# 2. Atoms and Bohr Model

## 2.1 Introduction

- Concept of atom → John Dalton (1803)
- Electron → J. J Thompson (1897)

Proposed that as $e^-$ are negatively charged particles, hence atom must contain the positively charged particles too.

Hence, he suggested "Plum Pudding Model".

- Verification of Plum Pudding Model :-

RUTHERFORD SCATTERING EXPERIMENT

Geiger and Marsden carried out Alpha particle Scattering Experiment under Guidance of Rutherford.

→ $\alpha$- particle = positively charged particle
= actually a Helium Nucleus.

So if Plum Pudding Model is really true then most of the $\alpha$ particles would be deflected & hence one could conclude that positively charged particle is distributed all over atom.

But most of the $\alpha$ particle in that famous Gold foil experiment done under Rutherford, went without appreciable deflection.

Hence, Plum Pudding Model failed. Although from the center of the atom of Gold foil, there was great deflection, which concluded that at the center of atom there is positively charged particle - called NUCLEUS.

## Observations from Rutherford Nucleus Model.

- Most of the space is metal foil must be empty
- Positively charged matter must be center at/around single point

Hence Rutherford proposed planetary Model.

This model is Concentrated in tiny Nucleus. And electrons revolve around the nucleus.

## Critical Issues with Rutherford's Model.

- electron in a circle is continously revolving charged particle: That is, it is in acceleration
- And as per "classical electrodynamics", such accelerated charged particle must radiate out energy. Hence it should spiral and fall into the nucleus, which doesn't happen.

that is because spiralling electron would emit radiation of increasing frequency

But we all know — atoms don't radiate unless excited.

## 2.2 Atomic Spectra

All elements in atomic state $\rightarrow$ emit line spectra

bright lines separated by dark intervals.

From atomic spectroscopy it was found that each atom exhibits definite pattern / Series. We call them "spectral Series."

characteristics of atoms.

Study of atoms in such a way is termed "Spectroscopy".

In intial days – wavelength of such series was calculated empirically or Semi-empirically. One such effort was made by ~~Balt~~ Balmer in 1885.

Rydberg const : $1.097 \times 10^{7}\ m^{-1}$

$$\frac{1}{\lambda} = R\left(\frac{1}{2^2} - \frac{1}{n^2}\right)$$

longest wavelength of Balmer series is $6563\ \mathring{A}$.

for transition from $n$th energy level to energy level 2, of Hydrogen atom.

Later on other series like Balmer Series were identified. Generic formula is :-

$$\frac{1}{\lambda} = R\left[\frac{1}{n_1^2} - \frac{1}{n_2^2}\right]$$ ; where $n_2 > n_1$

Rydberg – Ritz Formula.

for Lyman Series $\equiv n_1 = 1$

" Balmer " $\equiv n_1 = 2$

" Paschen " $\equiv n_1 = 3$

" Brackett " $\equiv n_1 = 4$

" Pfund " $\equiv n_1 = 5$

## 2.3 Bohr Model of Hydrogen like Atom

In 1913 → Bohr Suggested → Theories of classical electrodynamics doesn't apply at atomic scale.

combined

Rutherford's Nuclear Model

and

Quantum Idea by Planck and Einstein

↓

Proposed theory for Hydrogen like atom. → although not entirely true, but still important milestone.

**Postulates Proposed :-**

I. electrons can revolve only in certain allowed orbits.

II. Angular Momentum is quantised (PYQ).

$L = n\hbar$

III. Electron make transition from lower to upper or upper to lower orbit.

- lower to upper energy level ⇒ Extra energy needed by absorbing a photon of energy $h\nu = E_2 - E_1$.

- higher to lower energy level ⇒ Extra energy released by emitting a photon of energy $h\nu = E_2 - E_1$.

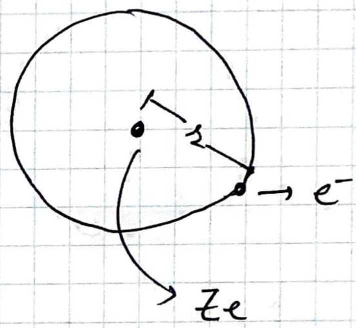
Based on above postulates one can find radius of orbit and velocity of electron orbitting :-

Let $Z$ = atomic no. of the atom (i.e nucleus).

