# DELHI TECHNOLOGICAL UNIVERSITY

# EP-205

# MODELLING HYDROGEN ATOM

Submitted by:-
**Sanmveg saini(**2k17/EP/70)
**Durgesh Kumar**(2k17/EP29)

Submitted to:-
**Mrs. Rinku Sharma**
Department of applied physics
Delhi Technological University

**Department of Applied Physics**
DELHI TECHNOLOGICAL UNIVERSITY
(Formerly Delhi College of Engineering)
Bawana Road, Delhi-110042

# CERTIFICATE

This is to certify that the contents of the project **Modelling Hydrogen Atom** is a bonafide work by Durgesh Kumar, Sanmveg Saini and is submitted to Mrs. Rinku Sharma in partial fulfillment of project work in Engineering Physics for 3rd semester.

**Mrs Rinku Sharma**

Department of Applied Physics

Delhi Technological University

# Acknowledgement

We would like to show our gratitude to **Mrs.Rinku sharma** for giving us the opportunity to work on this project and for giving us the required guidelines for the assignment throughout numerous consultations.

We would like to express our gratitude towards our friends and seniors who guided us in completing this project. The completion of this assignment gives us much pleasure. Many people, especially our classmates and team members itself, have made valuable comment suggestions on this proposal which gave us an inspiration to improve our assignment. We thank all the people for their help, directly and indirectly, in completing our assignment.

# Contents

# List of Tables

# List of figure

# List of symbols, abbreviations and Nomenclature

| | |
|---|---|
| $\hbar$ | Planck's constant |
| e | electronic charge |
| V(r) | potential at a radius r |
| u | radial wave function |
| n | Principal quantum no. |
| l | Azimuthal quantum no. |
| $\theta$ | Polar angle |
| $\phi$ | azimuthal angle |
| $\psi$ | Wave function |
| $\|\psi\|^2$ | Probability Density |
| L | Laguerre polynomial |
| $Y^l{}_m$ | Spherical harmonic |

**Chapter 1**
INTRODUCTION

The Hydrogen Atom consists of a heavy, essentially motionless proton, of charge e, together with a much lighter elecron From Coulomb's law potential enrgy is

$$V(r) = \frac{-e^2}{4\pi\epsilon r}$$

The radial equation is

$$\frac{-\hbar^2 d^2u}{2mdr^2} + \left[\frac{-e^2}{4\pi\epsilon r} + \frac{\hbar^2 l(l+1)}{2mr^2}\right] u = Eu \ldots (1)$$

Our problem is to solve this equation for $u(r)$, and determine the allowed energies, E. The coulomb potential admit continuum states $(E > 0)$. describing electron-proton scattering, as well as discrete bound states, representing the hydrogen atom.

# 1 The Radial Wave function

Let $\kappa \equiv \frac{-2mE}{h}$ for bound states E is negative and real

$$\frac{d^2u}{\kappa^2 dr^2} = \left[1 - \frac{me^2}{2\pi\epsilon h^2 \kappa(\kappa r)} + \frac{l(l+1)}{(\kappa r)^2}\right] u$$

This suggests that we introduce

$\rho \equiv \kappa r$, and $\rho_0 \equiv \frac{me^2}{2\pi\epsilon_0 h^2 \kappa}$ so that

$$\frac{d^2u}{d\rho^2} = \left[1 - \frac{\rho_0}{\rho} + \frac{l(l+1)}{\rho^2}\right] u$$

Next we examine the asymptotic form of th solutions as $\rho \to \infty$, the constnants term in the bracket dominates,so(approx.)

$$\frac{d^2u}{d\rho^2} = u$$

The general solution is

$$u(\rho) = Ae^{-\rho} + Be^{\rho}$$

but $e^{\rho}$ blows up (as $\rho \to \infty$), so $B = 0$. Evidently

$$u(\rho) \approx Ae^{-\rho}$$

for large $\rho$. On the other hand as $\rho \to 0$ the centrifugal term dominates approximately then:

$$\frac{d^2u}{d\rho^2} = \frac{l(l+1)}{\rho^2}u$$

The general solution is

$$u(\rho) = C\rho^{l+1} + D\rho^{-l}$$

but $\rho^{-l}$ blows up (as $\rho \to 0$), so $D = 0$ . Thus

$$u(\rho) = C\rho^{l+1}$$

for small $\rho$. The next step is to peel off the asymptotic behaviour introducing the new function $v(\rho)$:

$$u(\rho) = \rho^{l+1}e^{-\rho}v(\rho),$$

Differentiating:

$$\frac{du}{d\rho} = \rho^l e^{-\rho}\left[(l+1-\rho)v + \rho\frac{dv}{d\rho}\right]$$

and

$$\frac{d^2u}{d\rho^2} = \rho^l e^{-\rho}\left[[-2l-2+\rho+\frac{l(l+1)}{\rho}]v + 2(l+1-\rho)\frac{dv}{d\rho} + \rho\frac{d^2v}{d\rho^2}\right]$$

