=-2;
38     if (i<N)
39         T(i,i+1)=1;
40         T(i+1,i)=1
41     end
42 end

```

```

43
44 T_matrix = factor1*T; // Kinetic Energy Matrix final
    in MeV
45
46 // Potential energy matrix in MeV
47 U_matrix = zeros(N,N)
48 for i = 1:1:N
49 U_matrix(i,i)=V(i)
50 end
51
52 // Hamiltonian matrix
53 Ham = T_matrix+U_matrix;
54 [u,eigen] = spec(Ham);
55 eigval_numeric = spec(Ham)
56
57
58 disp ('The first five eigen values obtained using
    FDM are:')
59 disp(eigval_numeric(1:5))
60
61 //Plotting the eigenvalues obtained by numerical
    computation
62
63 for n =1:1:5
64     eigvalue_num = eigval_numeric(n)
65     eigvalue_num_vector = eigvalue_num*ones(1,N);
66     plot(rmat,eigvalue_num_vector,'r')
67 end
68
69
70 // normalisation check (The value comes out to be 1)
71 normalisation = sum((u(:,1).*conj(u(:,1))))
72
73 // plotting the eigen functions.
74 //(plot of mod psi squared). Done the scaling of
    eigen function magnitude
75
76 psisq1 = (1/normalisation)*(u(:,1).*conj(u(:,1)))

```

```

77 plot(rmat(1,:),8000*psisq1'+eigval_numeric(1),'k')
78
79 psisq2 = (1/normalisation)*(u(:,2).*conj(u(:,2)))
80 plot(rmat(1,:),8000*psisq2'+eigval_numeric(2),'k')
81
82 psisq3 = (1/normalisation)*(u(:,3).*conj(u(:,3)))
83 plot(rmat(1,:),8000*psisq3'+eigval_numeric(3),'k')
84
85 psisq4 = (1/normalisation)*(u(:,4).*conj(u(:,4)))
86 plot(rmat(1,:),8000*psisq4'+eigval_numeric(4),'k')
87
88 psisq5 = (1/normalisation)*(u(:,5).*conj(u(:,5)))
89 plot(rmat(1,:),8000*psisq5'+eigval_numeric(5),'k')
90
91 title('Plot of first 5 probability density functions
', 'fontsize',2);
92 xlabel('r (in fm) —>', 'fontsize',2)
93 ylabel('Energy(in MeV)and scaled probability density
functions)', 'fontsize',2)
94
95 legend(['Potential Plot', 'Eigenvalues'])

```

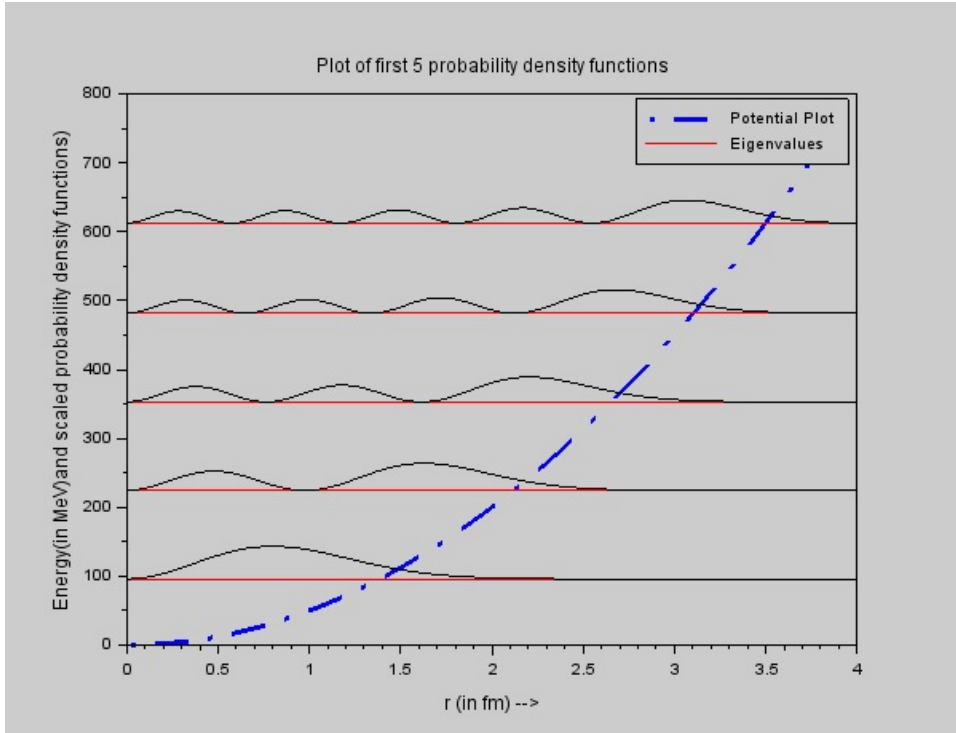


Figure 3.1: Harmonic Oscillator

