Assignment 1 - Correspondence Principle

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Lab Assignment #1

(Correspondance Principle)

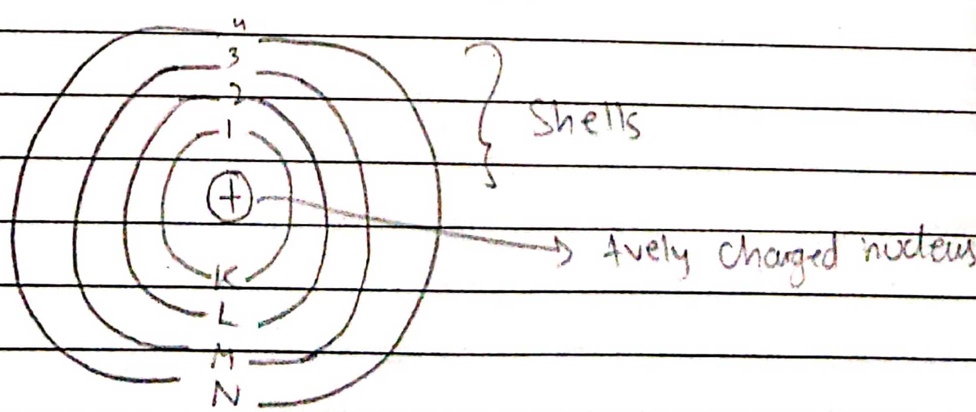
Theory :

(a) Bohr's Model for atom

Bohr theory modified the atomic structure model by explaining that e^- move in fixed orbitals (shells) and not anywhere in between and each orbit has a fixed energy

Bohr's model consists of a small nucleus (+ve chaged) surrounded by -ve e^- moving around the nucleus in orbits.

e^- away from the nucleus has more energy and closer to nucleus has less energy.



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Postulates of Bohr Model

1. The $-ve$ e^- moves around the $+ve$ nucleus (proton) in a circular orbit. All electron orbits are centered at the nucleus. Not all classically possible orbits are available to an e^- bound to the nucleus.

2. The allowed e^- orbits satisfy the first quantization condition: In the n^{th} orbit, the angular momentum L_n of the e^- can take only discrete values:

$$L_n = n\hbar \quad \text{where } n = 1, 2, 3 \ldots$$

→ Angular monetum is quantized.

$$\boxed{m_e v_n r_n = n\hbar}$$

v_n → velocity of e^- in n^{th} orbit

r_n → radius of n^{th} orbit.

3. An e^- is allowed to make transitions from one orbit where its energy is E_n to another orbit where energy is E_m.
When atom absorbs a photon, e^- goes to a higher state.
When atom emits a photon, e^- returns to lower energy state.
This happens instantaneously

→ Second quantization condition:

$$\boxed{h\nu = |E_n - E_m|}$$

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(b) $m_e \rightarrow$ mass of e^- $\quad$ $r_n \rightarrow$ radius of n^{th} orbit.
$-e \rightarrow$ charge on e^- $\quad$ $v_n \rightarrow$ Velocity of e^-
$+e \rightarrow$ charge on nucleus $\quad$ $Z \rightarrow$ no. of e^-
$n \rightarrow$ principal quantum no

Coulomb's force (F_e) = Centripetal force (F_{cp})

$$\therefore \frac{Ze^2}{4\pi\varepsilon_0 r_n^2} = \frac{m_e v_n^2}{r_n}$$

$$v_n^2 = \frac{Ze^2}{4\pi\varepsilon_0 r_n m_e} \quad — (1)$$

by bohr's postulate,

$$m_e r_n v_n = \frac{nh}{2\pi}$$

$$m_e^2 v_n^2 r_n^2 = \frac{n^2 h^2}{4\pi^2}$$

$$v_n^2 = \frac{n^2 h^2}{4\pi^2 m_e^2 r_n^2} \quad — (2)$$

equate (1) and (2)

$$\frac{n^2 h^2}{\cancel{4}\pi^2 m_e^2 r_n^2} = \frac{Ze^2}{\cancel{4\pi}\varepsilon_0 \cancel{r_n}\, \cancel{m_e}}$$

$$r_n = \left(\frac{\varepsilon_0 h^2}{\pi m_e Z e^2}\, n^2\right)$$

$$\boxed{r_n = \frac{\varepsilon_0 h^2}{\pi m_e e^2}\, n^2}$$ for $Z=1$ (Hydrogen)