In terms of $v(\rho)$, then the radial equation reads

$$\rho\frac{d^2v}{d\rho^2} + 2(l+1-\rho)\frac{dv}{d\rho} + [\rho_0 - 2(l+1)]v = 0$$

Finally, we assume the solution$v(\rho)$can be expressed as a power series in $\rho$ :

$$v(\rho) = \sum_{j=0}^{\infty} c_j \rho^j$$

Differentiating term by term to detemine the coefficients:

$$\frac{dv}{d\rho} = \sum_{j=0}^{\infty} j c_j \rho^{j-1} = \sum_{j=0}^{\infty} (j+1) c_{j+1} \rho^j$$

Differentiating again and adjusting the dummy index j;

$$\frac{d^2 u}{d\rho^2} = \sum_{j=0}^{\infty} j(j+1) c_{j+1} \rho^{j-1}$$

Solving;

$$\sum_{j=0}^{\infty} j(j+1) c_{j+1} \rho^j + \sum_{j=0}^{\infty} (j+1) c_{j+1} \rho^j - 2 \sum_{j=0}^{\infty} j c_j \rho^j + [\rho_0 - 2(l+1)] \sum_{j=0}^{\infty} c_j \rho^j = 0$$

Equating the coefficients of like power yields

$$c_{j+1} = \left[ \frac{2(j+l+1) - \rho_0}{(j+1)(j+2l+2)} \right] c_j$$

This recursion formula determines the coefficients and hence the function.

For large j the recursion formula can be approximated to

$$c_{j+1} \cong \frac{2j}{j(j+1)} c_j = \frac{2}{j+1} c_j$$

Suppose for a moment that this were exact.Then

$$c_j = \frac{2^j}{j!} c_0$$

so

$$v(\rho) = c_0 \sum_{j=0}^{\infty} \frac{2^j}{j!} \rho^j = c_0 e^{2\rho}$$

and hence

$$u(\rho) = c_0 \rho^{l+1} e^{\rho}$$

which blows up at large $\rho$ because of exponential factor
For finding solution that we are interested in the series must terminate such that

$$c_{(j_{max}+1)} = 0$$

then, $2(j_{max} + l + 1) - \rho_0 = 0$ defining

$$n \equiv j_m ax + l + 1$$

n = principal quantum number
$\rho_0 = 2n$

so the allowed energies

$$E = \frac{-\hbar^2 \kappa^2}{2m} = \frac{me^4}{8\pi^4 \epsilon_0^4 \hbar^2 \rho_0^4}$$

this is the bohr formula.

Above equations give

$$\kappa = \left[\frac{me^2}{4\pi\epsilon_0 \hbar^2}\right] \frac{1}{an} = \frac{1}{an}$$

where

$$\text{Bohr's Radius} = a \equiv \frac{4\pi\epsilon_0\hbar^2}{me^2} = 0.529 \times 10^{-10}$$

It follows that $\rho = \frac{r}{an}$ and the spatial wave function for hydrogen are labelled by three quantum numbers (n,l,m)

$$\psi_{nlm}(r, \theta, \phi) = R_{nl}(r) Y_l^m(\theta, \phi)$$

where

$$R_{nl}(r) = \frac{\rho^{l+1} e^{-\rho} v(\rho)}{r}$$

and $v(\rho)$ is a polynomial of degree $j_{max} = n - l - 1$ whose coefficeints are determined by the recursion formula.

$$c_{j+1} = \left[ \frac{2(j + l + 1 - n)}{(j + 1)(j + 2l + 2)} \right] c_j$$

The ground state (n=1) is $E_1 = -13.6eV$. Evidently the binding energy is 13.6 eV.