So, centripetal Force of $e^-$ revolving = Coulomb Force in b/w $e^-$ and Nucleus.

$$\Rightarrow \frac{mv^2}{r} = \frac{1}{4\pi\epsilon_0} \cdot \frac{(Ze)\cdot(e)}{r^2}$$

$$\Rightarrow \frac{mv^2}{r} \cdot mr^2 = [RHS]\, mr^2$$




$$\Rightarrow m^2v^2r^2 = [RHS]\cdot mr^2 \cdot r$$

$$\Rightarrow L^2 = \frac{Ze^2 \cdot mr^3}{4\pi\epsilon_0 \cdot r^2}$$

$$\Rightarrow n^2\hbar^2 = \frac{Ze^2 \cdot mr}{4\pi\epsilon_0}$$

$$\Rightarrow \boxed{r = r_n = \frac{4\pi\epsilon_0 \cdot n^2\hbar^2}{Ze^2 \cdot m}}$$

and similarly velocity (speed) of $e^-$ in the orbit is — $\boxed{V_n = \frac{Ze^2}{(4\pi\epsilon_0)\hbar n}}$

Radius when $Z=1$, $n=1$

Or in simpler form → $a_0 = \frac{4\pi\epsilon_0\hbar^2}{me^2}$

$$r_n = (0.529)\frac{n^2}{Z} \; \mathring{A}$$

$$V_n = (2.18\times10^6)\frac{Z}{n} \; m/s.$$

• Remember it!

Now one can find Total Energy →

$$T.E = \text{Kinetic Energy} + \text{Potential Energy}$$

$$= \frac{1}{2}mv^2 + \frac{1}{4\pi\epsilon_0} \cdot \frac{Q_1 \cdot Q_2}{r}$$

$$= \frac{1}{2}m \cdot \left[\frac{Ze^2}{4\pi\epsilon_0 \hbar n}\right]^2 + \frac{1}{4\pi\epsilon_0} \cdot \frac{(Ze)(-e)}{(4\pi\epsilon_0)n^2\hbar^2/Ze^2m}$$

$$\boxed{T.E = -\frac{m}{2\hbar^2}\left(\frac{Ze^2}{4\pi\epsilon_0}\right)\left(\frac{1}{n^2}\right)}$$ } imp. relation keep in mind

or $$T.E = (-13.6)\frac{Z^2}{n^2} \text{ eV}.$$

## Summary

- $$r_n = \frac{(4\pi\epsilon_0)n^2\hbar^2}{Ze^2m} = 0.529\frac{n^2}{Z} \text{ Å}$$

- $$V_n = \frac{Ze^2}{(4\pi\epsilon_0)\hbar \cdot n} = 2.18\times 10^6 \frac{Z}{n} \text{ m/s}$$

- $$E_n = -\frac{m}{2\hbar^2}\left(\frac{Ze^2}{4\pi\epsilon_0}\right)\frac{1}{n^2}$$

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

## Frequency and wavelength of Radiation in the Transition from $n_2 \rightarrow n_1$

Recalling energy difference relation :-

$$h\nu = E_{n_2} - E_{n_1}$$

$$\Rightarrow \nu = \frac{E_{n_2} - E_{n_1}}{h} = \frac{E_{n_2} - E_{n_1}}{2\pi\hbar}$$

$$\Rightarrow \nu = \frac{m}{4\pi\hbar^3}\left(\frac{Ze^2}{4\pi\epsilon_0}\right)\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)$$

$$\Rightarrow \frac{c}{\lambda} = \frac{m}{4\pi\hbar^3}\left(\frac{Ze^2}{4\pi\epsilon_0}\right)^2\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)$$

$$\Rightarrow \boxed{\frac{1}{\lambda} = R_\infty Z^2\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)}$$

where $R_\infty \rightarrow \frac{m}{4\pi c\hbar^3}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2$

Rydberg constant.

$\infty$ sign hints that infinite nuclear mass has been assumed.

It is combination of fundamental constants and is remarkably close to empirical value $\rightarrow$ $1.097 \times 10^7 \ m^{-1}$

In atomic physics You will study "Infinite Nuclear Mass Correction".