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Now,

$$\frac{m_e v_n^2}{r_n} = \frac{1}{4\pi\varepsilon_0} \times \frac{e^2}{r_n^2}$$

$$m_e v_n^2 = \frac{1}{4\pi\varepsilon_0} \times \frac{e^2}{r_n} \quad \text{---(1)}$$

$$K.E = \frac{1}{2} m_e v_n^2$$

$$= \frac{1}{2} \times \frac{1}{4\pi\varepsilon_0} \times \frac{e^2}{r_n} \quad \text{from (1)}$$

$$K.E = \frac{e^2}{8\pi\varepsilon_0 r_n}$$

$$P.E = \frac{1}{4\pi\varepsilon_0} \frac{e}{r_n} (-e)$$

$$P.E = \frac{-e^2}{4\pi\varepsilon_0 r_n}$$

$$T.E = \frac{e^2}{8\pi\varepsilon_0 r_n} + \left(-\frac{e^2}{4\pi\varepsilon_0 r_n}\right)$$

$$E_n = \frac{-e^2}{8\pi\varepsilon_0 r_n}$$

we know, $r_n = \left(\frac{\varepsilon_0 h^2}{\pi m_e e^2}\right) n^2$

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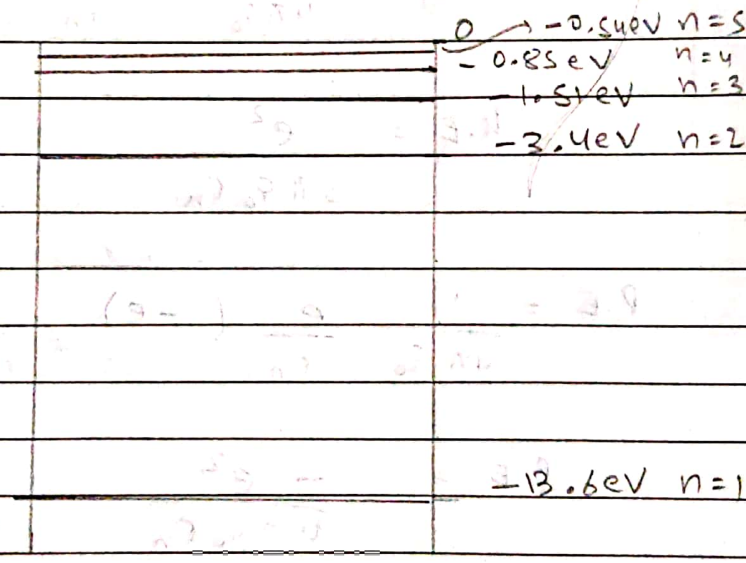
$$E_n = -\frac{1}{8\pi\varepsilon_0} \frac{e^2}{\left(\frac{\varepsilon_0 h^2}{\pi m_e e^2}\right) n^2}$$

$$E_n = -\left(\frac{m e^4}{8 \varepsilon_0^2 h^2}\right) \frac{1}{n^2}$$

$$\boxed{E_n = \frac{-m e^4}{32\pi^2 \varepsilon_0^2 \hbar^2} \frac{1}{n^2} = \frac{-13.6\,eV}{n^2}} \quad n = 1, 2, 3 \ldots$$



We know that,

$$r_n = r_0 n^2$$

$$r_n = 0.529\,\mathring{A}\, n^2$$

for radius $\approx$ 1mm

$$\frac{1\,mm}{0.529\,\mathring{A}} = n^2$$

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$$\frac{10^{-3}\ m}{0.529 \times 10^{-10}\ m} = n^2$$

$$n^2 = 1.89 \times 10^7$$
$$n^2 = 18.9 \times 10^6$$

$$\boxed{n = 4.347 \times 10^3}$$

(c) The correspondance principle states that the behaviour of systems described by the theory of quantum mechanics reproduces classical physics in the limit of large quantum numbers.
In other words, it says that for large orbits and for large energies, quantum calculations most agree with classical calculations.

(d) we know,

$$\frac{2\pi r_n}{T} = v_n$$

using eqs of r_n and v_n and $\nu = \frac{1}{T}$ (ν → f_{cln})

$$f_{cln} \times 2\cancel{\pi} \times \frac{\varepsilon_0 h^2}{\cancel{\pi} m_e e^2} n^2 = \frac{e^2}{2\varepsilon_0 n h}$$

$$f_{cln} = \frac{m_e e^4}{4\varepsilon_0^2 h^3 n^3}, \qquad \text{now } \hbar = \frac{h}{2\pi}$$