For hydrogen, after limitaions l=0,m=0 ,so, $\psi_{100}(r, \theta, \phi) = R_{10}(r) Y_0^0(\theta, \phi)$
The recursion formula truncates after the first term so $v(\rho)$is a constant($c_0$), and

$$R_{10}(r) = \frac{c_0}{a} e^{-r/a}$$

After normalizing it we get $c_0 = 2 \times \sqrt{a}$ and $Y_0^0 = 1/\sqrt{4\pi}$
Therefore, the ground state of hydrogen is

$$\psi_{100}(r, \theta, \phi) = \frac{1}{\sqrt{\pi}} e^{-r/a}$$

For arbitray n, the possible values of $l$ are $l = 0, 1, 2, \ldots, n-1$ and for each $l$ there are $(2l + 1)$ possible values of $m$,so the total degeneracy of the energy level $E_n$ is $d(n) = \sum_{l=0} n - 1 = n^2$. The formula for $v(\rho)$ is a function well known to applied mathematician; apart from normalization ,it can be written as

$$v(\rho) = L_{n-l-1}^{2l+1}(2\rho)$$

where

$$L_{q-p}^{p}(x) \equiv (-1)^p \frac{d}{dx}^{P} L_q(x)$$

is an associated Laguerre polynomial, and

$$L_q(x) = e^x \frac{d}{dx}^{q} (e^{-x} x^q)$$

is the $q^{th}$ Laguerre Polynomial.The normalized hydrogen wavefunctions are

$$\psi = \sqrt{\left(\frac{2}{na}\right)^3 \frac{(n-l-1)!}{2n((n+1)!)^3}} \times e^{-r/na} \times \frac{2r}{na}^{l} \times \left( L_{n-l-1}^{2l+1} \times \frac{2r}{na} \right) \times Y_l^m(\theta, \phi)$$

This is one of the very few realistic systems that can be solved at all in exact closed form.The wave function depend on all three quantum numbers whereas the energies are determined by n alone.

# Chapter 2

## MATLAB code

### **HAWF.m** Hydrogen atom wave function

```
% HAWF hydrogen atom wave function
clear all; % clear all previously saved variables
close all; % close all windows
% n = principle quantum number
% l = Azimuthal quantum number
% m = magnetic quantum number
% take the input of n, l, and m
n = input('Enter Principle Quantum number: ');
l = input('Enter Azimuthal Quantum number: ');
m = input('Enter Magnetic  Quantum number: ');
% a is the bohars radius. in meters
a = 0.529*10^(-10);
% define shperical coordinate symbols
% th = theta
% phi = phi
% r = radial diatance
syms th phi r
% get the expression of normalized angular wave function
Y = NAWF(th, phi, l, m);
% get the expression of associated laguerre polynomial
L(r) = ALUP(r, n, l);
% replace all the occurance of r with 2*r/(n*a)
L(r) = L(2*r/(n*a));
% b and c are values which will be use later on to calculate RWA
b = sqrt(((2/(n*a))^3)*((factorial(n-l-1))/(2*n*(factorial(n+l))^3)) );
c = (2*r/(n*a))^l;
% wave function
psi(r, th, phi) = b*c*exp(-r/(n*a))*L*Y;
% RWA = Radial wave function
RWF(r) = exp(-r/(n*a))*L*c/(a*n);

% the following command will calculate the different value of r
r=linspace(0, 10^(-9), 100);
% v is basically a wave function for particular value of th and phi
v = psi(r, pi/4, 0);
% u is the probability density of of u
u = abs(v).^2;
% A is a constant employed for the sake of ploting
A = (a^1.5);
w = A*RWF(r);

% plot wave function and its probability density
plotyy(r, v, r, u); grid on;
```

```
legend('wave function', 'probability density');
title('Plot of wavefunction and its probability density');
gtext( {['Principle quantum number = ', num2str(n), ''], ['Azimuthal Quantum number = ', num2str(l)],
['Magnetic quantum number = ', num2str(m)]});
xlabel('Radial distance');
yyaxis left
ylabel('\psi');
yyaxis right
ylabel('|\psi|^2');
% plot Radial wave function
figure;
plot(r, w); grid on;
ylabel('a^{1.5}\times R_{nl}');
xlabel('Radial Distance');
gtext({['Principle quantum number = ', num2str(n), ''], ['Azimuthal Quantum number = ', num2str(l)], ['Magnetic
quantum number = ', num2str(m)]});
title('Plot of Radial wave function Vs Radial distance');
```

