SEMESTER VI

QUANTUM MECHANICS PRACTICAL **L T P C**

17PHU612A **- - 4 2**

1. Use C/C++/Scilab for solving the following problems based on Quantum Mechanics like

Solve the s-wave Schrodinger equation for the ground state and the first excited state of the hydrogen atom: corresponding wavefunctions. Note that the ground state energy of hydrogen atom is -13.6 eV. Take e = 3.795 $(eVÅ)^{1/2}$, ħc = 1973 (eVÅ) and m = $0.511x10^6$ eV/c^2.

2. Solve the s-wave radial Schrodinger equation for an atom: where m is the reduced mass of the system (which can be chosen to be the mass of an electron), for the screened coulomb potential

3. Find the energy (in eV) of the ground state of the atom to an accuracy of three significant digits. Also, plot the corresponding wavefunction. Take e = 3.795 $(eVÅ)^{1/2}$, m = $0.511x10^6$ eV/c^2 , and a = 3 Å, 5 Å, 7 Å. In these units ħc = 1973 (eVÅ). The ground state energy is expected to be above -12 eV in all three cases.

4. Solve the s-wave radial Schrodinger equation for a particle of mass m:
significant digits. Also, plot the corresponding wave function. Choose m = 940 MeV/c^2, k = 100 MeV fm^{-2}, b = 0, 10, 30 MeV fm^{-3} In these units, cħ = 197.3 MeV fm. The ground state energy I expected to lie between 90 and 110 MeV for all three cases.

5. Solve the s-wave radial Schrodinger equation for the vibrations of hydrogen molecule:
Find the lowest vibrational energy (in MeV) of the molecule to an accuracy of three significant digits. Also plot the corresponding wave function. Take: m = $940x10^6$ eV/C^2, D = 0.755501 eV, α = 1.44, r_o = 0.131349 Å

6. Study of Electron spin resonance- determine magnetic field as a function of the resonance frequency

7. Study of Zeeman effect: with external magnetic field; Hyperfine splitting

REFERENCE BOOKS:

1. Schaum's Outline of Programming with C++. J.Hubbard, 2000, McGraw Hill Pub.
2. Numerical Recipes in C:The Art of Scientific Computing, W.H. Press et.al., 3rd
3. Edn., 2007, Cambridge University Press.
4. A Guide to MATLAB, B.R. Hunt, R.L. Lipsman, J.M. Rosenberg, 2014, 3rd Edn., Cambridge University Press
5. Elementary Numerical Analysis, K.E. Atkinson, 3rd Ed. 2007, Wiley India Edition
6. Simulation of ODE/PDE Models with MATLAB®, OCTAVE and SCILAB: Scientific
7. Engineering Applications: A.V. Wouwer, P. Saucez, C.V. Fernández.2014 Springer Quantum Mechanics, Leonard I. Schiff, 3rd Edn. 2010, Tata McGraw Hill.

Program No:1

SOLUTION OF WAVE EQUATION

Aim:

To write a C program for the solution of wave equation .

Program:

```
#include<stdio.h>
#include<math.h>
#define X 5
#define T 5
float fun(int x)
{
   return x*x*(5-x);

}
main()
{
   float u[X+1][T+1],square_of_c, ut, ue;
   int i,j;
   printf("\n Enter the square of c: ");
   scanf("%d",&square_of_c);
   printf(" Enter the value of u[0][t]:");
   scanf("%f",&ut);
   printf(" Enter the value of u[%d][t]:",X);
   scanf("%f",&ue);
   for(j=0;j<=T;j++)
   {
      u[0][j]=ut;
      u[X][j]=ue;
   }
```

```
25    for(i=1;i<=X-1;i++)
26    u[i][1]=u[i][0]=fun(i);
27    for(j=1;j<=T-1;j++)
28    for(i=1;i<=X-1;i++)
29    u[i][j+1]=u[i-1][j]+u[i+1][j]-u[i][j-1];
30    printf(" The values of u[i][j] are: \n");
31    for(j=0;j<=T;j++)
32    {
33       for(i=0;i<=X;i++)
34       printf("%6.1f",u[i][j]);
35       printf("\n");
36
37    }
38
39 }
```

Output:

```
Enter the square of c: 16
Enter the value of u[0][t]:0
Enter the value of u[5][t]:0
The values of u[i][j] are:
  0.0   4.0  12.0  18.0  16.0   0.0
  0.0   4.0  12.0  18.0  16.0   0.0
  0.0   8.0  10.0  10.0   2.0   0.0
  0.0   6.0   6.0  -6.0  -6.0   0.0
  0.0  -2.0 -10.0 -10.0  -8.0   0.0
  0.0 -16.0 -18.0 -12.0  -4.0   0.0

Process returned 10 (0xA)   execution time : 160.035 s
Press any key to continue.
```

Result:

The above program for solution of wave equation using C has been executed and output is verified.

Program No:2

EIGEN VALUE AND EIGEN VECTOR USING POWER METHOD

Aim:

To write a C program for the Eigen value and Eigen vector using power method.

