Scilab Manual for CC-XI: Quantum Mechanics & Applications (32221501) by Dr Neetu Agrawal Physics Daulat Ram College, University Of Delhi ¹

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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} \text{ eV}/\text{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)<sup>1</sup>/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*
      h b a r_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
       T(i,i) = -2
30
```

```
31
       if i<N-1 then
32
            T(i, i+1) = 1
            T(i+1,i) = 1
33
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
       V_{matrix(i,i)} = -(e*e)/r(i);
43
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
                                                       \mathrm{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 \operatorname{disp}(\operatorname{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 \text{ 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<sup>2</sup>| as a function of
76 figure(2);
77 // scf()
78 R_wave_1s=u(:,1)./r; //Radial wavefuction
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)

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=-(hbarc^2)/(2*mcsq*s^2);
21 // this factor is (hbar2*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 \text{ for } i=1:N-1
       T(i,i) = -2
26
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 \text{ for } i=1:N-1
       r(i)=r_min+i*s
38
39
       V_vector(i,1) = -((e*e)/r(i))*exp(-r(i)/a);
       V_{matrix(i,i)} = -((e * e)/r(i)) * exp(-r(i)/a);
40
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 \operatorname{disp}(\operatorname{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



Figure 2.2: Screened coulomb potential



Figure 2.3: Screened coulomb potential

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 \text{ 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
       rmat(1,i)=r_min+(i-1)*s
24
25 end
26
27 for ir = 1:1:size(rmat,2)
       r = rmat(ir);
28
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)</pre>
39
           T(i, i+1) = 1;
           T(i+1,i) = 1
40
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 \text{ for } i = 1:1:N
49 U_matrix(i,i)=V(i)
50 \text{ 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
       eigvalue_num = eigval_numeric(n)
64
65
       eigvalue_num_vector = eigvalue_num*ones(1,N);
       plot(rmat,eigvalue_num_vector,'r')
66
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) \longrightarrow', '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



Figure 3.2: Harmonic Oscillator

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: $m = 940 \times 106 \text{ eV/c2}$, D = 0.755501 eV, = 1.44, r0 = 0.131349 //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 106
     eV/c2, D = 0.755501 eV, = 1.44, ro = 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
      particular 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<sup>o</sup>
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 \text{ 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) \rightarrow >>(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
     to make the conventional plot with 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
      '])
```

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

```
"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 :"
  37.637235
  150.54828
  338.73117
  602.18259
  940.89795
 "The Eigen values (eV) obtained from Analytic Formula are :"
  37.737723
  150.95089
  339.63951
  603.80357
  943.44308
-->
```



```
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 elctron volt
16 Angst = 1e-10; // value of one angstrom
17
18 \text{ 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
       x(1,i) = x_{min} + (i-1) * s
31
32 end
33 // Kinetic energy matrix (Using central difference
      formula)
34 \quad T=zeros(N,N)
35 for i=1:1:N
       T(i,i) = -2;
36
       if (i<N)</pre>
37
38
           T(i,i+1) = 1;
           T(i+1,i)=1
39
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 \text{ 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
       temp1 = eigval_numeric(n)
72
       eigval_numeric_vector = temp1*ones(1,N);
73
       plot(x/Angst,eigval_numeric_vector,'r-', '
74
          linewidth', 2)
       xlabel('x (in angstrom units)', 'fontsize',3)
75
       ylabel('Eigenvalue (eV)', 'fontsize',3)
76
       title('Eigenvalues for first 5 Eigen functions',
77
          '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)', 'r', 'linewidth', 2)
93 subplot(5,1,3)
94 plot(x(1,:)/Angst,psisq(:,3)', 'r', 'linewidth', 2)
95 ylabel("Probability density", 'fontsize',3)
96 subplot(5,1,4)
97 plot(x(1,:)/Angst,psisq(:,4)', 'r', 'linewidth', 2)
98 subplot(5,1,5)
99 plot(x(1,:)/Angst,psisq(:,5)', 'r', 'linewidth', 2)
100 xlabel("x (in angstrom units)", 'fontsize',3)
```