## **NAWF.m** Normalized angular wave function

```
% NAWF = normalized angular wave function
function Y = NAWF(th, phi, l, m)
  % l should be positive integer and m should be an integer
  % the following condition will check for the above constraint
  if ( ~isnumeric(l) || ~isnumeric(m)) || ( ceil(abs(m)) ~= abs(m) || ceil(abs(l)) ~= abs(l) )
    ME = MException('MyComponent:variabletypeError', 'l should be positive integer and m should be an
integer');
    throw(ME);
  end
  eps = 0; % this is a constant which will be used later in this function file
  % its value will is calculated below
  if m <= 0
    eps = 1;
  else
    eps = (-1)^m;
  end
  if abs(m) <= l
    % if the absolute of magnetic number is less than or equal to
    % azimuthal quantum number then
    % get the associated Legendre polynomial
    % define a symbol for the working
    syms x;
    % get the Associated Legendre function
    P(x) = ALP(x, l, m);
    % change all the aoourance of x by cos
    P(x) = P(cos(th));
    % calculate some other function
    Q(phi) = exp(m*phi*1i);
    c = sqrt(((2*l+1)/(4*pi))* (factorial(l-abs(m))) /(factorial(l+abs(m))) );
```

```
        % get the final expression of normalized angular wave function
        Y = eps*c*P(x)*Q(phi);
    else
        % if absolute of magnetic number is less than azimuthal quantum
        % number then normalized angular wave function is 0
        Y =0;
    end
end
```

## **ALP.m** Associated Legendre polynomial

```
function g = ALP(v, l, m) % ALP = associated legendre polynomial
    % both l amd m should be integers
    % the following condition will check for the above constraint
    if ( ~isnumeric(l) || ~isnumeric(m)) || ( ceil(abs(m)) ~= abs(m) || ceil(abs(l)) ~= abs(l) )
        ME = MException('MyComponent:variabletypeError', 'l should be positive integer and m should be an
integer');
        throw(ME);
    else
        if abs(m) <= l
            % if m is in between -l and l then  find
            % legendre polynomial
            lp = legendreP(l,v);
            % Associated legendre polynomial
            f(v) = ((1-v^2)^(abs(m)/2))*diff(lp, abs(m));
            % return the calculated Associated Lengendre polynomial
            g = f;
        else
            g = 0;
        end
    end
end
```

## **ALUP.m** Associated Laguerre polynomial

```
% ALUP - associated Laguerre Polynomial
function L = ALUP(r, n, l)
    % both l amd n should be integers
    % the following condition will check for the above constraint
    if ~isnumeric(n) || ~isnumeric(l)
        throw(MException('MyComponent:InvalidDataType', 'n and l should be numbers'));
    elseif n < 0 || ceil(abs(n)) ~= abs(n) || l < 0 || ceil(abs(l)) ~= abs(l)
        throw(MException('MyComponent:InvalidDataType', 'n and l should be positive integers'));
    elseif ~(l <= n-1)
        throw(MException('MyComponent:InvalidDataType', 'l should be less than n'));
    end
    % define some constants
    a = 0.529*10^(-10); % in meters
    p = 2*l+1;
    q = n+l;
```

```matlab
    % get the coefficients of the Laguerre polynomial in order
    f = fliplr(coeffs(laguerreL(q, r), r));
    % return the polynomial after calculating it
    L = ((-1)^p)*diff(laguerreL(q, r)/abs(f(1)), p) ;%(2*r/(n*a))
end
```

# Chapter 3

## Tables and figures.

| |
|---|
| $Y_0^0 = \left(\frac{1}{4\pi}\right)^{\frac{1}{2}}$ |
| $Y_1^0 = \sqrt{\frac{3}{4\pi}} \times \cos\theta$ |
| $Y_2^{\pm 1} = \mp \sqrt{\frac{3}{8\pi}} \times \sin\theta \times e^{\pm i\phi}$ |
| $Y_2^0 = \sqrt{\frac{5}{16\pi}} \times (3\cos^2\theta - 1)$ |
| $Y_2^{\pm 1} = \mp \sqrt{\frac{15}{8\pi}} \sin\theta \times \cos\theta$ |

**Table 1.** The first few spherical Harmonics, $Y_l^m(\theta, \phi)$

| |
|---|
| $R_{20} = \frac{1}{\sqrt{2}} a^{-\frac{3}{2}} \left(1 - \frac{1}{2}\frac{r}{a}\right) \exp\left(-\frac{r}{2a}\right)$ |
| $R_{21} = \frac{1}{\sqrt{24}} a^{-\frac{3}{2}} \times \frac{r}{a} \exp\left(-\frac{r}{2a}\right)$ |
| $R_{32} = \frac{4}{81\sqrt{30}} a^{-\frac{3}{2}} \times \left(\frac{r}{a}\right)^2 \exp\left(-\frac{r}{3a}\right)$ |
| $R_{42} = \frac{1}{64\sqrt{5}} a^{-\frac{3}{2}} \times \left(1 - \frac{1}{12}\frac{r}{a}\right) \left(\frac{r}{a}\right)^2 \exp\left(-\frac{r}{4a}\right)$ |
| $R_{43} = \frac{1}{768\sqrt{35}} a^{-\frac{3}{2}} \times \left(\frac{r}{a}\right)^3 \times \exp\left(-\frac{r}{4a}\right)$ |