# 3. WAVE NATURE OF MATTER

## 3·1 DE BROGLIE HYPOTHESIS

As we studied that radiation has dual nature according to theories / observation of Planck, Einstein and compton.

de Broglie Hypothesis.

Lateron In 1924, Louis deBroglie extended the idea that " Radiation behaves as Matter" to it reverse analogous part "Matter too has wave nature".

we know that energy is :-

$$E^2 = p^2c^2 + E_0^2$$

→ Rest Mass Energy. (RME)

for photon we could write :-

$$(h\nu)^2 = p^2c^2 \qquad \left\{ \text{RME is Zero for photon} \right\}$$

$$\Rightarrow \quad p = h/\lambda$$

$$\Rightarrow \quad \boxed{\lambda = \frac{h}{p}} \quad \Rightarrow \text{de Broglie wavelength}$$

Now as $k = 2\pi/\lambda$

hence $p = \hbar \cdot k$

and $E = \hbar\omega$

Hence.

| | | |
|---|---|---|
| I. | $\lambda = h/p$ | Basic Relations of Quantum Theory |
| II. | $p = \hbar k$ | |
| III. | $E = \hbar\omega$ | |

Other usefull expression related to de Broglie wavelength

I. $$\boxed{\lambda = \frac{h}{\sqrt{2mKE}}}$$ as $KE = \frac{p^2}{2m}$

II. $$\lambda = \frac{h}{\sqrt{2mqV}}$$ as $KE = qV$

charge

Accelerating Potential

or $$\boxed{\lambda = \frac{12.3}{\sqrt{V}}\ \mathring{A}}$$

III. In case of Relativistic energy / speed

$$E^2 = p^2c^2 + m_0^2c^4$$

$$\Rightarrow p^2 = \frac{E^2 - E_0^2}{c^2}$$

and thus $$\lambda = \frac{h}{\sqrt{KE(KE + 2m_0c^2)}}$$

and $$\boxed{\lambda = \frac{12.3}{\sqrt{V(1 + \alpha/2)}}\ \mathring{A}}$$

where $\alpha = \frac{qV}{E_0}$

## 3.2 EXPERIMENTAL VERIFICATION OF DE-BROGLIE HYPOTHESIS

- If you accelerates electron with 100 volts, then by using one can find $\lambda = \frac{12.3}{\sqrt{100}}\,\mathring{A} = 1.23\,\mathring{A}$
- So, de Broglie wavelength associated with $e^-$ accelerated by 100 volts is $\sim 1.23\,\mathring{A}$, which is of same order as of interplanner spacing in b/w crystalls of atom.
- Hence, matter waves' existence may be demostrated by using X-ray diffraction by crystells.

Davisson-Germer Experiment is such an experiment. { Similar experiment was also conducted by G.P Thomson. }

### Davisson - Germer Experiment (1927).

**Prelude** Both were studying → Scattering of $e^-$ from a solid

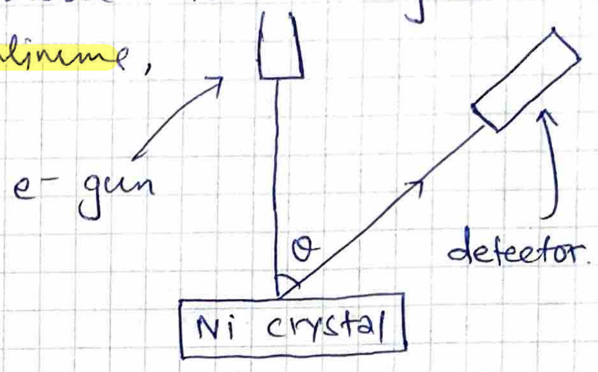
The energy of the electrons in primary beam, the angle at ~~they~~ which they reach the target and position of detector - all could be varried.

**Classical Prediction**

Scattered electrons would energe in all ~~directions~~ directions, with only a moderate dependence on — intensity upon scattering angle
— energy of primary electrons.

