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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);

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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

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