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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

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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
0053     plot(r(i),U(i,3),"b-","linewidth",2,"markersize",2)
0054     xgrid()
0055     legend("Ground State","First Excited State")
0056     ylabel("Wave Function u(r)")
0057     xlabel("r")
0058     title('Numerical')
0059     subplot(2,2,2)
0060
0061     plot(r(i),U(i,2)**2,"r*","linewidth",2,"markersize",2)
0062
0063     plot(r(i),U(i,3)**2,"b-","linewidth",2,"markersize",2)
0064     xgrid()
0065     legend("Ground State","First Excited State")
0066     ylabel("Probability Density u(r)*u(r)")
0067     xlabel("r")
0068     title('Numerical')
0069     subplot(2,2,3)
0070
0071     x = [0:0.1:10]
0072     plot((2/b^(3/2))*x.*exp(-x/b),'r')
0073
0074     plot(1/b^(3/2)*(x.*exp(-x/(2*b)) - 1/(2*b)*x^2.*exp(-x/(2*b))))
0075     xgrid()
0076     legend("Ground State","First Excited State")

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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
0084         plot((1/b^(3/2)*(x.*exp(-x/(2*b)) - 1/(2*b)*x^2.*exp(-x/(2*b))))^2)
0085         xgrid()
0086         legend("Ground State","First Excited State")
0087         ylabel("Probability Density u(r)*u(r)")
0088         xlabel("r")
0089         title('Theoretical')
0090     end

```