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Advanced quantum concepts through soft computing using matlab

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ABSTRACT

The behavior of electron and the nucleons are simulated through soft computing using MatLab language meant for Science and Engineering. Since the electrons and nucleons movement confined around nucleus and within the nucleus, to visualize the behavior the coordinates were taken with incremental value of 0.001 and less to visualize the behaviour. The graphical output shows the path and tendency of electron movement around the nucleus of Hydrogen atom. These curves show that the energy of electron is not constant but increases with the principal quantum number(n) and azimuthal quantum number(l).Some quantum mechanical problems have been solved and reported.

Introduction

Quantum mechanics, a subject deals the microscopic subatomic particles like electrons, protons and neutrons is a difficult subject to comprehend and interpret the results that we arrived through mathematical expressions.

Quantum mechanics needs a lot of mathematics like integration, differentiation, polynomial etc., to understand the nature of the particles / bodies. Problem solving in Quantum Mechanics with C, C++ or JAVA is cumbersome task. So the MATLAB language meant for science and engineering in employed in problem solving and concept explanation.

MatLab- short form of Matrix Laboratory is a special purpose computer program optimized to perform engineering and scientific calculations.

The MatLab program implements MATLAB language and provides extensive library predefined functions to make technical programming task much easier and solve technical problems using MatLab than other language.

Methodology

Though numbers of simulations are possible in quantum mechanics using MatLab, only four simulations which are widely used for B.Sc, and M.Sc, physics teaching and learning were taken and solved to explain the employability of MatLab.

They are

1. Wavefunction and Probability of a particle in a box
2. Wavefunction of Harmonic oscillator
3. Normalized Wave function and probability of electron of Hydrogen atom
4. Redial function of electron of Hydrogen atom

The above programs deal the movement of electron around the nucleus of Hydrogen atom The program.1 deals the eigen function and probability of an electron, program 2 and 3 deal the wave functions and , wave associated with electron and probability of electron to remain in an atom when moving around the nucleus.

The wave function and probability of a particle in a box is given by the equations

$$\psi=\sqrt{\frac{2}{L}} * sin((n * pi * x)/L) \quad \text{.............(1)}$$

$$P=\psi*\psi \quad \text{.........................(2)}$$

where

ψ =wavefunction of the particle for the principal quantum number n

P=probability of finding the particle at the location x

L=length of the box

n=principal quantum number=1,2,3,4……..

pi=3.14159

and x=position of the particle at any instant

m=mass of the particle executing simple harmonic motion

The wavefunction of the harmonic oscillator can be obtained from the equation

ψ=(2*m*nu/hx)^(1/4)*(2n*p!)^(-1/2)Hn(y)exp(-y*y/2)..3

'nu' is the frequency of oscillation, 'hx=1.05e-34 J', n=principal quantum number=0,1,2,3,4,5

'Hn' Hermite polynomial for n, p=factorial value for n

The equations given the program No.3describes the normalized wave function of electron in Hydrogen atom. Since the solutions are different for different principal and azimuthal quantum numbers they are not shown here. They are given in programs.

Similiarly the radial function of electron of Hydrogen atom is given in Program No.4.Since the solutions are different for different principal and azimuthal quantum numbers they are not shown here. They are indicated in program.

Program: 1

When a particle moves inside a box, it moves from one end to another end with certain velocity. According to quantum concepts, whenever a particle moves a wave is associated with it and it is described by wavefunction. From wavefunction probability of finding a particle inside the box is determined. The wavefunction and probability of the particle can be visualized in graphics window by executing the program. This concept is applied to electrons and nucleons of atoms.

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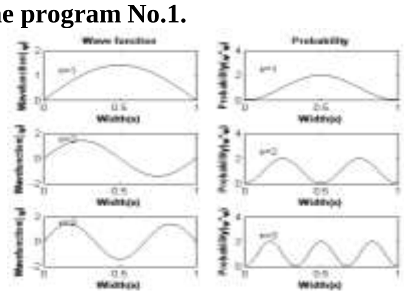
Program No. 1

```
disp('1 Wave function and probability of a particle .');
si=eigen function(wave function)
P=Probability
L=1;x=[0:.001:L];
a=sqrt(2/L);
n=1;b=n*pi;
si=a*sin(b*x/L);
subplot(321);plot(x,si,'r');
xlabel('\bfWidth(x)','color','r');
ylabel('\bfWavefunction \psi','color','m');
text(.1,1.2,'n=1','color','b');
title('\bfWave function','fontsize',10,'color','r');
P=si.^2;
subplot(322);plot(x,P,'r');
xlabel('\bfWidth(x)','color','r');
ylabel('\bfProbability(\psi*\psi)','color','m');
text(.1,2.5,'n=1','color','b');
title('\bfProbability','fontsize',10,'color','b');
p1=a^2*int('sin(b*x/L)^2',.45,.55);
n=2;c=n*pi;
si=a*sin(c*x./L);
subplot(323);plot(x,si,'g');
xlabel('\bfWidth(x)','color','r');
ylabel('\bfWavefunction \psi','color','m');
text(.1,1.5,'n=2','color','b');
P=si.^2;
subplot(324);plot(x,P,'g');
xlabel('\bfWidth(x)','color','r');
ylabel('\bfProbability(\psi*\psi)','color','m');
text(.1,2.5,'n=2','color','b');
p2=a^2*int('sin(c*x/L)^2',.45,.55);
n=3;d=n*pi;
si=a*sin(d*x./L);
subplot(325);plot(x,si,'m');
xlabel('\bfWidth(x)','color','r');
ylabel('\bfWavefunction \psi','color','m');
text(.1,1.5,'n=3','color','b');
P=si.^2;
subplot(326);plot(x,P,'m');
xlabel('\bfWidth(x)','color','r');
ylabel('\bfProbability(\psi*\psi)','color','m');
text(.1,2.5,'n=3','color','b');
```

