

Welcome to



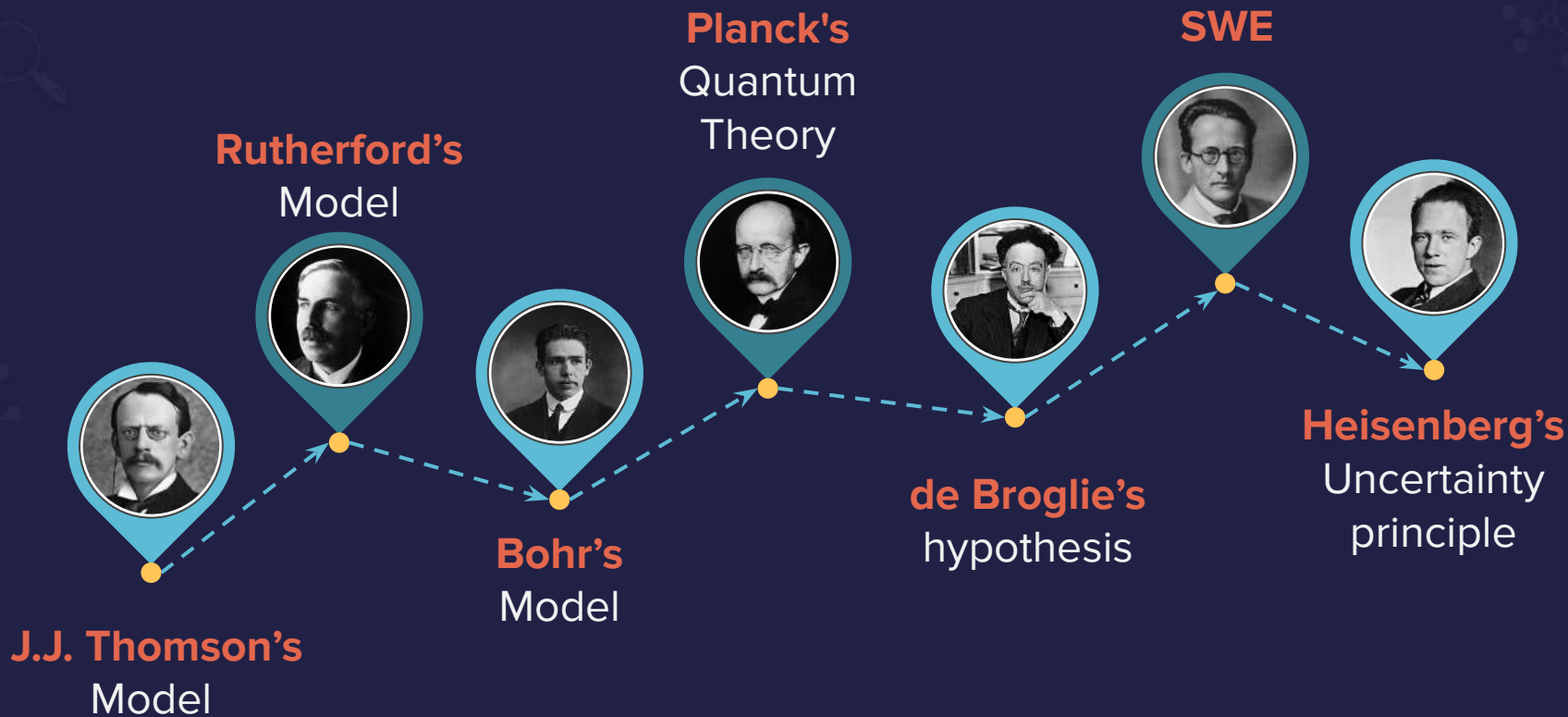
Aakash



BYJU'S LIVE

Atomic Structure





Discovery of electron

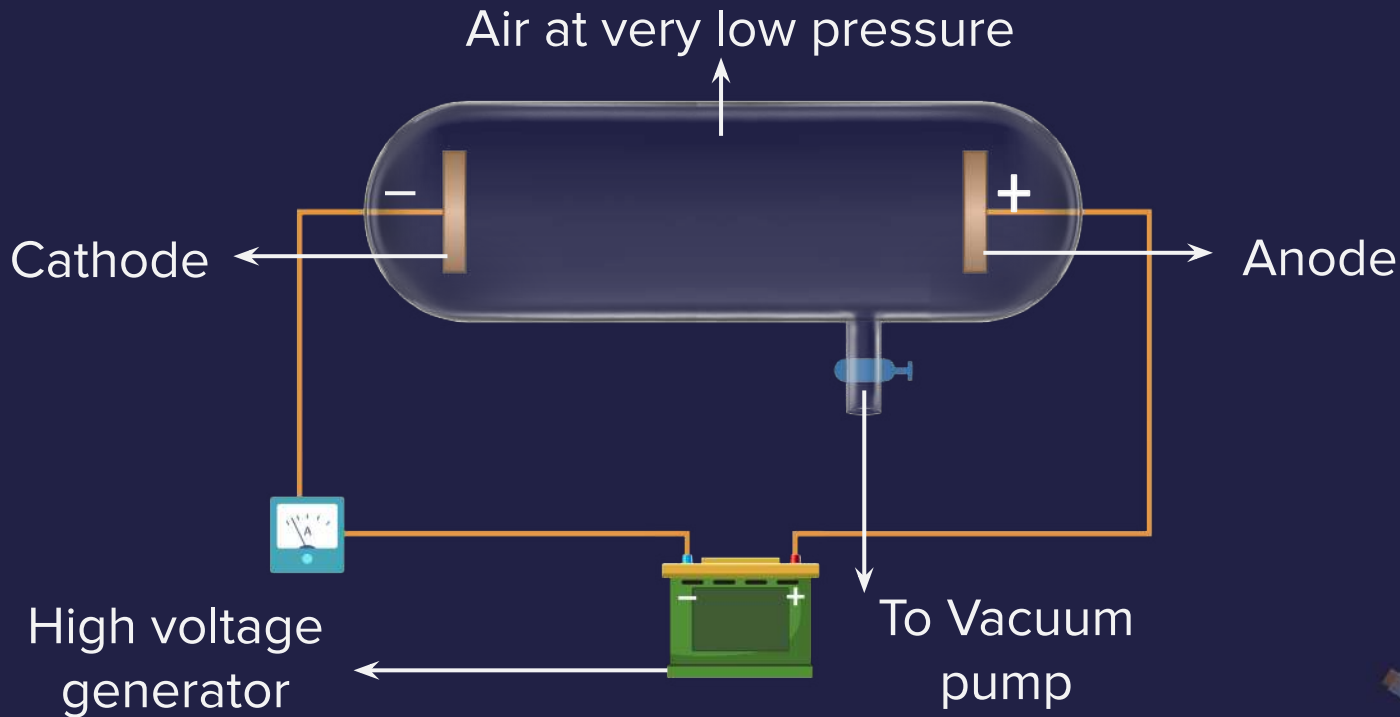
Cathode rays

In 1891, George Johnstone Stoney named the fundamental unit of electricity as 'electron'

J. J. Thomson and his team identified electron as a particle in 1897

Discovery of electron

Discharge tube: Cylindrical hard glass tube fitted with **two metallic electrodes** connected to a **battery**.

