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2020PH41201

QM Lab Assignment - 1

Correspondence Principle

1. (a) After the failure of Rutherford's model of atom, Bohr's concluded that classical laws do not apply on the atomic scale. After that, Bohr's modified Rutherford's model of atom by combining classical & early quantum concepts and gave his semi classical model of atom in the form of 3 postulates :-

i) Bohr's first postulate was that an electron in an atom could revolve in certain stable orbits without the emission of radiant energy. According to this postulate, each atom has certain ~~scientific~~ definite stable states in which it can exist and each possible state has definite total energy. These are called stationary states of an atom.

ii) Bohr's second postulate defines these stable orbits. This postulate states that the electron ~~was~~ revolves around the nucleus only in those orbits for which the angular momentum is some integral multiple of $\frac{h}{2\pi}$ where h is Planck's constant. Thus, the angular momentum (L) of the orbiting electron is quantised.

iii) Bohr's third postulate ~~was~~ incorporated into atomic theory the early quantum concepts that had been developed by Planck and Einstein. It states that an electron might make a transition from one of its specified non-radiating orbits to another of lower energy. When it does so, a photon is emitted having energy equal to the energy difference between the initial & final states. The frequency of emitted photon is then given by

$$\boxed{h\nu = E_i - E_f}$$

b) * Radius of n^{th} orbit of in Bohr's model

Centripetal force is provided by the electrostatic force:-

$$F_c = F_e$$

$$\frac{mv^2}{r} = \frac{1}{4\pi\epsilon_0}\frac{q_1 q_2}{r^2}$$

Here, $q_1 = e$ & $q_2 = +Ze$

$$\frac{mv^2}{r} = \frac{Ze^2}{4\pi\epsilon_0 r^2} \quad — (1)$$

& also $mvr = \frac{nh}{2\pi}$ — (2)

(2)^2 ÷ (1)

$$\frac{\cancel{m^2} \cancel{v^2} r^2}{\frac{\cancel{m} \cancel{v^2}}{r}} = \frac{\frac{n^2h^2}{4\pi^2}}{\frac{Ze^2}{\cancel{4}\pi\epsilon_0 r^2}}$$

$$mr^3 = \frac{n^2h^2\epsilon_0}{\pi Z e^2}$$

$$\Rightarrow \boxed{r_n = \frac{n^2 h^2 \epsilon_0}{\pi m Z e^2}}$$

For hydrogen atom, $Z = 1$

$$\Rightarrow \boxed{r_n = \frac{n^2 h^2 \epsilon_0}{\pi m e^2}}$$

* Energy in the n^{th} energy level :-

Kinetic energy, $KE = \frac{1}{2} m v_n^2$

In Bohr's model, velocity in n^{th} orbit is given by

$$\boxed{v_n = \frac{Ze^2}{2h\epsilon_0 n}}$$

$$\Rightarrow KE = \frac{1}{2} m \left(\frac{Z^2 e^4}{4h^2 \epsilon_0^2 n^2} \right)$$

$$\Rightarrow \boxed{KE = \frac{m Z^2 e^4}{8h^2 \epsilon_0^2 n^2}}$$

Potential energy, $PE = \frac{1}{4\pi\epsilon_0} \frac{q_1 q_2}{r_n}$

$$\Rightarrow PE = \frac{1}{4\pi\epsilon_0} \frac{(-e)(+Ze)}{\left(\frac{n^2 h^2 \epsilon_0}{\pi m e^2 Z} \right)} \qquad \left[\because r_n = \frac{n^2 h^2 \epsilon_0}{\pi m Z e^2} \right]$$

$$\Rightarrow \boxed{PE = \frac{-m Z^2 e^4}{4 n^2 h^2 \epsilon_0^2}}$$

Now, $E_n = KE + PE$

$$\Rightarrow E_n = \frac{mZ^2e^4}{8h^2\epsilon_0^2n^2} - \frac{mZ^2e^4}{4n^2h^2\epsilon_0^2}$$

$$\Rightarrow E_n = \frac{mZ^2e^4}{8h^2\epsilon_0^2n^2} - \frac{2mZ^2e^4}{8n^2h^2\epsilon_0^2}$$