Output of the program No.1.



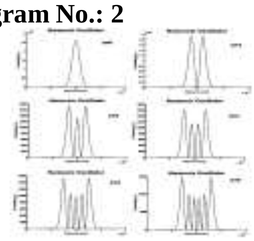
Program:2

When a particle moves inside a box and if the movement of the particle is harmonic, it moves from one end to another end with certain velocity. According to quantum concepts, whenever a particle moves a wave is associated with it and is described by wavefunction. From wavefunction and probability of finding a particle inside box is determined. If we assume that the movement of electron is harmonic,one can understand the behavior of the electron in an atom.The wavefunction and and probability of the particle can be visualized in graphics window on executing the program.

Program No.2

```
disp(' 2.  Harmonic Oscillator');
hx=1.054e-34;m=9.11e-31;
x=[-2:.0001:2]*1e-4;nu=4e4;
y=sqrt(2*pi*m*nu/hx)*x.*1;
n=input('Energy state=n=');
if     n==0;
p=1;    Hn=1;
text(1e-4,2.5e4,'n=0','fontsize',20,'color',[.8 .2 .7]);
elseif n==1
p=1;   Hn=2*y;
text(1.2e-4,1.6e4,'n=1','fontsize',20,'color',[.8 .2 .7]);
elseif n==2
p=2;   Hn=4*y.^2-2;
text(1.2e-4,14000,'n=2','fontsize',20,'color',[.8 .2 .7]);
elseif n==3
p=6;   Hn=8*y.^3-12*y;
text(1.3e-4,14000,'n=3','fontsize',20,'color',[.8 .2 .7]);
elseif n==4
p=24;  Hn=16*y.^4-48*y.^2+12;
text(1.3e-4,14000,'n=4','fontsize',20,'color',[.8 .2 .7]);
elseif n==5
p=120; Hn =32*y.^5-160*y.^3+120*y;
text(1.3e-4,14000,'n=5','fontsize',20,'color',[.8 .2 .7]);
end
hold on
a=(2*m*nu/hx)^(1/4);
b=(2^n*p)^(-1/2);
c=exp(-y.^2/2);
P=(a*b*Hn.*c).^2;
plot(x,P);
xlabel('Displacement(x)','color','m');
ylabel('Probability(\psi*\psi)','color','b');
title('\bfHarmonic Oscillator','fontsize',20,'color','r');
```

