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0001 //SOLVE Schrodinger equation for H-atom in Morse potential
      (using Finite Difference Method)
0002
0003 clc; clear; clf;      //Clearing console, variables and fig
0004
0005 //Describing Constants
0006 h=1973; D=0.755501; m=940*10^6; a=1.44; ro=0.131349;
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 Morse Potential using given formula
0013 V=zeros(n,n);
0014 for i=1:n
0015     rp=(r(i)-ro)/r(i);
0016     V(i,i)=D*(exp(-2*a*rp)-exp(-a*rp));
0017 end
0018
0019 //Defining Kinetic Energy using given formula
0020 K=eye(n,n)*(-2);
0021 for i=1:(n-1)
0022     K(i,i+1)=1;
0023     K(i+1,i)=1;
0024 end
0025
0026 //Defining Hamiltonian Matrix using given formula
0027 H=(-(h^2)/(2*m*d^2))*K+V;
0028
0029 //Evaluating Eigenvalues & Eigenvectors of H matrix
      using "spec" function
0030 [U,EV]=spec(H); //U=Eigenvectors(used to plot
      Wavefunction) & EV=Eigenvalues(used to find Energies)
0031 E=diag(EV); //Extracting diagonal elements of EV matrix
      using "diag" function
0032 format(6);      //changing number format
0033
0034 disp("Grounded State Energy (in eV)",E(1),"1st Excited
      State Energy (in eV)",E(2));
0035
0036 //Plotting Wavefunctions at GS State & 1st Excited State
0037 plot(r',[abs(U(:,1))**2,abs(U(:,2))**2],"linewidth",3);
0038 legend("Ground State","1st Excited State",1);

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0039 xlabel("r","fontsize",5);
0040 ylabel("Probability Density","fontsize",5);
0041 xgrid(5);
0042
0043 //Finding Bohr Radius (using SI unit)
0044 E= -13.6; //Energy required to separate electron and
    proton, eV
0045 e= 1.6*(10^(-19)); //charge of an electron, C
0046 E= E*e; //converting to J
0047 Po= 8.85*(10^(-12)); //Permittivity of free space, F/m
0048 r= e^2/(8*(%pi)*Po*E); //radius, m
0049 r=-r;
0050 disp("Bohr Radius(in m) = ",r);
0051
0052 //NOTE : U here is not the radial function. Instead U/r is
    the radial function
0053
0054 //SECOND PART OF PROGRAM to find Dissociation Energy &
    plot potential
0055 //Defining Morse Potential using given formula
0056 rmin=0.001; rmax=10; n=1000;
0057 r=linspace(rmin,rmax,n); //linspace = linearly spaced
    vector
0058 V=zeros(n,1);
0059 for i=1:n
0060     V(i)=D*( (1-exp(-a*(r(i)-ro))) ** (2));
0061 end
0062 scf(2);
0063 plot(r',V,"linewidth",3);
0064 legend("Morse Potential Graph",2);
0065 xlabel("Internuclear Distance (r)","fontsize",5);
0066 ylabel("Morse Potential (V(r))","fontsize",5);
0067 xgrid(5);
0068
0069 //D is the well depth (defined relative to the dissociated
    atoms)
0070 Dissociation_Energy = V(n)-V(1)
0071 disp("Dissociation Energy = ",Dissociation_Energy)
0072
0073 //OUTPUT
0074 //
0075 // "Grounded State Energy (in eV)"
0076 //
0077 // -0.155

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0078  //
0079  //  "1st Excited State Energy (in eV)"
0080  //
0081  //  -0.143
0082  //
0083  //  "Bohr Radius(in m) = "
0084  //
0085  //    5.D-11
0086  //
0087  //  "Dissociation Energy = "
0088  //
0089  //    0.723
```