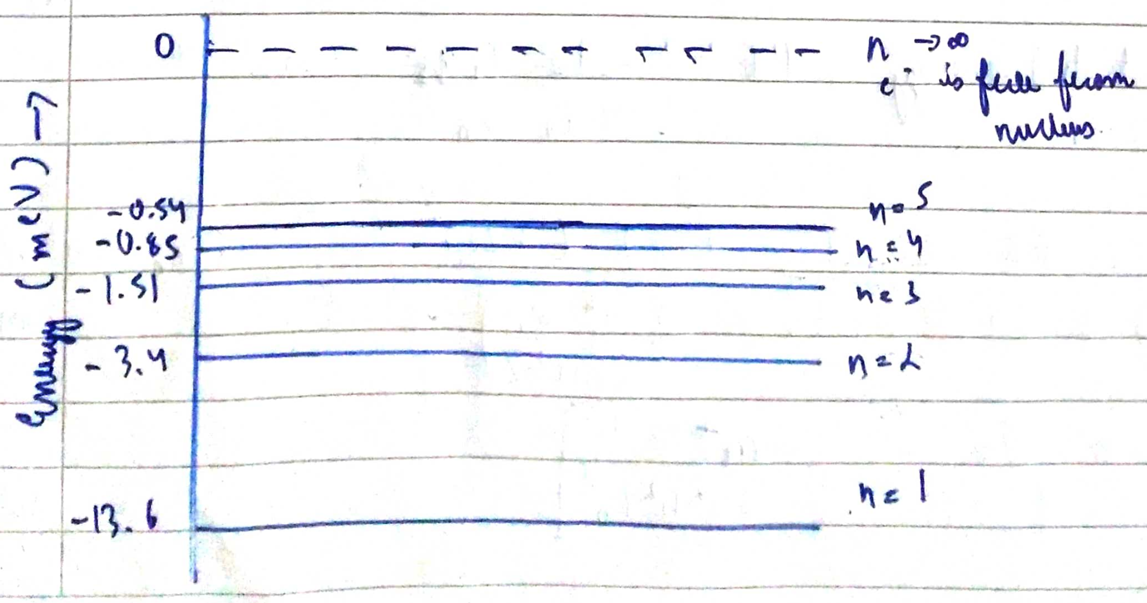
$$\Rightarrow \boxed{E_n = -\frac{mZ^2e^4}{8h^2\epsilon_0^2n^2}}$$

or $\boxed{E_n = \frac{-mZ^2e^4}{32\pi^2\epsilon_0^2\hbar^2n^2}}$ $\because$, $\hbar = \frac{h}{2\pi}$

For hydrogen atom, $Z = 1$

$$\Rightarrow \boxed{E_n = \frac{-me^4}{32\pi^2\epsilon_0^2\hbar^2n^2}}$$

* Energy level diagram :-



→ If the atom size is 1mm.

$$r_n = \frac{1mm}{2} \Rightarrow 0.5 \times 10^7 A^\circ$$

$$\Rightarrow 0.5 \times 10^7 A^\circ = 0.529 \frac{n^2}{Z} A^\circ$$

$$\frac{0.5 \times 10^7 \times Z}{0.529} = n^2$$

$$0.9452 \times 10^7 \times Z = n^2$$

$$9.452 \times 10^6 \times Z = n^2$$

For hydrogen atom $Z = 1$

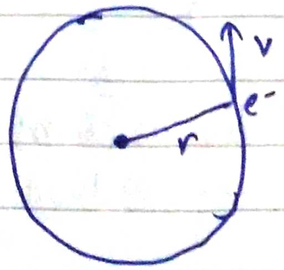
$$n^2 = 9.452 \times 10^6$$

$$\Rightarrow \boxed{n = 3.07 \times 10^3}$$

c) Bohr's correspondence principle states that "The predictions of quantum mechanics must reproduce the predictions of classical physics in the limit of large quantum ~~no~~ numbers."

