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Lab Assignment 1 (Corresponding Principle)

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1. Bohr's Model for atom and it's postulates...

Ans. Bohr's model explains the structure of atom that electrons moves in fixed orbitals. These orbitals have probability of presence of electrons. According to Bohr's model, atom consists of positively charged nucleus and negatively charged electrons moving around it. Electrons located away from nucleus have more energy compared to electrons which are near to nucleus.

Postulates of Bohr's Model

1. Electrons revolve around nucleus in fixed circular path called orbits.
2. Each orbit has fixed energy
3. Energy levels are represented by an integer ($n=1,2,3 --$) known as quantum number. At $n=1$, electrons attain lowest energy level and said to be in at ground state.
4. Electrons move from lower energy level to higher energy level by gaining energy and vice versa.

(b) Obtain the expression for radius (r_n) of n^{th} orbit in Bohr's model and value of energy in n^{th} energy level.

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

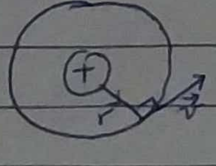
Ans: According to Coloumb's law of attraction

Force btw proton and electron

$$F = \frac{k q_1 q_2}{r_n^2} = \frac{k(e)(-e)}{r_n^2}$$

Taking magnitude of force

$$|F| = \frac{ke^2}{r_n^2} = \underbrace{\frac{mv^2}{r_n}}_{\text{centripital force}} \Rightarrow \frac{ke^2}{r_n} = mv^2 \quad -(1)$$



Angular momentum $(\vec{L}) = \vec{r} \times \vec{p}$

$$\vec{L} = \vec{r}_n m \vec{v} \sin\theta$$

$$L = mvr_n$$

According to Bohr's model, angular momentum is quantized

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$L = mvr_n = n\frac{h}{2\pi}$

$$\boxed{v = \frac{nh}{2\pi m r_n}} \quad -(2)$$

Putting value of v from (2) in (1)

$$\frac{ke^2}{r_n} = m\left(\frac{nh}{2\pi m r_n}\right)^2$$

$$\frac{ke^2}{\cancel{r_n}} = \frac{mn^2h^2}{4\pi^2 m^2 r_n^{\cancel{2}}}$$

$$r_n = \frac{\cancel{m}n^2h^2}{4\pi^2 m^{\cancel{2}} ke^2} = \frac{n^2h^2}{4\pi^2 m ke^2} = \frac{n^2h^2 \times 4\pi\varepsilon_0}{4\pi^2 m e^2} = \frac{n^2h^2\varepsilon_0}{\pi m e^2}$$

putting all values, $r = 6.3 \times 10^{-11}$ m

→ To derive expression for energy in n^{th} orbit

From (1) $\frac{ke}{r_n} = mv^2$

Dividing by 2 on both sides

$$\frac{1}{2}\frac{ke^2}{r} = \frac{1}{2}mv^2 = K.E. = \frac{1}{2 \times 4\pi\varepsilon_0}\frac{e^2}{r_n} = \frac{e^2}{8\pi\varepsilon_0 r_n}$$

$$\text{Potential Energy } (V_E) = \frac{-ke^2}{r_n} = \frac{-1}{4\pi\varepsilon_0 \times r_n}e^2$$

$$(E_T)_n = K.E. + V_E = \frac{1}{2}\frac{ke^2}{r_n} - \frac{ke^2}{r_n} = \frac{-1}{2}\frac{ke^2}{r_n} = \frac{-1 \times e^2}{8\pi\varepsilon_0 r_n}$$

$$E_n = \frac{-1e^2}{8\cancel{\pi}\varepsilon_0} \times \frac{\cancel{\pi} me^2}{n^2h^2\varepsilon_0} = -\left(\frac{me^4}{8\varepsilon_0^2h^2}\right)\frac{1}{n^2} = \frac{-me^4}{8\varepsilon_0^2 \times (\hbar \times 2\pi)^2 n^2}$$

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

Putting values of $m, e, \varepsilon_0, \hbar, \pi$, we'll get

$$E_n = \frac{-13.6}{n^2} \text{ eV}$$

$E_1 = \frac{-13.6}{1^2}$ $\quad E_2 = \frac{-13.6}{4} = -3.4$ eV $\quad E_3 = -1.51$ eV

$E_4 = -0.85$ eV

$E_5 = -0.544$ eV

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Energy Level Diagram

$n=5$ ———————— $-0.544\,eV$

$n=4$ ———————— $-0.85\,eV$

$n=3$ ———————— $-1.51\,eV$

$n=2$ ———————— $-3.4\,eV$

$n=1$ ———————— $-13.6\,eV$

→ As $r_n = \dfrac{n^2 h^2 \varepsilon_0}{\pi m e^2}$

If we take $r_n = 1\,mm$

then $n^2 = \dfrac{r_n \pi m e^2}{h^2 \varepsilon_0}$

$n \sim 11$

For value, $n \geq 11$ Size of Bohr's atom will become a lab sized object.