Program:

```
#include<stdio.h>
#include<conio.h>
#include<math.h>
void main()
{

   int i,j,n;
   float A[40][40],x[40],z[40],e[40],zmax,emax;
   printf("\nEnter the order of matrix:");
   scanf("%d",&n);
   printf("\nEnter matrix elements row-wise\n");
   for(i=1; i<=n; i++)
   {
      for(j=1; j<=n; j++)
      {
         printf("A[%d][%d]=", i,j);
         scanf("%f",&A[i][j]);
      }
   }
   printf("\nEnter the column vector\n");
   for(i=1; i<=n; i++)
   {
      printf("X[%d]=",i);
      scanf("%f",&x[i]);
```

```
25  }
26  do
27  {
28      for(i=1; i<=n; i++)
29      {
30          z[i]=0;
31          for(j=1; j<=n; j++)
32          {
33              z[i]=z[i]+A[i][j]*x[j];
34          }
35      }
36      zmax=fabs(z[1]);
37      for(i=2; i<=n; i++)
38      {
39          if((fabs(z[i]))>zmax)
40              zmax=fabs(z[i]);
41      }
42      for(i=1; i<=n; i++)
43      {
44          z[i]=z[i]/zmax;
45      }
46      for(i=1; i<=n; i++)
47      {
48          e[i]=0;
49          e[i]=fabs((fabs(z[i]))-(fabs(x[i])));
50      }
51      emax=e[1];
52      for(i=2; i<=n; i++)
```

```
53      {
54          if(e[i]>emax)
55              emax=e[i];
56      }
57      for(i=1; i<=n; i++)
58      {
59          x[i]=z[i];
60      }
61  }
62  while(emax>0.001);
63  printf("\n The required eigen value is %f",zmax);
64  printf("\n\nThe required eigen vector is :\n");
65  for(i=1; i<=n; i++)
66  {
67      printf("%f\t",z[i]);
68  }
69  getch();
70  }
```

Output:

```
Enter the order of matrix:3

Enter matrix elements row-wise
A[1][1]=2
A[1][2]=-1
A[1][3]=0
A[2][1]=-1
A[2][2]=2
A[2][3]=-1
A[3][1]=0
A[3][2]=-1
A[3][3]=2

Enter the column vector
X[1]=1
X[2]=0
X[3]=0

 The required eigen value is  3.414214

The required eigen vector is :
0.708459        -1.000000       0.705754
```

Result:
The above program for Eigen value and Eigen vector using C has been executed and output is verified.

Program No:3 A

NUMBER OF PHOTONS EMITTED PER SECOND

Aim:
To write a sci program for calculation of number of photons emitted per second.

Program:

```
E =40
lembda=6000*10**-10
h=6.63*10**-34
c=3*10**8

n=(E*lembda)/(h*c)

printf("\n Number of photons emitted per second are given by %0.2f *10**19" ,n *10** -19)
printf("\n The answers vary due to round off error")
```

Output:

```
Number of photons emitted per second are given by 12.07 *10**19
The answers vary due to round off error
```

Result:
The above program for number of photons emitted per second using sci has been executed and output is verified.

Program No:3 B

KINETIC ENERGY OF THE PHOTOELECTRON

Aim:
To write a sci program for calculation of kinetic energy of the photoelectron.

Program:

```
a =3.2
energy =3.8
```

e =1.6*10** -19

c= energy -a
Energy =c*e

printf ("\n Kinetic energy of the photoelectron is given by %e Joule" ,Energy)

Output:
Kinetic energy of the photoelectron is given by 9.600000e-20 Joule

Result:
The above program for calculation of kinetic energy of the photoelectron using sci has been executed and output is verified.

Program No:4 A

MAXIMUM WAVELENGTH OF PHOTON

Aim:
To write a sci program for calculation of maximum wavelength of photon.

Program:
W =3.45
h =6.63*10**-34
c =3*10**8
e =1.6*10**-19

lembda =(h*c)/(W*e)

printf ("\n Maximum wavelength of photon is %0.0f A",lembda *10**10)

Output:
Maximum wavelength of photon is 3603 A

Result:
The above program for calculation of maximum wavelength of photon using sci has been executed and output is verified.

Program No:4 B

THRESHOLD VOLTAGE , MAXIMUM ENERGY OF PHOTOELECTRON AND STOPPING POTENTIAL

Aim:

To write a sci program for calculation of threshold voltage, maximum energy of photoelectron and stopping potential.

Program:

```
W=3
h =6.63*10**-34
e =1.6*10**-19
lembda =3.0*10**-7
c =3*10**8

v0 =(W*e)/h
v=c/lembda
E=h*(v-v0)
E1 =(h*(v-v0))/(1.6*10**-19)
V0=E

printf ("\n (a) Threshold frequency %0.2f *10**15 HZ",v0*10**-15)
printf ("\n (b) Maximum energy of photoelectron %0.2f eV" ,E1)
printf ("\n (c) Stopping potential %0.2f V" ,V0)
```

Output:

(a) Threshold frequency 0.72 *10**15 HZ
(b) Maximum energy of photoelectron 1.14 eV
(c) Stopping potential 0.00 V

Result:

The above program for calculation of threshold voltage, maximum energy of photoelectron and stopping potential using sci has been executed and output is verified.