$h \to \hbar . 2\pi$

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$$f_{cen} = \frac{m_e \; e^4}{4\varepsilon_0^2 \hbar^3 \; 8\pi^3} \cdot \frac{1}{n^3}$$

$$\boxed{f_{cen} = \frac{m e^4}{32\pi^3 \varepsilon_0^2 \hbar^3} \cdot \frac{1}{n^3}}$$

(e) we know,

$$E_n = \frac{-me^4}{32\pi^2 \varepsilon_0^2 \hbar^2} \cdot \frac{1}{n^2}$$

$$E_{qn} = |E_n - E_{n-1}|$$

$$= \left| \frac{-me^4}{32\pi^2 \varepsilon_0^2 \hbar^2} \cdot \frac{1}{n^2} + \frac{me^4}{32\pi^2 \varepsilon_0^2 \hbar^2} \cdot \frac{1}{(n-1)^2} \right|$$

$$= \left| \frac{me^4}{32\pi^2 \varepsilon_0^2 \hbar} \left[\frac{1}{(n-1)^2} - \frac{1}{n^2} \right] \right|$$

$$= \left| \frac{me^4}{32\pi^2 \varepsilon_0^2 \hbar} \left[\frac{\cancel{n^2} - (\cancel{n^2}+1-2n)}{n^2(n-1)^2} \right] \right|$$

$$\boxed{E_{qn} = \frac{me^4}{32\pi^2 \varepsilon_0^2 \hbar^2} \cdot \frac{2n-1}{n^2(n-1)^2}}$$

we know that,

$$\hbar = \frac{h}{2\pi}$$

$$E = h\nu$$

$$h = \hbar . 2\pi$$

$$f_{qn} = \frac{E_{qn}}{\hbar \cdot 2\pi}$$

$$\boxed{f_{qn} = \left(\frac{me^4}{64\pi^3 \varepsilon_0^{\,2} \hbar^3}\right) \frac{2n-1}{n^2(n-1)^2}}$$

In the limit of large n:

$$2n - 1 \approx 2n$$

$$n - 1 \approx n$$

Using this approximation,

$$= \frac{me^4}{32\,\cancel{64}\,\pi^3 \varepsilon_0^2 \hbar^3} \; \frac{2\cancel{n}}{n^{\cancel{2}} \cdot n^2}$$

$$= \frac{me^4}{32\pi^3 \varepsilon_0^2 \hbar^3} \cdot \frac{1}{n^3} \Rightarrow f_{cln}$$

Thus, $f_{cln} \approx f_{qn}$ for a large value of n.

For radius of 1 mm

$n \rightarrow 4347$

$f_{cln}(4347) = 80100.6624$ Hz

$f_{qn}(4347) = 80128.3108$ Hz

They come out to be approximately equal.

Programming

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

#constants
m = 9.1093837015e-31
e = 1.602176634e-19
eps = 8.8541878128e-12
h_c = 1.05457182e-34


def f_cln(n):
    return (m*(e**4))/(32*(np.pi**3)*(eps**2)*(h_c**3)*(n**3))

def f_qn(n):
    return ((m*(e**4))/(64*(np.pi**3)*(eps**2)*(h_c**3)))*((2*n-1)/(n**2*(n-1)**2))

p = 0
n_val=[]
logn_val = []
per_val = []
f_class = []
f_quant = []

tol = 1

while tol > 10e-6:
    p = p + 0.5
    n = 10**p

    log_n = np.log(n)
    n_val.append(n)
    logn_val.append(log_n)

    deltaF = abs(f_qn(n) - f_cln(n))
    rel_diff = deltaF/f_qn(n)
    rel_diff_per = rel_diff * 100

    per_val.append(rel_diff_per)

    f_class.append(f_cln(n))
    f_quant.append(f_qn(n))

    tol = rel_diff


data = {

  'n': n_val,
  'f_cln': f_class,
  'f_qn': f_quant,
  'Rel. Error %' : per_val

}

df = pd.DataFrame(data)
print(df)

plt.plot(logn_val, per_val)
plt.scatter(logn_val, per_val)
plt.grid()
plt.title('% Relative Difference as a function of ln(n)')
plt.xlabel('ln(n)')
plt.ylabel('% Rel. Diff.')
plt.plot()
```