(c) Bohr's Correspondence principle---

According to this principle for large number of quantum numbers, the classical and quantum theory gives same results.

Frequency of radiation from classical mechanicsr

Time period (T) of revolution of e^- revolving around nucleus in circular orbit of radius(r) with velocity (v) is given by

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

Frequency of revolution (ν) $= \dfrac{1}{T} = \dfrac{v}{2\pi r}$ — (1)

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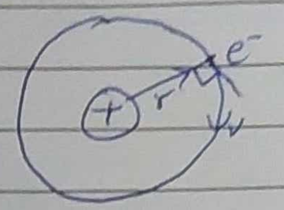
Comparing centripital force and Columbic force



$$\frac{mv^2}{r} = \frac{ke^2}{r^2}$$

$$v^2 = \frac{ke^2}{rm}$$

$$v^2 = \frac{e^2}{4\pi\varepsilon_0 rm} \quad -(2)$$

According to Bohr's postulate, quantisation of angular momentum,

$$mvr = \frac{nh}{2\pi}$$

$$v = \frac{nh}{2\pi mr} \quad -(3)$$

Squaring on both sides

$$v^2 = \frac{n^2h^2}{4\pi^2m^2r^2} \quad -(4)$$

Comparing (2) and (4)

$$\frac{e^2}{4\pi\varepsilon_0 rm} = \frac{n^2h^2}{4\pi^2m^2r^2}$$

$$\frac{e^2}{\varepsilon_0} = \frac{n^2h^2}{\pi mr}$$

$$r = \frac{n^2h^2\varepsilon_0}{\pi me^2} \quad -(5)$$

Dividing (2) by (3)

$$v = \frac{v^2}{v} = \frac{e^2}{4\pi\varepsilon_0 rm} \times \frac{2\pi mr}{nh} = \frac{e^2}{2\varepsilon_0 nh} \quad -(6)$$

Using (6) & (5) in (1)

$$\nu = \frac{v}{2\pi r} = \frac{\frac{e^2}{2\varepsilon_0 nh}}{2\pi \times \frac{n^2h^2\varepsilon_0}{\pi me^2}} = \frac{me^4}{4\varepsilon_0^2 n^3h^3} = \frac{me^4}{32\pi^3\varepsilon_0^2h^3n^3}$$

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(c) Using $E_n = \frac{me^4}{32\pi^2 \varepsilon_0^2 \hbar^2 n^2}$ to determine

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

As we know $E_n = \hbar\nu = \hbar \times 2\pi \times \nu$

$$\nu = \frac{me^4}{64\pi^3 \varepsilon_0^2 \hbar^3 n^2}$$

when the electron makes transition from orbit n to n-1 then,

$$\nu = \frac{me^4}{64\pi^3 \varepsilon_0^2 \hbar^3} \times \left(\frac{1}{(n-1)^2} - \frac{1}{n^2} \right)$$

$$= \frac{me^4}{64\pi^3 \varepsilon_0^2 \hbar^3} \times \left(\frac{n^2 - (n^2+1-2n)}{(n-1)^2 n^2} \right)$$

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

If n is very large i.e. $n >> 1$ then

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

$$\nu = \frac{me^4}{64\pi^3 \varepsilon_0^2 \hbar^3} \times \frac{2n}{n^4} = \frac{me^4}{32\pi^3 \varepsilon_0^2 \hbar^3}$$

which is same as frequency for classical system. So, for large value of n classical and quantum physics overlaps.

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Discussion: Energy Level Diagram shows that as the value of n increases (Size of atom increase), the difference between two consecutive Energy levels reduces.

Graph between Relative Difference (%) and $\log_{10}(n)$ shows that when value of n is very large, then classical results ~~and~~ for frequency of electron and results obtained quantum mechanically matched.