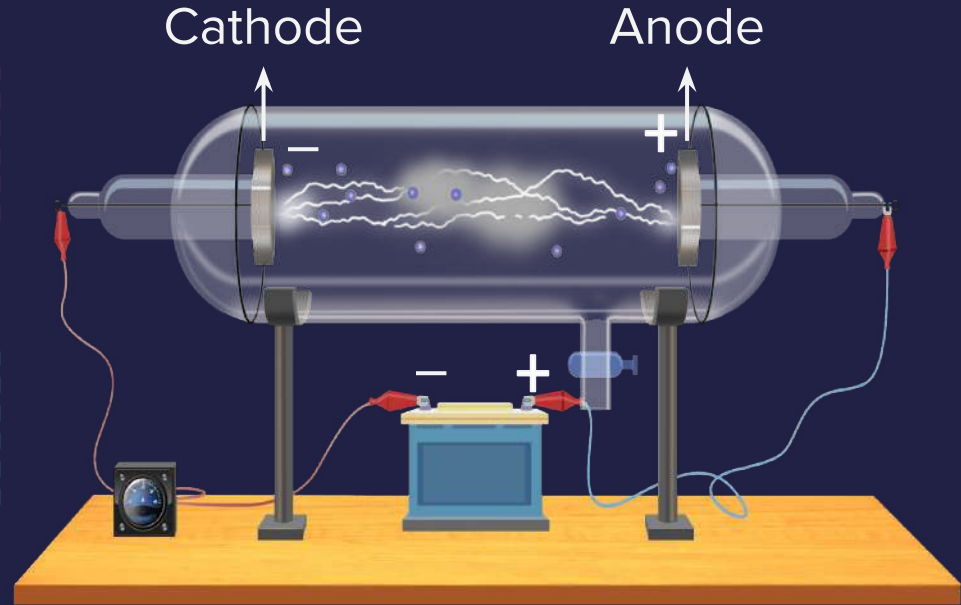


Discovery of electron

Observations

Readings of electric current was observed

Anode end of the tube showed a greenish glow on the ZnS screen







Discovery of electron

Why are Gases used under LOW pressure?

At high pressure, more number of gas molecules are present and so there is more obstructions in the paths of electrons which prevents electrons from reaching the anode.



Discovery of electron

Observation and Characteristics

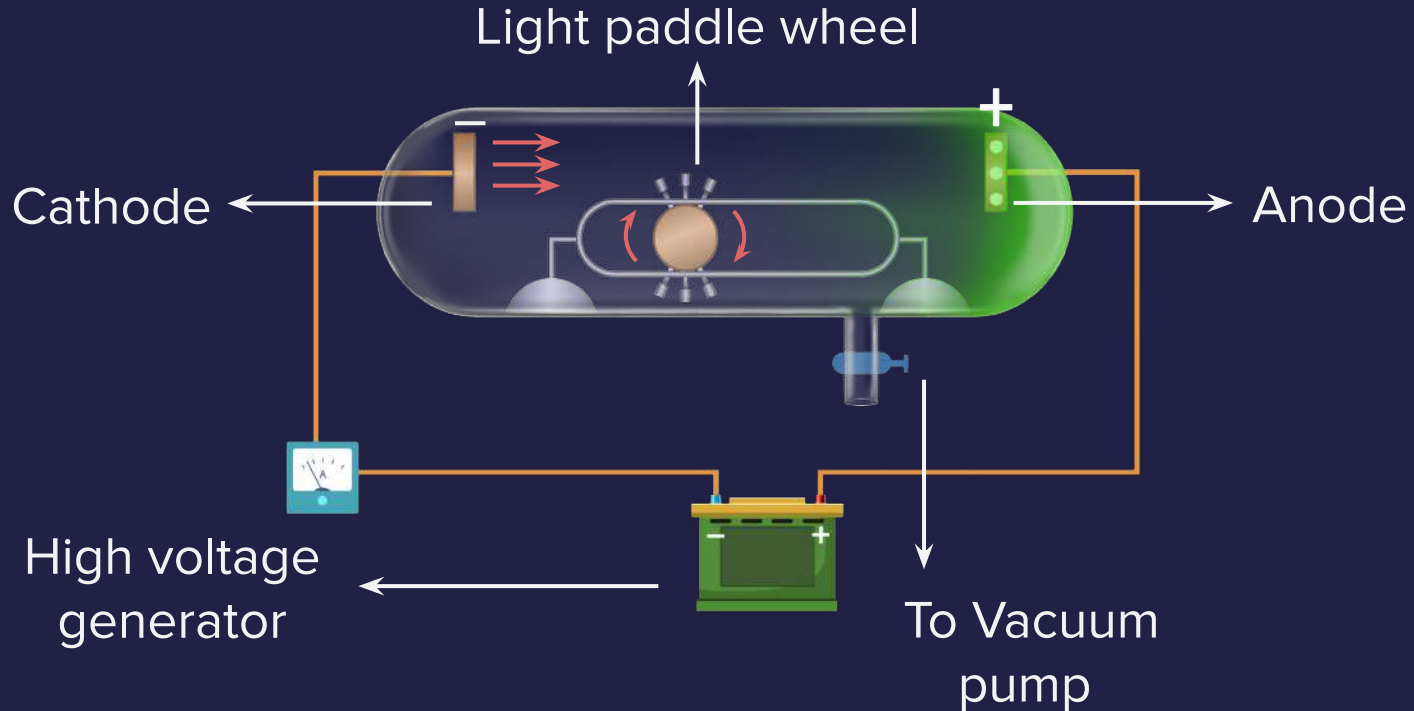
1. Cathode rays move from cathode to anode.