```

Scilab 6.1.0 Console

"The value of b in the potential is chosen to be:"

0.
Input the number of intervals (should be around 500 to 1000 for good computation: )700

"The first five eigen values obtained using FDM are:"

96.011767
224.45556
352.969
481.69927
612.51479

--> |

```

Figure 3.2: Harmonic Oscillator

Experiment: 4

Solve the s-wave radial Schrodinger equation for the vibrations of hydrogen molecule. Find the lowest vibrational energy (in MeV

Scilab code Solution 4.0 Morse Potential

```
1 //This program solves the s-wave radial Schrodinger
  equation for the vibrations of hydrogen molecule
  for the Morse potential
2 //Find the lowest vibrational energy (in MeV) of the
  molecule. Also plot the corresponding wave
  function. //Take: m = 940x106 eV/c2, D = 0.755501
  eV, r0 = 1.44, //Where s
  the reduced mass of the two-atom system for the
  Morse potential //Find the lowest vibrational
```

```

Enter the number of intervals(should be around 500 to 1000 for good computation)750
Warning : redefining function: eval . Use funcprot(0) to avoid this message

The Eigenvalues calculated using FDM are

0.4042986
0.7535893
0.8403509
0.9841226

-->

```

Figure 4.1: Morse Potential

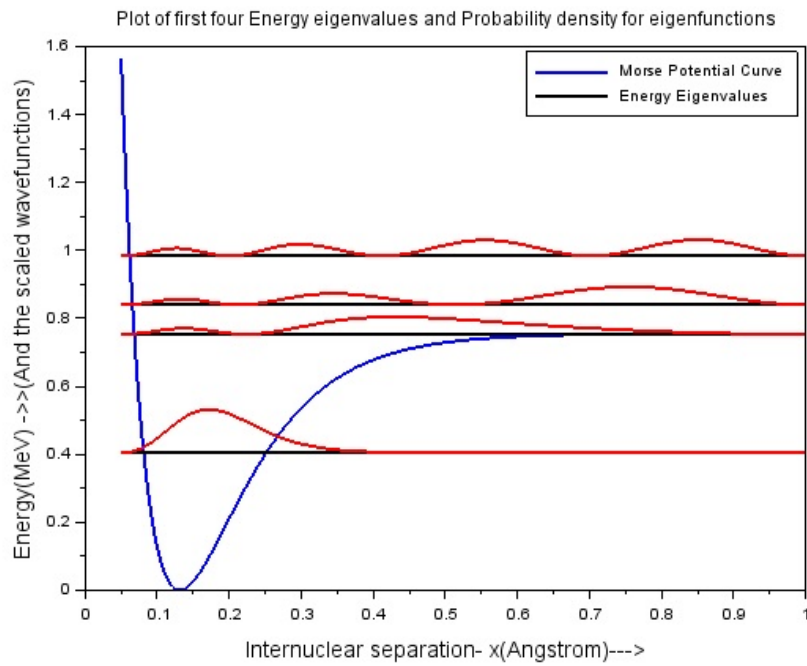


Figure 4.2: Morse Potential

energy (in MeV) of the molecule to an accuracy of three significant digits. Also plot the // corresponding wave function. //Take: $m = 940 \times 10^6$ eV/c², $D = 0.755501$ eV, $\alpha = 1.44$, $x_0 = 0.131349$