d) We know that time period of an electron in an orbit is given by :-

$$T = \frac{2\pi r}{v}$$



& $\nu = \frac{1}{T}$

$$\Rightarrow \boxed{\nu = \frac{v_n}{2\pi r_n}} \quad \text{—} \ (1)$$

& Radius is given by $\boxed{r_n = \frac{n^2 h^2 \epsilon_0}{\pi m e^2}}$

& velocity is given by $\boxed{v_n = \frac{e^2}{2h\epsilon_0 n}}$

Put r_n & v_n in eq. (1)

$$\nu = \frac{\frac{e^2}{2h\epsilon_0 n}}{\frac{2\pi n^2 h^2 \epsilon_0}{\pi m e^2}}$$

$$\Rightarrow \nu = \frac{e^2}{2h\epsilon_0 n} \times \frac{\pi m e^2}{2\pi n^2 h^2 \epsilon_0}$$

$$\Rightarrow \boxed{\nu = \frac{m e^4}{4h^3 \epsilon_0^2 n^3}}$$

or $\boxed{\nu_{cln} = \frac{m e^4}{32\pi^3 \epsilon_0^2 \hbar^3 n^3}}$ $\because \hbar = \frac{h}{2\pi}$

This is the expression for classical frequency of radiated by electron.

c) The energy of n^{th} orbit is given by:

$$E_n = \frac{-me^4}{32\pi^2 \epsilon_0^2 \hbar^2} \frac{1}{n^2}$$

& Energy of $(n-1)^{th}$ orbit is given by:-

$$E_{n-1} = \frac{-me^4}{32\pi^2 \epsilon_0^2 \hbar^2} \frac{1}{(n-1)^2}$$

Now, $\Delta E = E_n - E_{n-1}$

$$\Rightarrow h\nu = \frac{-me^4}{32\pi^2 \epsilon_0^2 \hbar^2} \frac{1}{n^2} + \left(\frac{-me^4}{32\pi^2 \epsilon_0^2 \hbar^2} \frac{1}{(n-1)^2} \right)$$

$$\Rightarrow h\nu = \frac{-me^4}{32\pi^2 \epsilon_0^2 \hbar^2} \left[\cancel{\frac{1}{n^2}} \frac{1}{n^2} - \frac{1}{(n-1)^2} \right]$$

$$\Rightarrow h\nu = \frac{-me^4}{32\pi^2 \epsilon_0^2 \hbar^2} \left[\frac{(n-1)^2 - n^2}{n^2 (n-1)^2} \right]$$

$$\Rightarrow h\nu = \frac{me^4}{32\pi^2 \epsilon_0^2 \hbar^2} \left[\frac{2n-1}{n^2 (n-1)^2} \right]$$

$$\Rightarrow \nu = \frac{me^4}{2 \times 32\pi^3 \epsilon_0^2 \hbar^3} \left[\frac{2n-1}{n^2 (n-1)^2} \right]$$

$$\Rightarrow \boxed{\nu_{n} = \frac{me^4}{64\pi^3 \epsilon_0^2 \hbar^3} \left[\frac{2n-1}{n^2 (n-1)^2} \right]}$$

This is the expression of for quantum frequency of radiation radiated by electron.

Now, if n is very large i.e. $n \gg 1$

$\Rightarrow 2n-1 \approx 2n$ & $n-1 \approx n$

$$\Rightarrow \nu = \frac{me^4}{\cancel{64}_{32}\pi^3 \epsilon_0^2 h^3} \left[\frac{\cancel{2}\cancel{n}}{n^{\cancel{4}}} \right].$$

$$\Rightarrow \boxed{\nu_{cn} = \frac{me^4}{32\pi^3 \epsilon_0^2 h^3} \cdot \frac{1}{n^3}}$$

which is the expression for classical frequency.