2. Cathode rays travel in a straight line with high velocity in the absence of electric & magnetic fields.

3. Cathode rays are more efficiently observed with the help of a fluorescent or phosphorescent material like ZnS.

4. Cathode rays rotate the light paddle wheel placed in their path. It shows that the particles of cathode ray particles are **material particles** which have **mass** and **velocity**.

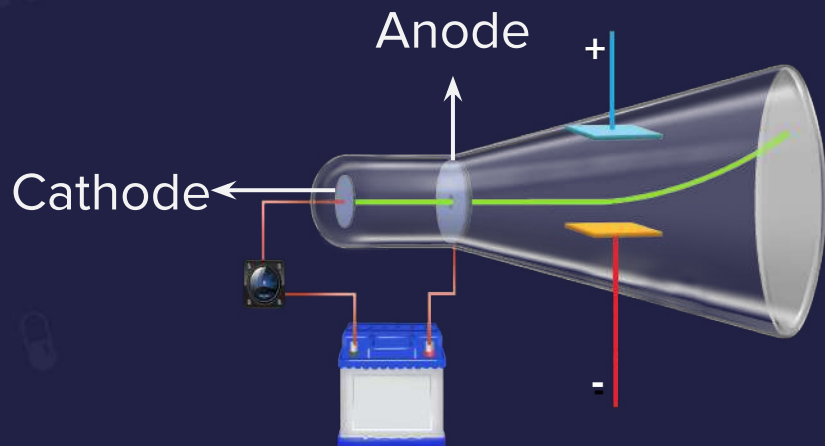
Discovery of electron



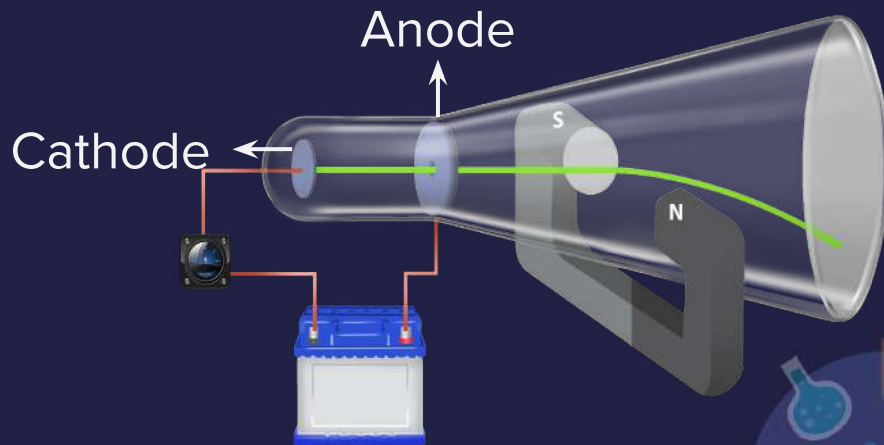
Discovery of electron

Observation and Characteristics

5. Cathode rays are deflected in the presence of an electric field.



6. Cathode rays are deflected in the presence of a magnetic field.



Discovery of electron

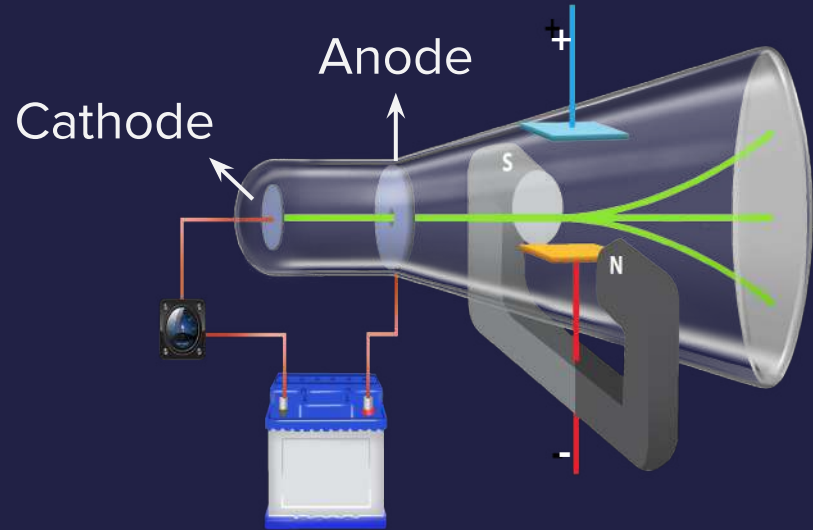
Conclusions

Cathode rays consist of negatively charged particles and identified as **electrons**.

Charge to mass ratio

In 1897, **J.J. Thomson**

- Measured the charge (e) to mass (m) ratio of an electron.