**Scattering** Block of Nickel was used.

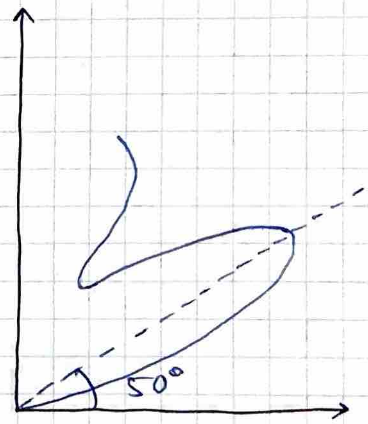
Accidently, air entered the apparatus and to correct they heated the Nickel, in hot oven. But now results were different. Now they could observe distinct Maxima & Minima, instead of continous variation.




So why did this happen?

<u>Answer</u> de Broglie hypothesis suggested that after Nickel was baked to remove the humidity, the ~~crystal~~ ~~plane~~ ~~set~~ atoms actually got crystallized and electrons were diffracted. This proved wave nature of electron.

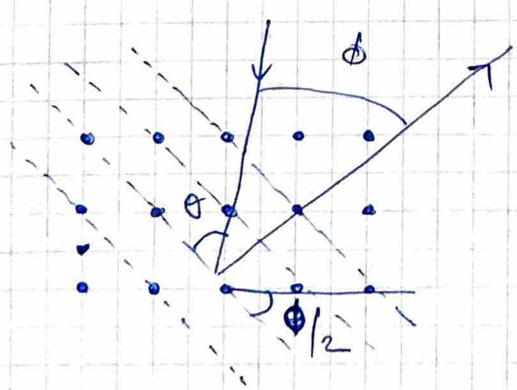
<u>Mathematical description</u>




Remember that increased intensity must have been the result of constructive interference.

Hence, Bragg's condition for the constructive interference is :-

$$n\lambda = 2d\sin\theta \quad ; \quad d \rightarrow \text{spacing b/w alternate bragg's plane}$$




→ for clear image you can see figure 4.4 of Mc Jain

Hence, $\theta + \phi + \theta = 180$

$$\theta = \frac{\pi}{2} - \frac{\phi}{2}$$

and from geometry $d = D \sin \frac{\phi}{2}$

interatomic spacing

So, $n\lambda = 2d\sin\theta$

$$= 2d\sin(\pi/2 - \phi/2)$$

$$= 2D\sin\frac{\phi}{2} \cdot \cos\frac{\phi}{2}$$

$$n\lambda = D\sin\phi$$

we know that for Nickel ~~D = 1~~ $D = 2.15\,\mathring{A}$ and first order diffraction $n = 1$. Assuming the peak for $\phi = 50^\circ$, we get.

$$\lambda = 2.15 \times \sin 50^\circ \ \mathring{A}$$

$$\boxed{\lambda = 1.65\ \mathring{A}}$$

Now, according to deBroglie hypothesis, we accl.ed electrons through a potential difference of 54 volt. so. $\lambda = \frac{12.3}{\sqrt{54}}\,\mathring{A} \approx 1.66\,\mathring{A}$.

$$\Rightarrow \boxed{\lambda = 1.66\,\mathring{A}}$$

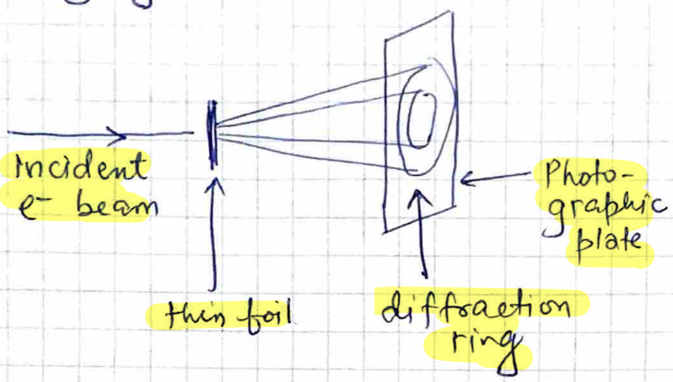
we can see that wavelength from both process is remarkably close. This leds to conclusion that electron's behaved as wave with wavelength and went for constructive ~~interference~~ interference and thus intensity peeks were formed at angle $\phi = 50^\circ$ with incident energy of electron beam to be ~~g~~. corresponding to voltage of 54 V.

## 3.3 GP Thomson's Experiment

highly accelerated $e^-$ → Polycrystalline Material

↓

$e^-$ passes and are observed on Photographic plate.