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A1.py

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```python
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt

#ENERGY:
E=[]
n=[]
for i in range(1,21):
    n.append(i)
    E_n= (-13.6/(i**2))
    E.append(E_n)

for i in range(len(E)):
    plt.axhline(y=E[i], xmin=0.1, xmax=0.8, color='g', linewidth=3, label='n= '+ str(n[i]))
    plt.ylabel('Energy')
    plt.title('Energy Level Diagram')
    plt.legend()
plt.grid()
plt.show()

m=9.1*10**(-31)
e=-1.6*10**(-19)
e_0=8.85*10**(-12)
h_bar=1.054*10**(-34)

#fcln
def freq(p):

    fcln= ((m * e**4)/(32* (np.pi)**3 * (e_0)**2 * (h_bar)**3))/ (10**p)**3
    fqn= ((m * e**4)/(64* (np.pi)**3 * (e_0)**2 * (h_bar)**3)) * ((2*(10**p) - 1)/(((10**p)**2)*((10**p)-1)**2))
    return fcln,fqn

Q=[]
```

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File Edit Selection View Go Run Terminal Help — A1.py - Visual Studio Code

A1.py

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```python
def freq(p):

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    fqn= ((m * e**4)/(64* (np.pi)**3 * (e_0)**2 * (h_bar)**3)) * ((2*(10**p) - 1)/(((10**p)**2)*((10**p)-1)**2))
    return fcln,fqn

Q=[]
C=[]
p=0.5
a,b=freq(p)
Q.append(b)
C.append(a)

n=1
while abs(a-b)>10**(-5):
    n+=1
    p+=0.5
    a,b=freq(p)
    Q.append(b)
    C.append(a)
N=[]
for i in range(n):
    N.append(10**i)
df=abs(np.array(Q)-np.array(C))
error=df/np.array(Q)

plt.plot(np.log(np.array(N)),error,color = 'y')
plt.title('Error Plot')
plt.grid()
plt.show()

print(pd.DataFrame({'n':N,'QUANTUM FREQUENCY':Q,'CLASSICAL FREQUENCY':C,'ERROR':error}))
```