Output of the Program No.: 2



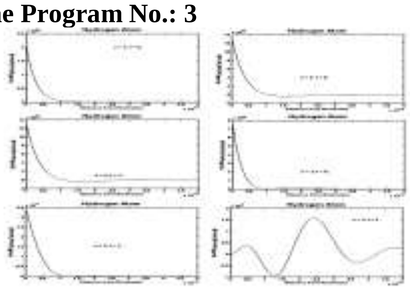
Program: 3

In a hydrogen atom electron moves around the nucleus in a circular path according to Neils Bohr. As mentioned in the above two article a wave associates with it.The wavefunction of the wave gives all the details of the electron such as position, time, energy. From wavefunction one can say the most probable position of the electron in an atom. On executing the Program No.3 and 4 one can get the most probable value and visualize the behavior of electron.

```
disp('3. Hydrogen Atom: Normalised Wave function and Probability of Hydrogen atom.');
r=[0:.01:5]*1e-10;a=.53e-10;d=a^(3/2);
e=r./a;t=linspace(0,2*pi,501);
n=input('n=');l=input('l=');
if n==1 & l==0
si=exp(-e)/(sqrt(pi)*d);P=exp(-2*e)/(pi*d^2);
plot(r,P,'r');
text(1.5e-10,.5e30,'n = 1; l = 0;','color',[.4 .1 .8]);
elseif n==2 & l==0
si=(2-e).*exp(-e/2)./(4*sqrt(2*pi)*d);P=((2-e)./(4*sqrt(2*pi)*d)^2).*exp(-e);
plot(r,P,'r');
```

```
text(2e-10,4e28,'n = 2; l = 0;','color',[.4 .1 .8]);
elseif n==2 & l==1
si=e.*exp(-e/2).*cos(t)./(4*sqrt(2*pi)*d);P=((2-
e)./(4*sqrt(2*pi)*d)^2).*exp(-e);
plot(r,P,'r');
text(2e-10,1e28,'n = 2; l = 1;','color',[.4 .1 .8]);
elseif n==3 & l==0
b=1/(81*sqrt(3*pi)*d);
c=27-18*e+2*e.^2;
si=b*c.*exp(-e/3);P=b^2*c.^2.*exp(-2*e/3);
plot(r,P,'r');
text(2e-10,2e28,'n = 3; l = 0;','color',[.4 .1 .8]);
elseif n==3 & l==1
b=sqrt(2)./(81*pi^(1/2)*e.*1);
c=(6-e).*e;
si=b.*c.*cos(t).*exp(-e/3);P=b.^2.*c.^2.*exp(-
2*e/3).*cos(t).^2;
plot(r,P,'r');
text(2e-10,1.55e-3,'n = 3; l = 1;','color',[.4 .1 .8]);
elseif n==3 & l==2
b=1./(81*sqrt(6*pi)*e);
c=e.^2;
si=b.*c.*exp(-e).*(3*cos(t).^2-1);P=b.^2.*c.^2.*exp(-
2*e/3).*(3*cos(t).^2-1);
plot(r,P,'r');
text(1e-10,1e-5,'n = 3; l = 2;','color',[.4 .1 .8]);
end;
sl=[1:1:501];
distable=[sl;r;P];
fprintf('For the sl=%3.0d distance r=%1.4e for
P=%1.4e\n',distable);
[maxdis sl]=max(P);
xlabel('Distance from Nucleus(x)','color','m');
ylabel('\psi(r,\theta,\phi)*\psi(r,\theta,\phi)','color','b');
title('Hydrogen Atom','color','r','fontsize',15);
```

Output of the Program No.: 3

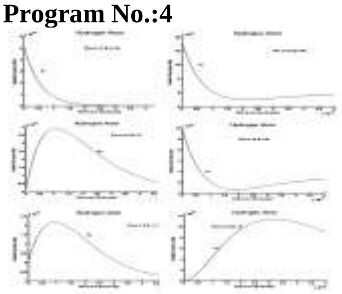


Program:4

disp(' 4. Hydrogen Atom; Radial function and Probability of finding electron);

```
r=[0:.01:5]*1e-10;a=.53e-10;
n=input('n='); l=input('l=');
if n==1 & l==0
R=(2/a^(3/2))*exp(-r/a);
text(2e-10,5e15,'For n =1 & l = 0;','color','k');
text(.5e-10,3e15,' 1s','color','b');
elseif n==2 & l==0
b=1/(2*2^(1/2)*a^(3/2));
c=2-(r./a);
R=b*c.*exp(-r./(2*a));
text(3e-10,15e14,'For n =2 & l =0','color','k');
text(.5e-10,10e14,' 2s','color','b');
elseif n==2 & l==1
b=1/(2*6^(1/2)*a^(3/2));
c=r./a;
R=b*c.*exp(-r./(2*a));
text(3e-10,3.5e14,'For n =2 & l =1','color','k');
text(2.5e-10,2.5e14,'2p','color','b');
elseif n==3 & l==0
b=2/(81*3^(1/2)*a^(3/2));
c=27-18*(r./a)+2*(r./a).^2;
R=b*c.*exp(-r./(3*a));
text(2e-10,8e14,'For n =3 & l =0','color','k');
text(.8e-10,2e14,' 3s','color','b');
elseif n==3 & l==1
b=4/(81*6^(1/2)*a^(3/2));
c=(6-(r./a)).*(r./a);
R=b*c.*exp(-r./(3*a));
text(3.5e-10,2e14,'For n = 3 & l = 1','color','k');
text(2e-10,1.5e14,' 3p','color','b');
elseif n==3 & l==2
b=4/(81*30^(1/2)*a^(3/2));
c=r.^2/a^2;
R=b*c.*exp(-r./(3*a));
text(1e-10,10e13,'For n =3 & l =2','color','k');
text(1e-10,6e13,' 3d','color','b');
end
hold on
sl=[1:1:501];
distable=[sl;r;R];
fprintf('For the sl=%3.0d distance r=%1.4e for
P=%1.4e\n',distable);
[maxdis sl]=max(R)
plot(r,R,'r');
title('Hydrogen Atom','fontsize',15,'color','r');
xlabel('Dist from Nucleus(r)','color','m');
ylabel('Radial Function R(r)','color','b');
```

Output of the Program No.:4



Conclusion

Matlab software is a powerful language tool to simulate any type of Science and Engineering even highly complicated problems like quantum mechanics .The same can be efficiently applied for graphical simulation also. Both the numerical and graphical simulations impart better understanding and knowledge about the subject.

References

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2. 2. Chapman, J.,Stephan,2004. Matlab Programming for Engineers, Thomson Learning, Third Edition-2004.