**Table 2.** First few radial wave function for hydrogen $R_{nl}(r)$

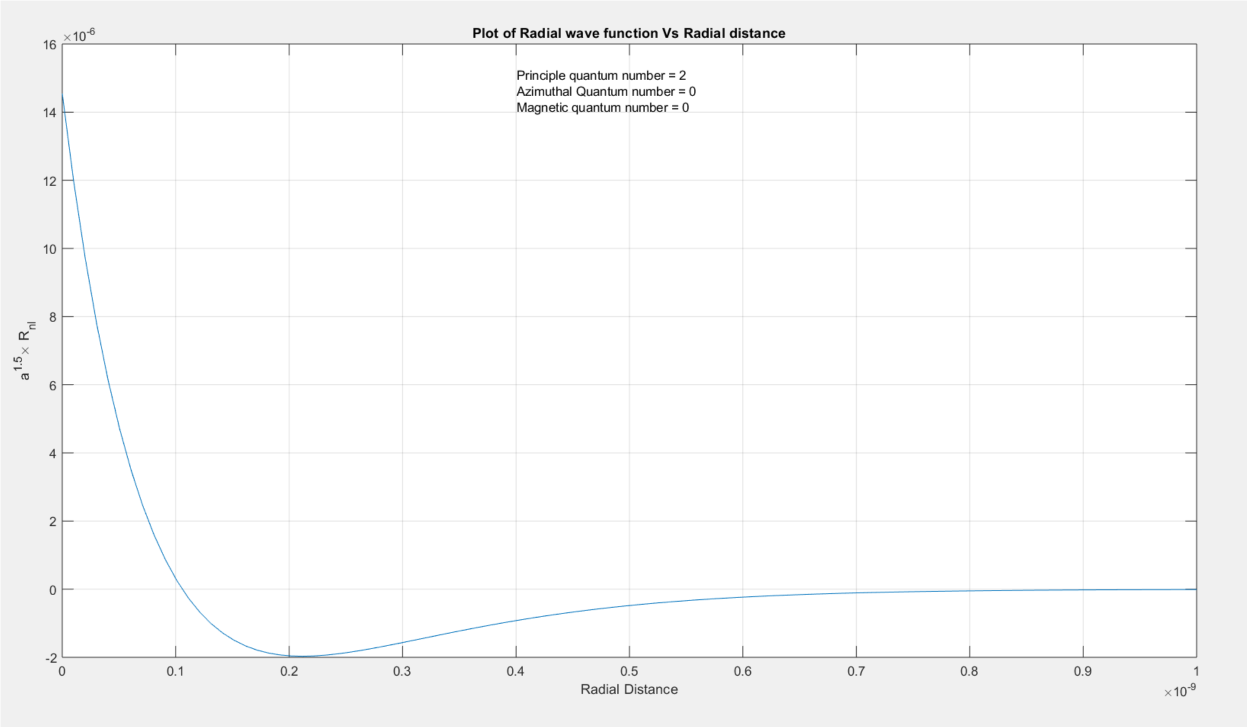


**Fig 1(a)** Wave function and probability density for n=2, l=0, m=0

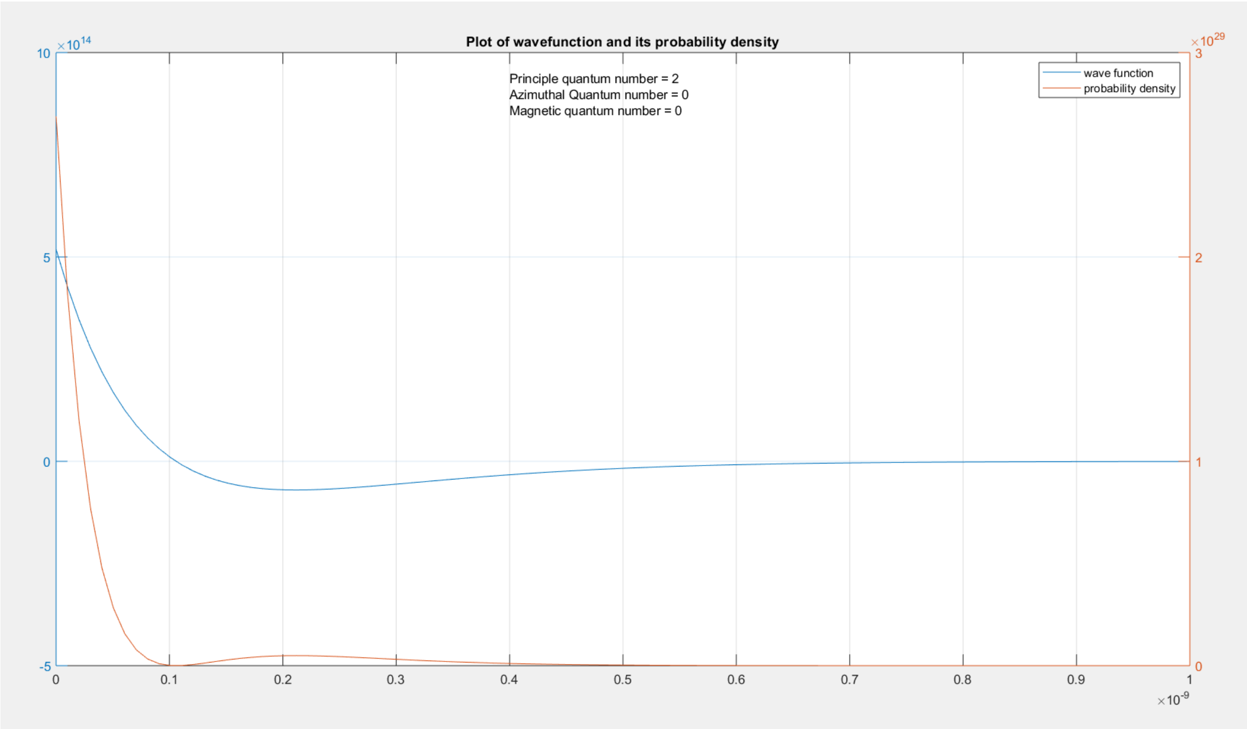