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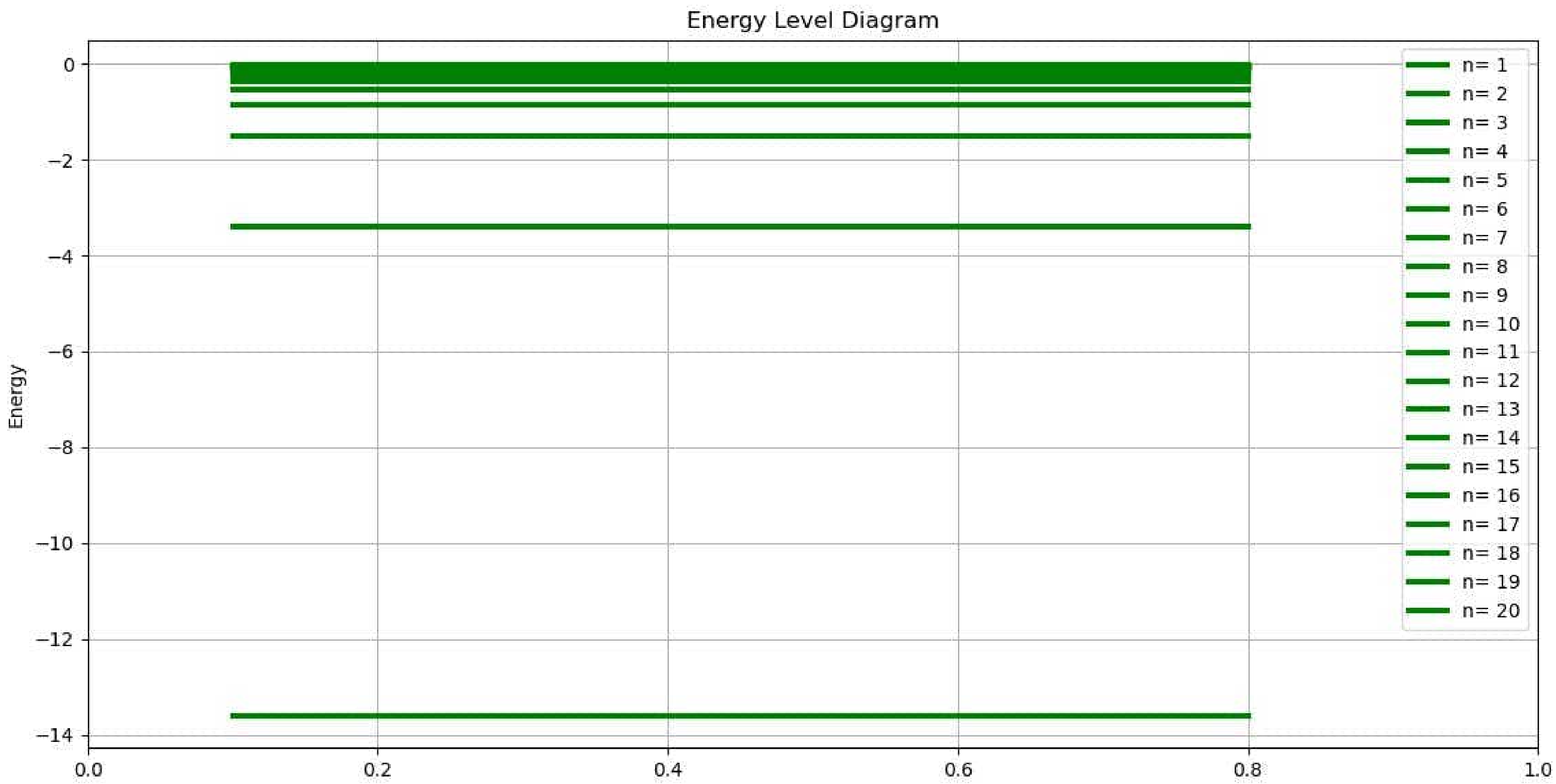
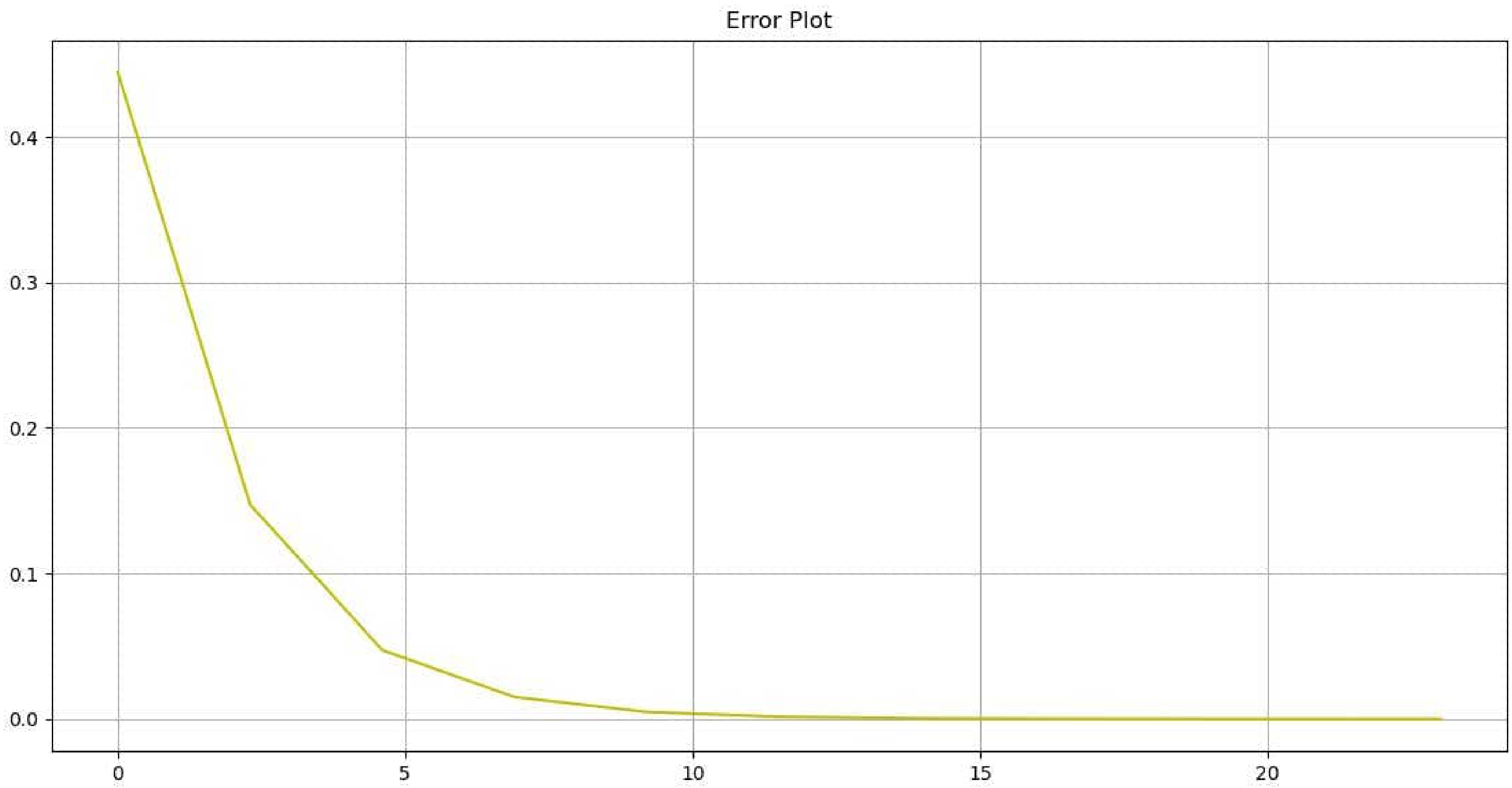