```

3
4 clear
5 close
6 clc
7
8 //Declaring the values of constants
9 hcutc=1973 //Planck's constant h divided by 2*pi (
    hcut=h/2*pi).This when multiplied by speed of
    light c gives hcutc(in units of eV A)
10 mcsq=940*10^6; //mass*c^2 in units of eV/c^2
11
12 x0=0.131349 //In units of Angstrom
13 alpha=1.44 //a*x0 where 'a' is a constant for
    particulare molecule
14 D=0.755501 //Dissociation Energy In units of eV
15
16 //Getting values of x to plot 'V(x)' v/s 'x' plot
17 xmin=0.05; //in units of A^o
18 xmax=1; //in units of A^o
19
20 n=input("Enter the number of intervals(should be
    around 500 to 1000 for good computation)");
21 s=(xmax-xmin)/n; //step size
22
23 for i=1:1:n
24 x(1,i)=xmin+s*(i-1); //x vector of 1 row and n
    columns to input values of internuclear
    seperation
25 x_(1,i)=(x(1,i)-x0)/x0 //x_ vector= (x-x0)/x0
26 end
27
28 factor1=-(hcutc^2)/(2*mcsq*s^2) //this factor is (
    hcut^2*c^2/2*m*c^2*s^2)

```

```

29
30 //plot of potential V(x) v/s x
31 V=zeros(n,n); //Potential energy matrix
32 for i=1:1:n
33 V_matrix(i,i)=(D*(1-exp(-alpha*x_(1,i)))^2) //
    formula for potential
34 end
35
36 for j=1:1:size(V_matrix,2)
37 V_vec(1,j)=V_matrix(j,j)
38 end
39 plot(x,(V_vec),"linewidth",2) //linewidth command to
    set width of line
40 title("Plot of first four Energy eigenvalues and
    Probability density for eigenfunctions","fontsize
    ",2) //title of the plot
41 xlabel('Internuclear separation - x(Angstrom)---->',"
    fontsize",3) //fontsize command to set the font
    size of labels
42 ylabel('Energy(MeV) ->>(And the scaled wavefunctions
    )',"fontsize",3)
43
44 for i=1:1:n
45 for j=1:1:n
46 if i==j then
47 K(i,j)=-2;
48 elseif i==(j-1) | i==(j+1) then
49 K(i,j)=1;
50 else
51 K(i,j)=0;
52 end
53 end
54 end
55 T_matrix=factor1*K; //Kinetic energy matrix
56 H_matrix=V_matrix+T_matrix; //Hamiltonian matrix
57 eval=spec(H_matrix); //eval stores the eigenvalues
    of matrix H
58 [a,b]=spec(H_matrix); //a stores the eigenvectors

```

```

59 disp("The Eigenvalues calculated using FDM are")
60 for i=1:1:4
61 disp(eval(i,1))
62 end
63
64 //Plotting the eigenvalues obtained by Numerical
    computation
65 for i=1:1:4
66 eval_num=eval(i)
67 eval_num_vec=eval_num*ones(1,n)
68 plot(x,eval_num_vec,'k',"linewidth",2)
69 end
70 //normalization check
71 normalisation=sum(a(:,1).*conj(a(:,1)));
72 //Plotting the first four Eigen functions (plot of
    mod psi square).We do the scaling of Eigen
    functions magnitudes by
73 //a factor of 15 and raise to level of eigen values
    and
74 //eigen functions on the same line
75 psisq1=(1/normalisation)*(a(:,1).*conj(a(:,1)))
76 psisq2=(1/normalisation)*(a(:,2).*conj(a(:,2)))
77 psisq3=(1/normalisation)*(a(:,3).*conj(a(:,3)))
78 psisq4=(1/normalisation)*(a(:,4).*conj(a(:,4)))
79 plot(x(1,:),15*psisq1'+eval(1),'r',"linewidth",1.5)
80 plot(x(1,:),15*psisq2'+eval(2),'r',"linewidth",1.5)
81 plot(x(1,:),15*psisq3'+eval(3),'r',"linewidth",1.5)
82 plot(x(1,:),15*psisq4'+eval(4),'r',"linewidth",1.5)
83 legend(['Morse Potential Curve','Energy Eigenvalues
    '])

```

Experiment: 5

Plot and analyse the wavefunctions for particle in an infinite potential well.

Scilab code Solution 5.0 1D Box potential