**Fig 1(b)** Radial wave function Vs radial distance for n=2, l=0, m=0

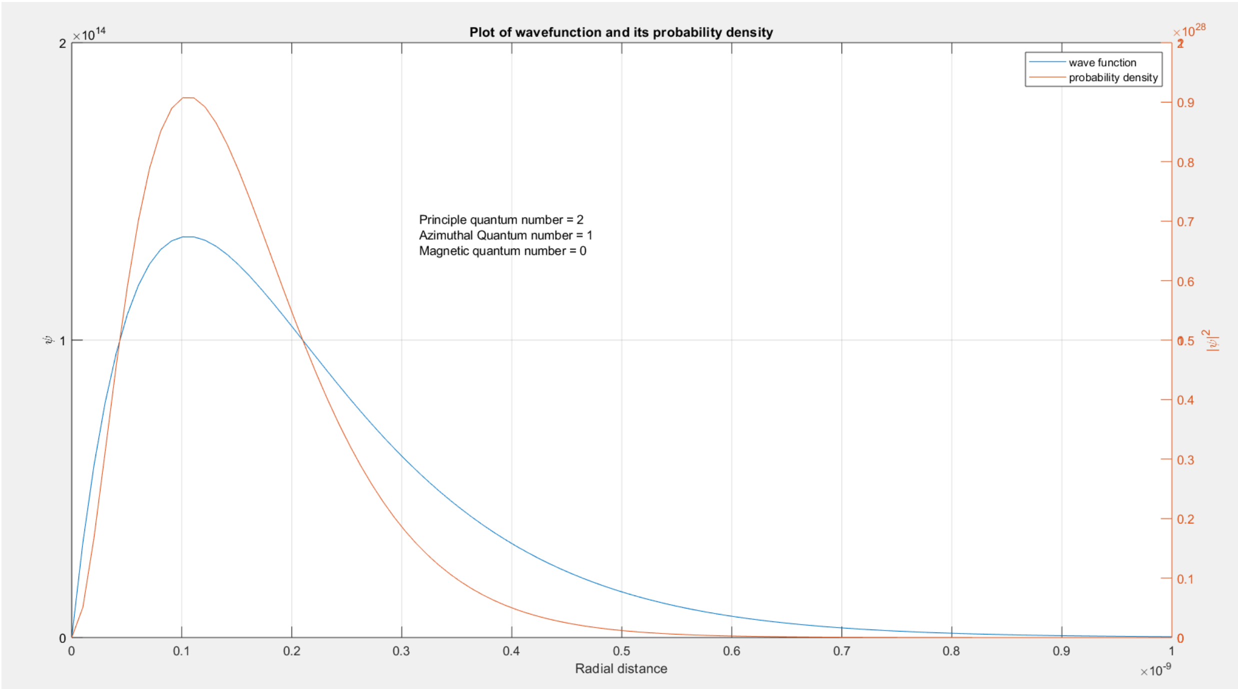


**Fig 2(a)** Wave function and probability density for n=2, l=1, m=0

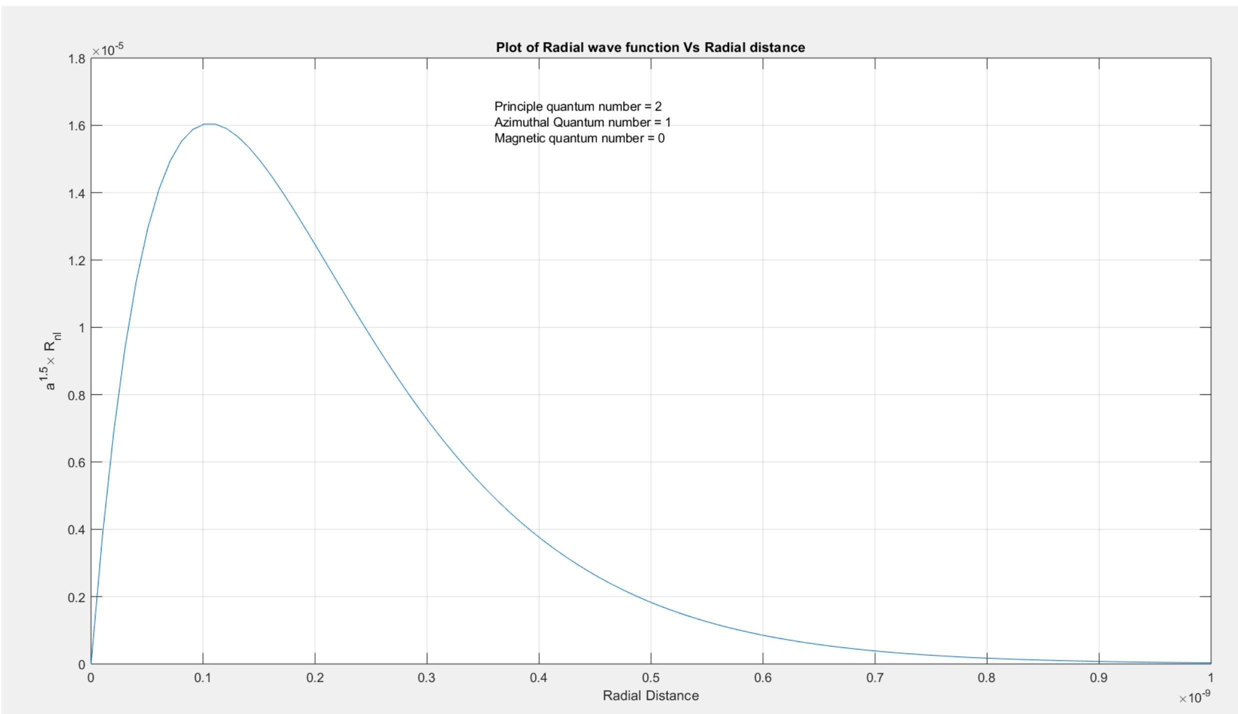