- Electric & magnetic fields were applied perpendicular to each other & to the path of electrons



$$\frac{e}{m}$$

=

$$1.758820 \times 10^{11} \text{ C/kg}$$

Charge to mass ratio

Charge to mass ratio is the same irrespective of

Nature of the gas

Material of Cathode

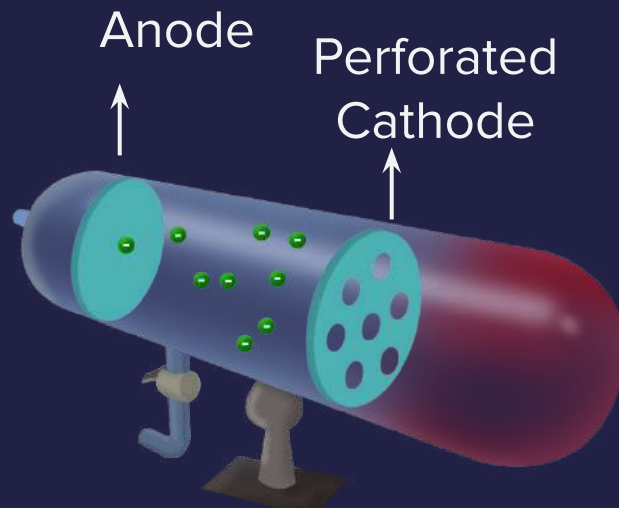
Electrons are fundamental particles

Discovery of Anode Rays

Discovered by Goldstein

He repeated experiment with a discharge tube by using a perforated cathode.

Existence of positively charged particles was shown using anode rays.



Red glow is due to anode particles which pass through perforated cathode and strike the wall of the tube at the cathode side.

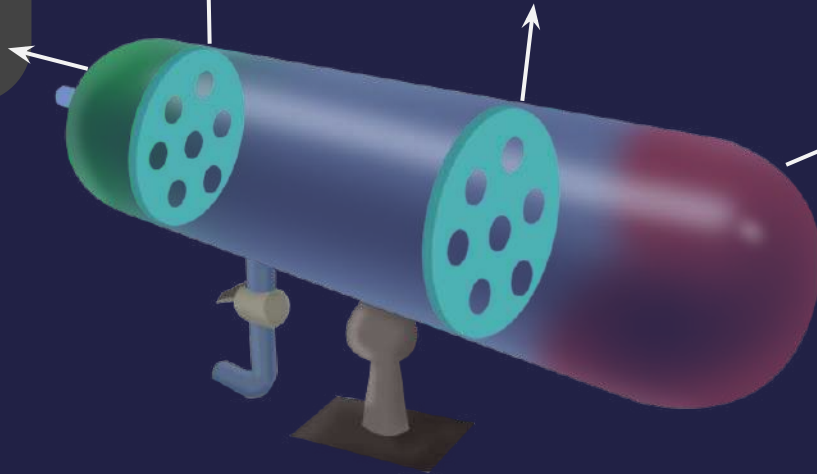
Discovery of Anode Rays

Green colour
fluorescence
observed due
to Cathode
rays

Perforated
Anode

Perforated
Cathode

Red colour
fluorescence
observed due
to Anode rays





Observations and Characteristics

1. Anode rays possess positive charge

Concluded by their directions of deflections in the presence of electric & magnetic fields