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PS C:\Users\adn19> & C:/Users/adn19/anaconda3/python.exe "d:/Sem 5/Quantum Mechanics/Lab/Assignments/Assignment 1.py"
                n          f_qn          f_cl  Relative Difference(%)
0        3.162278  3.723188e+11  2.067686e+11               44.464642
1       10.000000  7.668724e+09  6.538596e+09               14.736842
2       31.622777  2.170070e+08  2.067686e+08                4.718015
3      100.000000  6.637999e+06  6.538596e+06                1.497487
4      316.227766  2.077535e+05  2.067686e+05                0.474091
5     1000.000000  6.548417e+03  6.538596e+03                0.149975
6     3162.277660  2.068667e+02  2.067686e+02                0.047432
7    10000.000000  6.539577e+00  6.538596e+00                0.015000
8    31622.776602  2.067784e-01  2.067686e-01                0.004743
9   100000.000000  6.538694e-03  6.538596e-03                0.001500
10  316227.766017  2.067695e-04  2.067686e-04                0.000474
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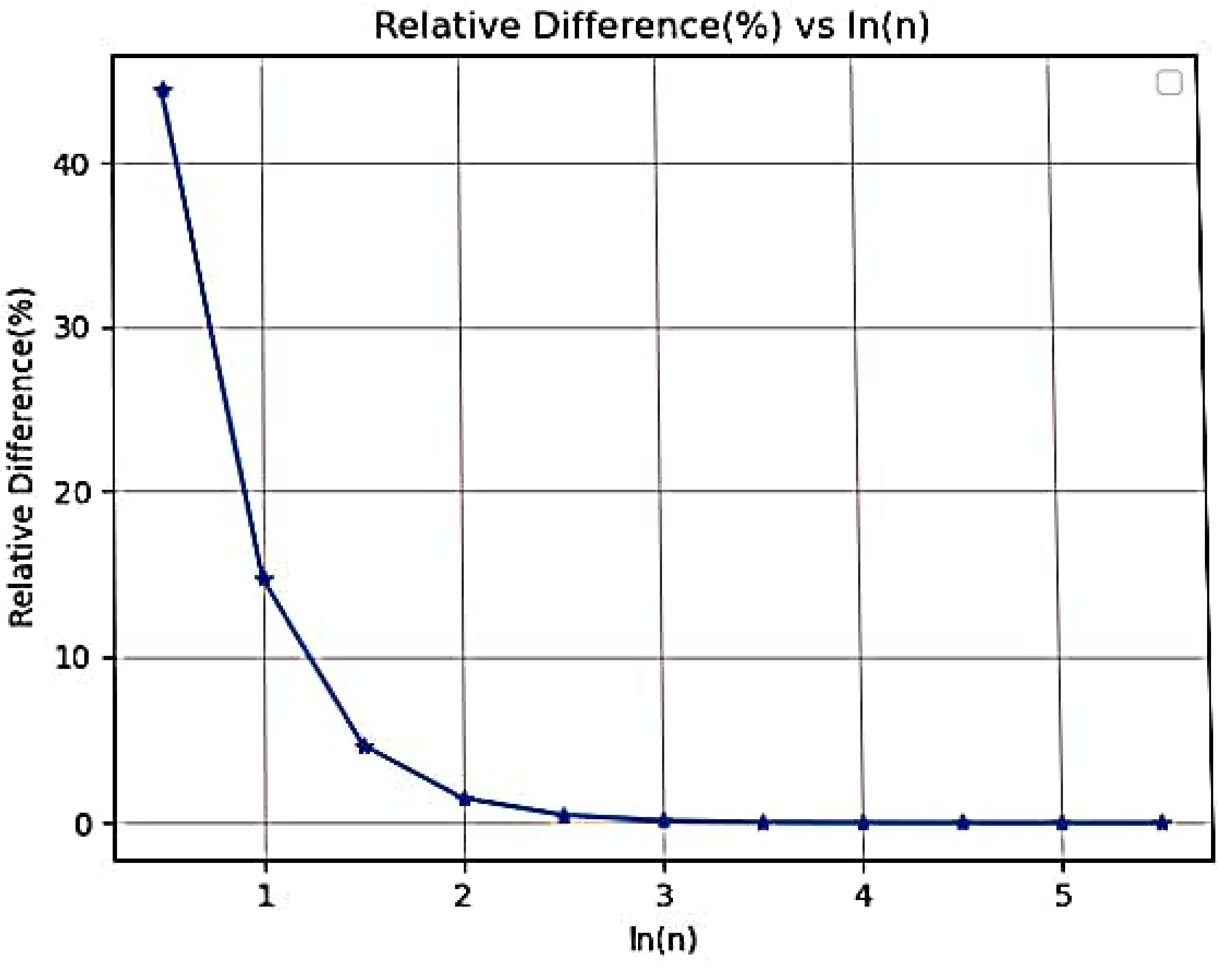
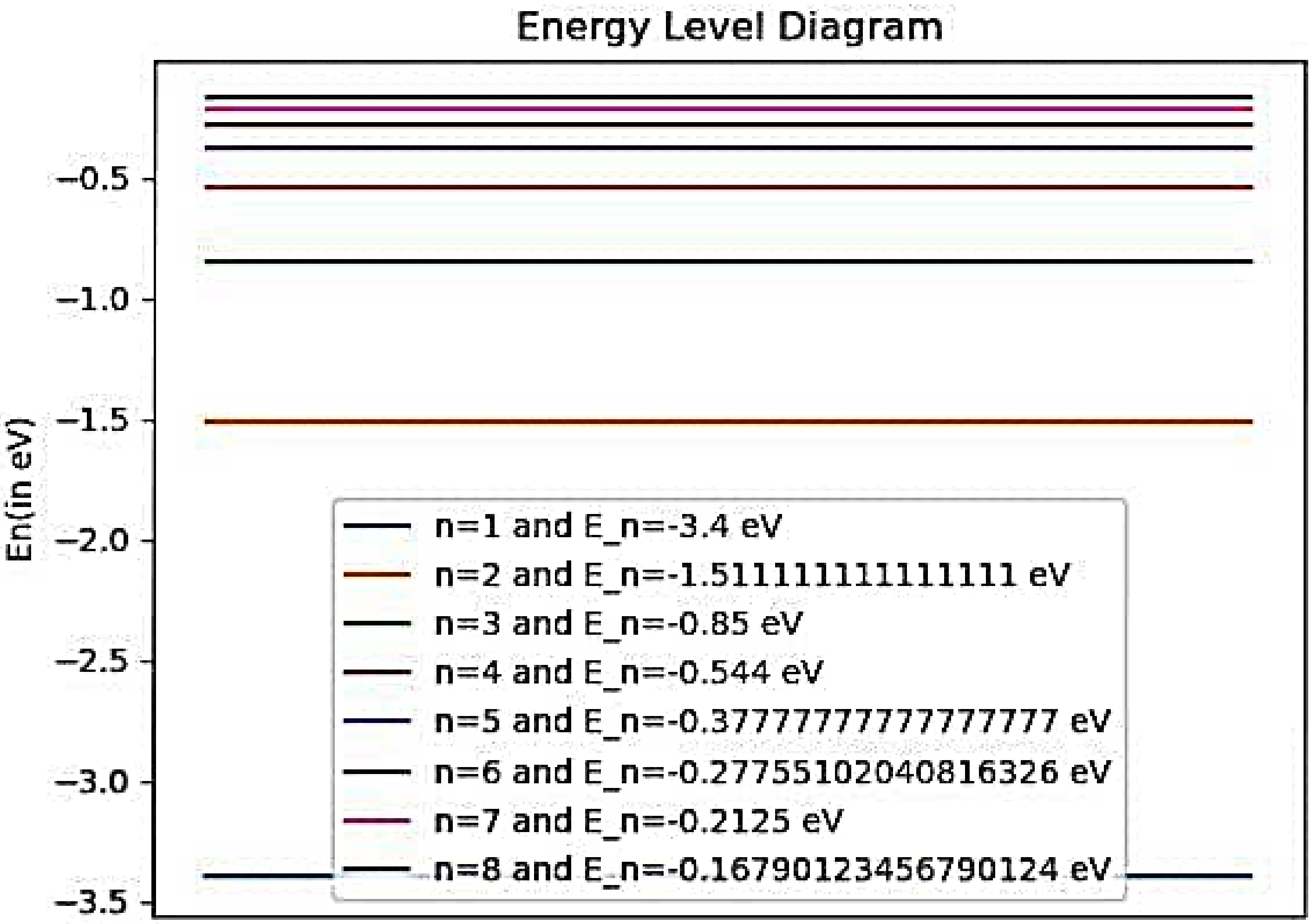


Relative Difference(%) vs ln(n)
Relative Difference(%)
ln(n)
0
10
20
30
40
1
2
3
4
5



Energy Level Diagram
En(in eV)
−0.5
−1.0
−1.5
−2.0
−2.5
−3.0
−3.5
n=1 and E_n=-3.4 eV
n=2 and E_n=-1.5111111111111111 eV
n=3 and E_n=-0.85 eV
n=4 and E_n=-0.544 eV
n=5 and E_n=-0.37777777777777777 eV
n=6 and E_n=-0.27755102040816326 eV
n=7 and E_n=-0.2125 eV
n=8 and E_n=-0.16790123456790124 eV