Energy Level Diagram
Energy
0
−2
−4
−6
−8
−10
−12
−14
0.0
0.2
0.4
0.6
0.8
1.0
n= 1
n= 2
n= 3
n= 4
n= 5
n= 6
n= 7
n= 8
n= 9
n= 10
n= 11
n= 12
n= 13
n= 14
n= 15
n= 16
n= 17
n= 18
n= 19
n= 20


Error Plot
0.4
0.3
0.2
0.1
0.0
0
5
10
15
20

```
PS C:\Users\Sarthak> python -u "c:\Users\Sarthak\Desktop\Important Stuff\QM Lab\A1\A1.py"
              n  QUANTUM FREQUENCY  CLASSICAL FREQUENCY     ERROR
0             1       3.732018e+14         2.072590e+14  0.444646
1            10       7.686913e+12         6.554104e+12  0.147368
2           100       2.175217e+11         2.072590e+11  0.047180
3          1000       6.653743e+09         6.554104e+09  0.014975
4         10000       2.082463e+08         2.072590e+08  0.004741
5        100000       6.563949e+06         6.554104e+06  0.001500
6       1000000       2.073573e+05         2.072590e+05  0.000474
7      10000000       6.555088e+03         6.554104e+03  0.000150
8     100000000       2.072688e+02         2.072590e+02  0.000047
9    1000000000       6.554203e+00         6.554104e+00  0.000015
10  10000000000       2.072600e-01         2.072590e-01  0.000005
```