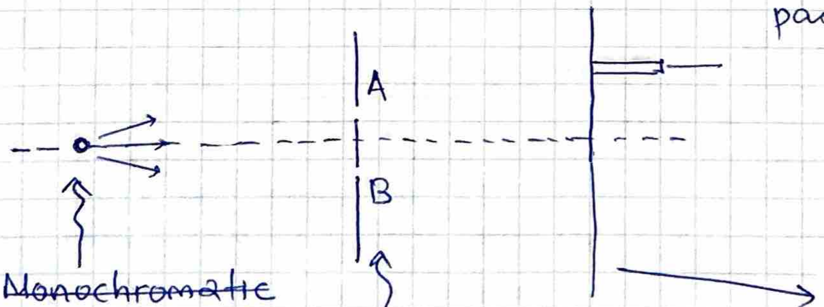

The observed pattern → similar to Debye-Scherrer X-ray

→ confirms wave nature of $e^-$

## 3.4 Double Pattern Experiment – but with particles this time

Double slit experiment → Excellent way to demonstrate WPD

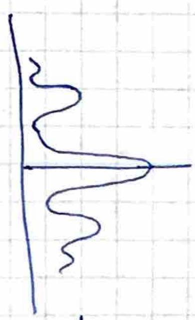
wave-particle duality




~~Monochromatic~~
Monoenergetic
Beam of electron

if wave then monochrometic
but;
as it is particle
so monoenergetic.

width & Spacing of slits having same order of de Broglie wave.



Observation

## 3.4 Need for wave function

The interference pattern with electrons in double slit experiment

↓

tells us that

↓

each particle interferes with itself in some way.

↓

But now → how do we describe a particle interfering with itself and, when they reach on any screen they create interference pattern.

↓

Solution

Solution is derived from classical physics — as we know that waves — are characterised by Amplitude and intensity of such waves is directly proportional to square of amplitude.

thus $I \propto |\psi(x,t)|^2 = \psi^*(x,t) \cdot \psi(x,t)$

we have assumed that each particle has associated wave function, such that absolute square of this function gives intensity.

Suppose we have two waves $\psi_1$ and $\psi_2$ moving to superimpose —

$I_1 = |\psi_1|^2$

hence, $\psi = \psi_1 + \psi_2$

$I_2 = |\psi_2|^2$

and $\psi_1 = |\psi_1| e^{i\alpha_1}$

$\psi_2 = |\psi_2| e^{i\alpha_2}$

where ~~[crossed out]~~ $|\psi_1|$ and $|\psi_2|$ are ~~absolu~~ absolute values and $e^{i\alpha_1}$ and $e^{i\alpha_2}$ are phases.

and we already know $|\psi_1| = \psi_1^* \psi_1$

complex conjugate of $\psi_1$

Thus intensity of combined (or superimposed wave) is →

$$
\begin{aligned}
I &= |\psi_1 + \psi_2|^2 \\
&= (\psi_1 + \psi_2)^* (\psi_1 + \psi_2) \\
&= \psi_1^* \psi_1 + \psi_1^* \psi_2 + \psi_2^* \psi_1 + \psi_2^* \psi_2 \\
&= |\psi_1|^2 + |\psi_2|^2 + \psi_1^* \psi_2 + \psi_2^* \psi_1 \\
&= |\psi_1|^2 + |\psi_2|^2 + |\psi_1||\psi_2| \left(e^{-i(\alpha_1-\alpha_2)} + e^{i(\alpha_1-\alpha_2)}\right)
\end{aligned}
$$

$$\Rightarrow I = |\psi_1|^2 + |\psi_2|^2 + 2\sqrt{I_1}\cdot\sqrt{I_2}\cdot \cos(\alpha_1 - \alpha_2)$$

## 3.5 Born's Interpretation

wave function was interpreted by Born (→ Max Born) statistically as wave functions in Q.M. seems abstract.

He postulated :-

1. wave function which describes a particle is actually wave of its probability.

   Hence $P(x)dx = |\psi(x,t)|^2 dx$.

   Probability of finding the particle in element $dx$ at time $t$.

   and $P(x) = |\psi(x,t)|^2$ is Position Probability Density.

II. Also particle must exist somewhere. So

$$\int_{-\infty}^{\infty} |\psi|^2 dx = 1.$$