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0001  //SOLVE Schrodinger equation for H-atom in Screened
      Anharmonic Oscillator potential (using Finite Difference
      Method)
0002
0003  clc; clear; clf;      //Clearing console, variables and fig
0004
0005  //Describing Constants : h, k, m, b1, b2, b3
0006  h=197.3; k=100; m=940; b1=0; b2=10; b3=30;
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)=(k*(r(i)^2))/2 + (b1*(r(i)^3))/3;
0016  end
0017  V2=zeros(n,n);
0018  for i=1:n
0019      V2(i,i)=(k*(r(i)^2))/2 + (b2*(r(i)^3))/3;
0020  end
0021  V3=zeros(n,n);
0022  for i=1:n
0023      V3(i,i)=(k*(r(i)^2))/2 + (b3*(r(i)^3))/3;
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);

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0041 [U3,EV3]=spec(H3);
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 b=0, 10 and
    30",[E1(1) E2(1) E3(1)],"1st Excited State Energy (in eV)for
    b=0, 10 and 30",[E1(2) E2(2) E3(2)])
0048
0049 //Plotting Wavefunctions at GS State & 1st Excited State
0050 subplot(3,1,1)
0051 plot(r',[abs(U1(:,1))**2,abs(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("b=0","position",[5 0.08])
0056
0057 subplot(3,1,2)
0058 plot(r',[abs(U2(:,1))**2,abs(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("b=10","position",[5 0.08])
0063
0064 subplot(3,1,3)
0065 plot(r',[abs(U3(:,1))**2,abs(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("b=30","position",[5 0.08])

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