Program No:5 A

WORK FUNCTION AND FREQUENCY

Aim:

To write a sci program for calculation of work function and frequency.

Program:

```
v0 =6*10**14
h =6.63*10**-34
e =1.6*10**-19
V0 =3

W=h*v0
W0 =(h*v0)/e
```

V=(e*V0+h*v0)/h

printf ("\ work function is given by %0.3f ev",W0)
printf ("\n frequency is given by %0.2f *10**15 s-1",V *10**-15)

Output:
work function is given by 2.486 ev
frequency is given by 1.32 *10**15 s-1

Result:
The above program for calculation of work function and frequency using sci has been executed and output is verified.

Program No:5 B

WAVELENGTH

Aim:
To write a sci program for calculation of wavelength.

Program:
n1 =3
n2 =2
E1 = -1.5
E2 = -3.4
h =6.63*10**-34
c =3*10**8
e =1.6*10**-19

v=(h*c)/((E1 -E2)*e)

printf ("\n Wavelength is %d Armstrom",v*10**10)
printf ("\n the answers vary due to round off error")

Output:
Wavelength is 6542 Armstrom
the answers vary due to round off error

Result:
The above program for calculation of wavelength using sci has been executed and output is verified.

Program No:6 A

KINETIC ENERGY

Aim:
To write a sci program for calculation of kinetic energy.

Program:
```
r =10.0**-14
h =1.054*10**-34
m =1.67*10**-27

p=h/r
E=(h**2/(2*m*(r**2)))/(1.6*10**-13)

printf ("\n Kinetic energy %0.2f Mev",E)
```

Output:
Kinetic energy 0.21 Mev

Result:
The above program for calculation of kinetic energy using sci has been executed and output is verified.

Program No:6 A

UNCERTAINITY IN THE ANGLE OF EMERGENCE

Aim:
To write a sci program for calculation of uncertainty in the angle of emergence.

Program:
```
clear
E =100
m =9.1*10**-31
e =1.6*10**-19
h =1.054*10**-34
x =10.0**-6

p= sqrt(2* m*E*e)
p1=h/x
theta =p1/p

printf ("\n uncertainty in the angle of emergence %0.1f *10**-4 radians",theta *10**4)
printf ("\n 4 seconds of arc")
```

Output:
uncertainty in the angle of emergence 0.2 *10**-4 radians

4 seconds of arc

Result:
The above program for calculation of uncertainty in the angle of emergence using sci has been executed and output is verified.

Program No:7 A

EIGEN FUNCTION FOR PARTICLE IN A POTENTIAL WELL

Aim:
To write a sci program for calculation of Eigen function for particle in a potential well.

Program:

```
m=9.1*10^-31
h=1.05*10^-34
ev=1.6*10^-19
n1=1
n2=2
n3=3
a=10^-10
pi=3.14

E1=(((n1^2*pi^2*h^2)/(8.0*m*a^2))/(1.6*10^-19))
E2=n2^2*E1
E3=n3^2*E1

printf("\n \n three lowest energy levels are %0.1f ev %0.1f ev and %0.2f ev",E1,E2,E3)
printf("\n their eigenfunction are 1/10^-5*cos(pi*x/2*10^-10),1/10^-5*sin(pi*x/10^-10) and
1/10^-5*cos(3*pi*x/2*10^-10)")
```

Output:

```
three lowest energy levels are 9.3 ev 37.3 ev and 83.99 ev
their eigenfunction are 1/10^-5*cos(pi*x/2*10^-10),1/10^-5*sin(pi*x/10^-10) and 1/10^-
5*cos(3*pi*x/2*10^-10)
```

Result:
The above program for calculation of Eigen function for particle in a potential well using sci has been executed and output is verified.

Program No:7 B

ENERGIES OF PARTICLE IN A POTENTIAL WELL

Aim:

To write a sci program for calculation of energies of particle in a potential well.

Program:

```
m=10.0*10^-3
l=10.0*10^-2
h=1.05*10^-34

n1=1
n2=2
n3=3

e1=(((3.14*h*n1)^2/(2.0*m*(1^2)))/(1.6*10^-19))
e2=(((3.14*h*n2)^2/(2.0*m*(1^2)))/(1.6*10^-19))
e3=(((3.14*h*n3)^2/(2.0*m*(1^2)))/(1.6*10^-19))

printf("\n energies are % ev,% ev,% ev",e1,e2,e3)
printf("\n energies are extermely small and close together and hence cant be measured")
printf("\n the answers vary due to round off error")
```

Output:

```
energies are  3.396940e-47v, 1.358776e-46v, 3.057246e-46v
energies are extermely small and close together and hence cant be measured
the answers vary due to round off error
```

Result:

The above program for calculation of energies of particle in a potential well using sci has been executed and output is verified.