**Fig 2(b)** Radial wave function Vs Radial distance for n=2, l=1, m=0

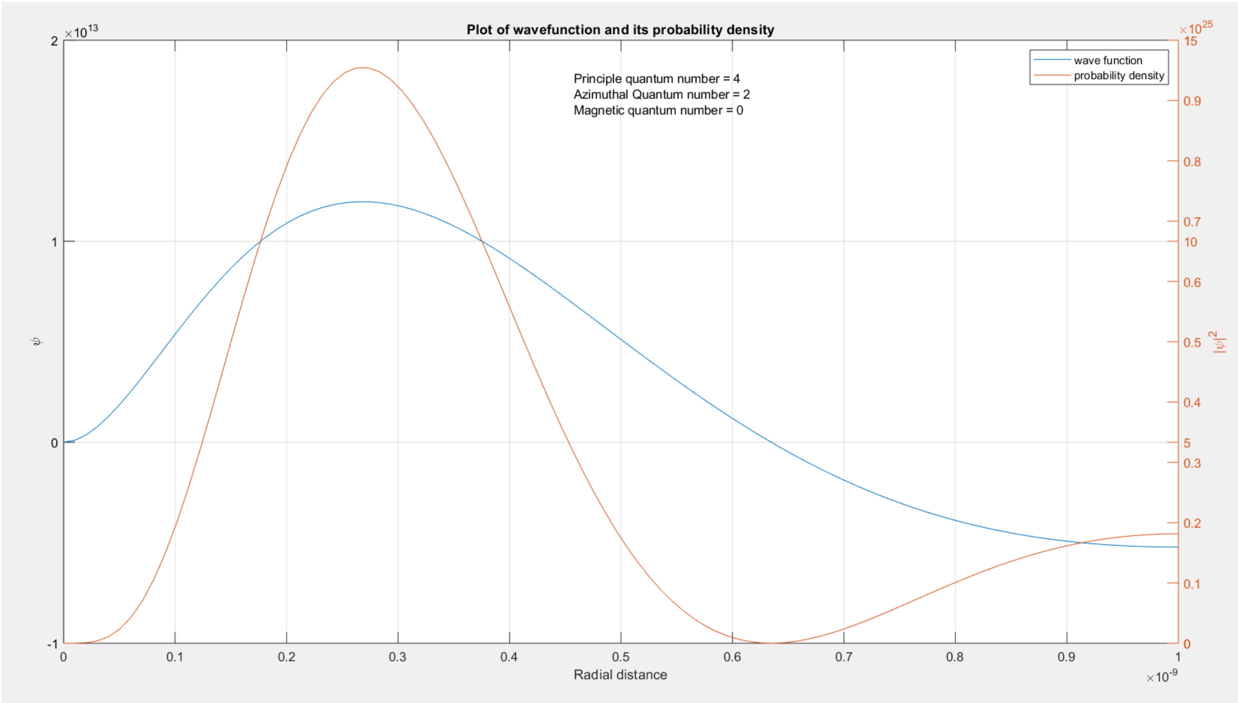


**Fig 3(a)** wave function and probability density for n=4, l=2, m=0

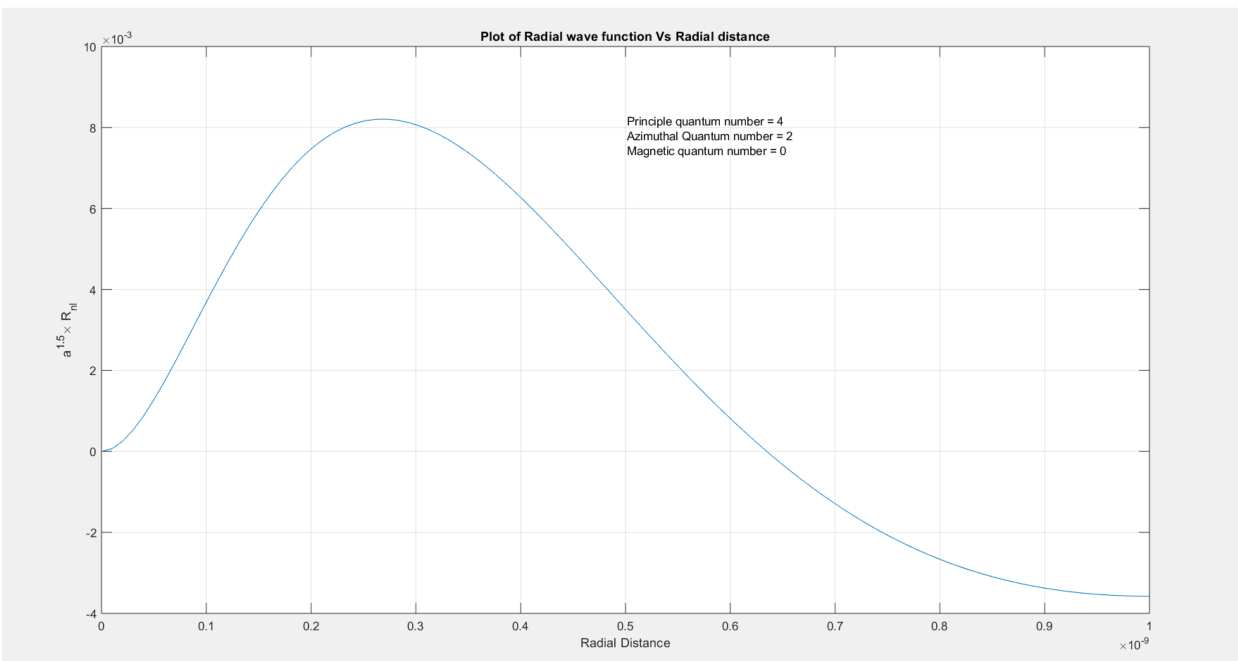


**Fig 3(b)** Radial wave function Vs radial distance for n=4, l=2, m=0

# References


[1] David J. Griffiths, Introduction To Quantum Mechanics. Pearson, 2005

[2] Documentation of MATLAB, https://in.mathworks.com/help/matlab/