```
plt.show()

def energy(n):
    return -13.6/(n**2)


for i in range(1,11):
    x_vals = range(1,11)
    e_val = energy(i)*np.ones(10)
    plt.plot(x_vals, e_val,label = f'n = {i}')

plt.title('Energy Diagram')
plt.ylabel('Energy(ev)')

plt.grid()
plt.legend()
plt.show()
```

Result and Discussion

	n	f_cln	f_qn	Rel. Error %
0	3.162278	2.080679e+14	3.746584e+14	44.464642
1	10.000000	6.579684e+12	7.716913e+12	14.736842
2	31.622777	2.080679e+11	2.183706e+11	4.718015
3	100.000000	6.579684e+09	6.679712e+09	1.497487
4	316.227766	2.080679e+08	2.090590e+08	0.474091
5	1000.000000	6.579684e+06	6.589567e+06	0.149975
6	3162.277660	2.080679e+05	2.081666e+05	0.047432
7	10000.000000	6.579684e+03	6.580671e+03	0.015000
8	31622.776602	2.080679e+02	2.080777e+02	0.004743
9	100000.000000	6.579684e+00	6.579783e+00	0.001500
10	316227.766017	2.080679e-01	2.080689e-01	0.000474

Figure 1: Table

It can be seen that as the value of n increases the relative error goes on decreasing. This shows that in the limit of large n the classical and quantum mechanical values of radiation frequencies are identical. This is an example of Bohr's correspondence theorem.

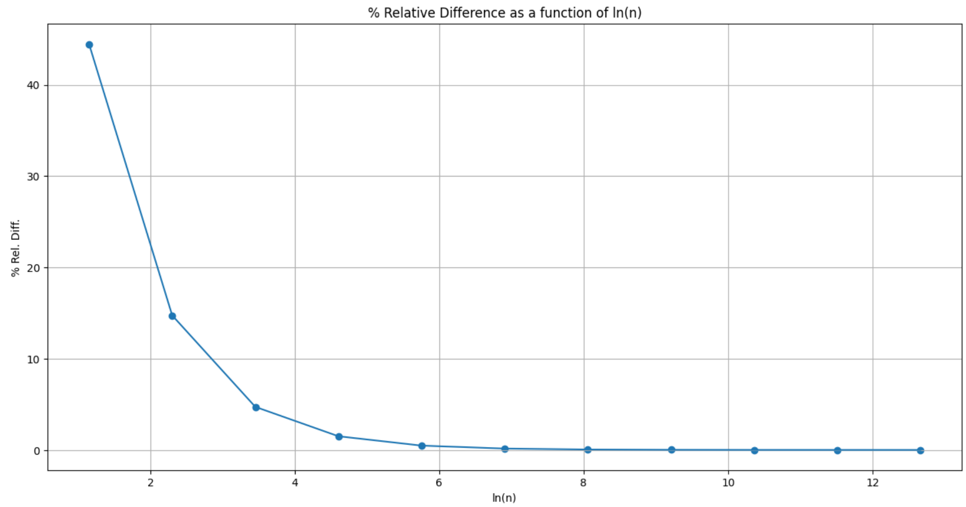

Figure 2: Rel. Error as a function of ln(n)

It can be noted that as the value of n increases the relative difference in % goes on decreasing which shows the two values are coming close to each other.

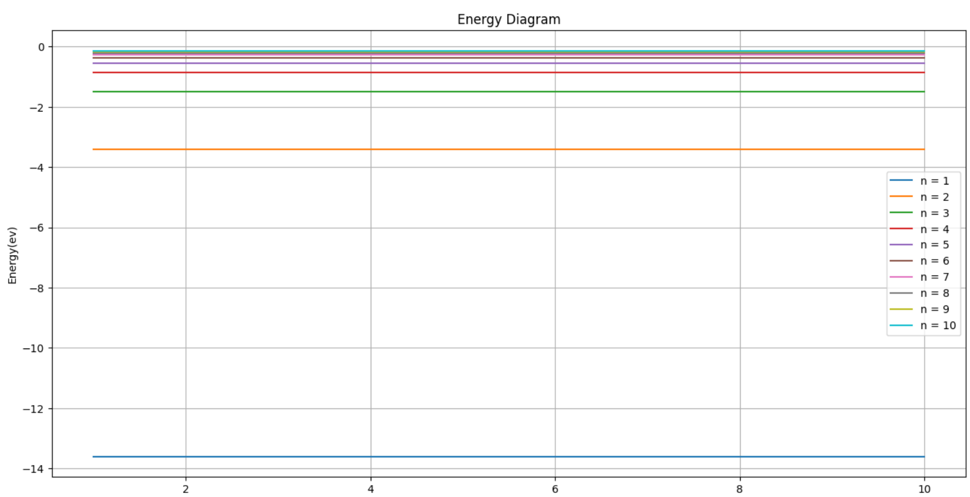

Figure 3: Energy Level Diagram

The energy levels go on becoming more closer as we increase the value of n. For $n = 1$, the lowest energy orbit(ground state) has an energy of -13.6eV.