```
1  close
2  clear
3  clc
4
5  //This is program calculates the energy eigen vaules
   and eigen functions
6  //for a particle in an infinite potential well of
   width a
7
8
9  // declaring constant values
```

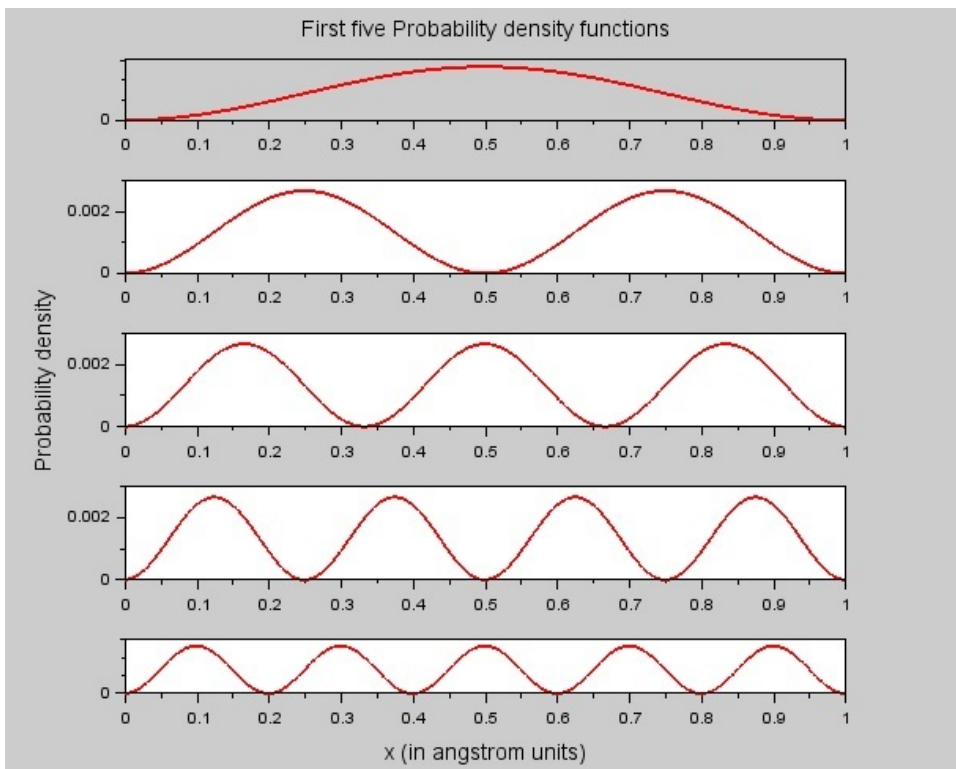


Figure 5.1: 1D Box potential

```

Scilab 6.1.0 Console

"The box size is (in meters):"

1.000D-10
Input the number of intervals (should be around 500 to 1000 for good computation)750

"The Eigen (eV) values obtained from Finite difference method are :"

```

Figure 5.2: 1D Box potential

```

10 m = 9.1e-31; // mass of electron
11 hplanck= 6.63*1e-34 // value of plancks constant
12 hbar = hplanck/(2*%pi) // value of h/2*pi (let we
    call it hbar)
13 hbarsqbytwo_m_term = (hbar^2)/(2*m); //(value of
    hbar square by 2*m)
14 eV = 1.6e-19; // vale of electron volt si units
15 MeV = (1e+6)*eV; // writing Mega electron volt
16 Angst = 1e-10; // value of one angstrom
17
18 x_min = 0;
19 x_max = 1*Angst; //This value can be changed to
    change width of 1D box
20
21 disp ('The box size is (in meters):' )
22 disp(x_max)
23
24 N = input("Input the number of intervals (should be

```

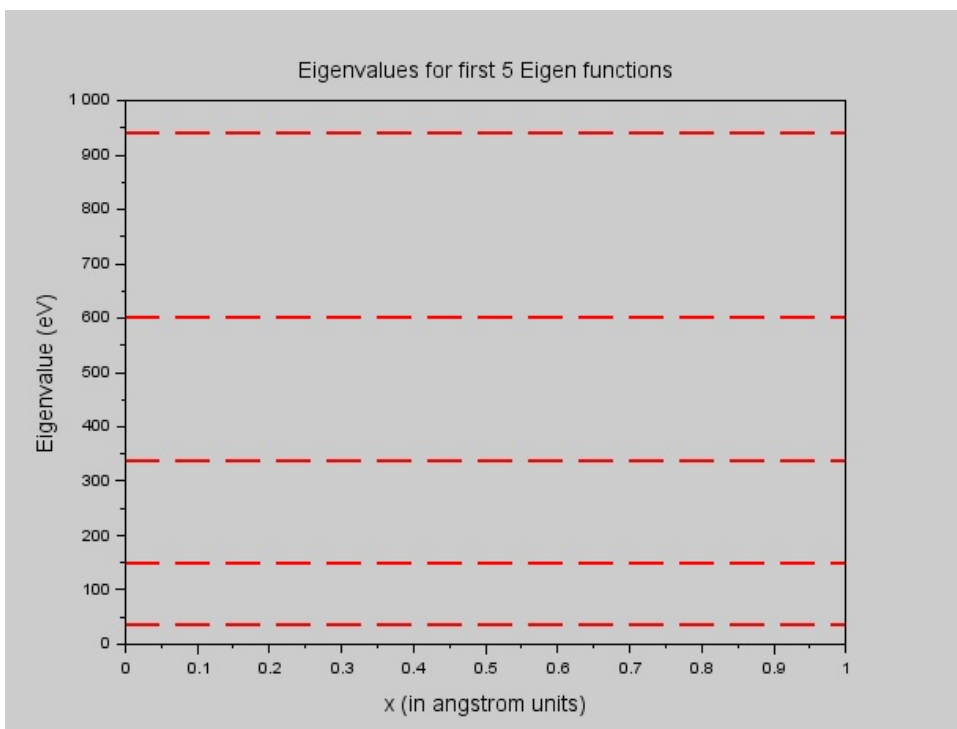


Figure 5.3: 1D Box potential

```

        around 500 to 1000 for good computation)”)
25 a = (x_max-x_min); // width of 1 d box
26 s = (x_max-x_min)/N; // step size
27 fac = -hbarsqbytwo_m_term/(s^2); // this factor
    is (hbar^2/2m) divided by h^2
28
29 // making a row vector to input x values
30 for i=1:1:N
31     x(1,i)=x_min+(i-1)*s
32 end
33 // Kinetic energy matrix (Using central difference
    formula)
34 T=zeros(N,N)
35 for i=1:1:N
36     T(i,i)=-2;
37     if (i<N)
38         T(i,i+1)=1;
39         T(i+1,i)=1
40     end
41 end
42 T_matrix = fac*T/eV; // Kinetic Energy Matrix in eV
43
44 // potential energy matrix
45 U_matrix = zeros(N,N)
46 for i = 1:1:N
47     U_matrix(i,i)=0;
48 end
49
50 // Hamiltonian matrix H=U+T
51 H_matrix = T_matrix+U_matrix;
52 [u,eigen] = spec(H_matrix);
53 eigval_numeric = spec(H_matrix)
54
55 // normalisation check
56 normalisation = sum((u(:,1).*conj(u(:,1))))
57
58 // By theoretically achieved Formulae
59 for n= 1:1:5

```

```

60 eigval_theory = (n^2*%pi^2*hbar^2)/(2*m*a^2) // in
    SI units
61 eigval_th_eV(n) = eigval_theory/eV // in eV
62 end
63
64 disp('The Eigen (eV) values obtained from Finite
    difference method are :')
65 disp(eigval_numeric(1:5))
66 disp('The Eigen values (eV) obtained from Analytic
    Formula are :')
67 disp(eigval_th_eV(1:5))
68
69 //Plotting the eigenvalues
70 figure;
71 for n =1:1:5
72     temp1 = eigval_numeric(n)
73     eigval_numeric_vector = temp1*ones(1,N);
74     plot(x/Angst,eigval_numeric_vector,'r—', '
        linewidth', 2)
75     xlabel('x (in angstrom units)', 'fontsize',3)
76     ylabel('Eigenvalue (eV)', 'fontsize',3)
77     title('Eigenvalues for first 5 Eigen functions',
        'fontsize',3)
78 end
79
80
81 // plotting the Probbility functions. (plot of mod
    psi squared)
82
83 figure;
84 for in =1:1:5
85     psisq(:,in) = (u(:,in).*conj(u(:,in)))
86 end
87
88 subplot(5,1,1)
89 title('First five Probability density functions',
    fontsize',3)
90 plot(x(1,:)/Angst,psisq(:,1)')', 'r', 'linewidth',2)

```

```
91 subplot(5,1,2)
92 plot(x(1,:)/Angst,psisq(:,2)','','linewidth', 2)
93 subplot(5,1,3)
94 plot(x(1,:)/Angst,psisq(:,3)','','linewidth', 2)
95 ylabel("Probability density",'fontsize',3)
96 subplot(5,1,4)
97 plot(x(1,:)/Angst,psisq(:,4)','','linewidth', 2)
98 subplot(5,1,5)
99 plot(x(1,:)/Angst,psisq(:,5)','','linewidth', 2)
100 xlabel("x (in angstrom units)",'fontsize',3)
```