2. Anode rays travel in straight lines in the absence of both electric and magnetic fields.





Observations and Characteristics

3. e/m ratio of the canal rays is different for different gases

Properties of anode rays depends on nature of the gas taken in the discharge tube

In 1919, Rutherford discovered that the smallest and the lightest positive ions are obtained from hydrogen and called them protons



Discovery of Neutrons



James Chadwick

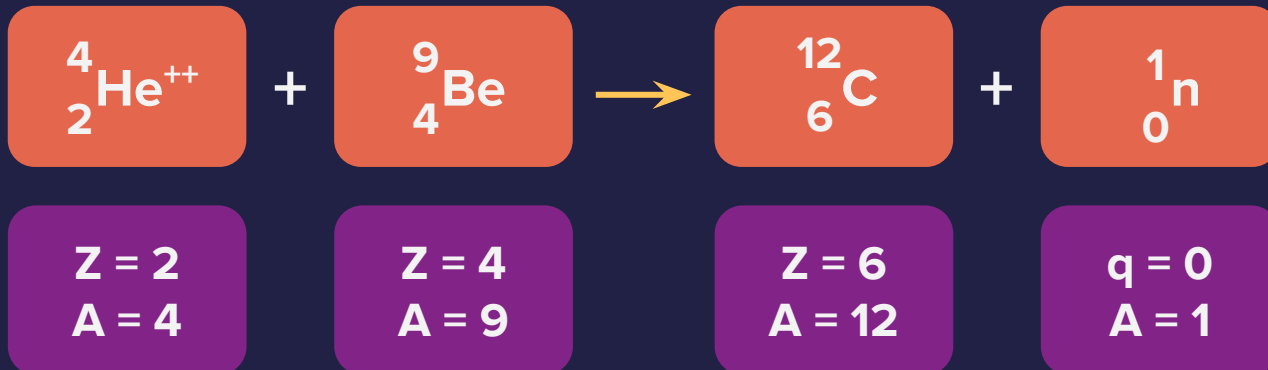
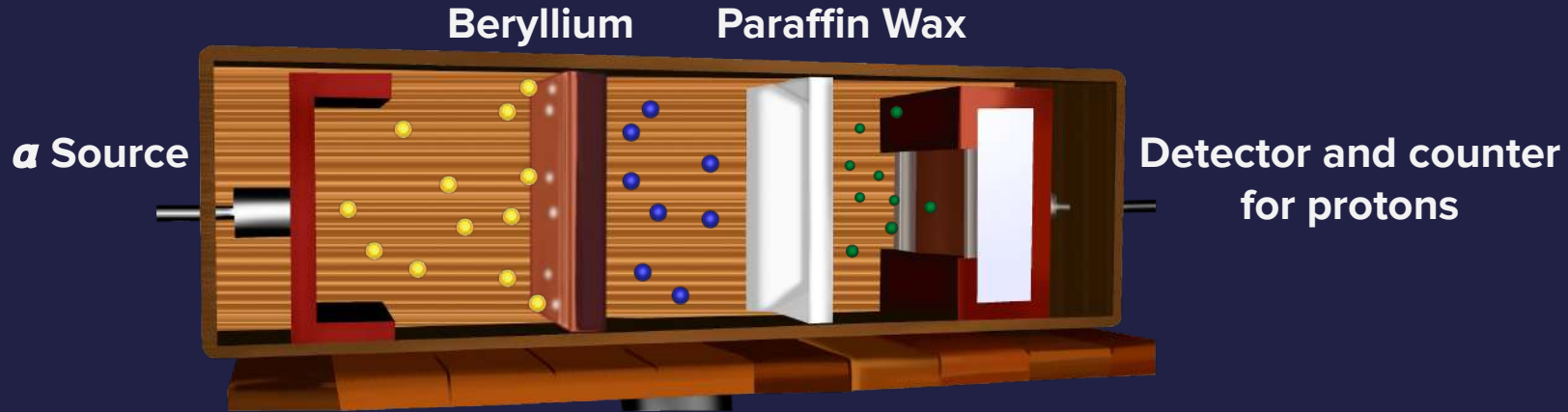
Named the electrically neutral particles emitted as neutrons

Discovered neutrons in 1932

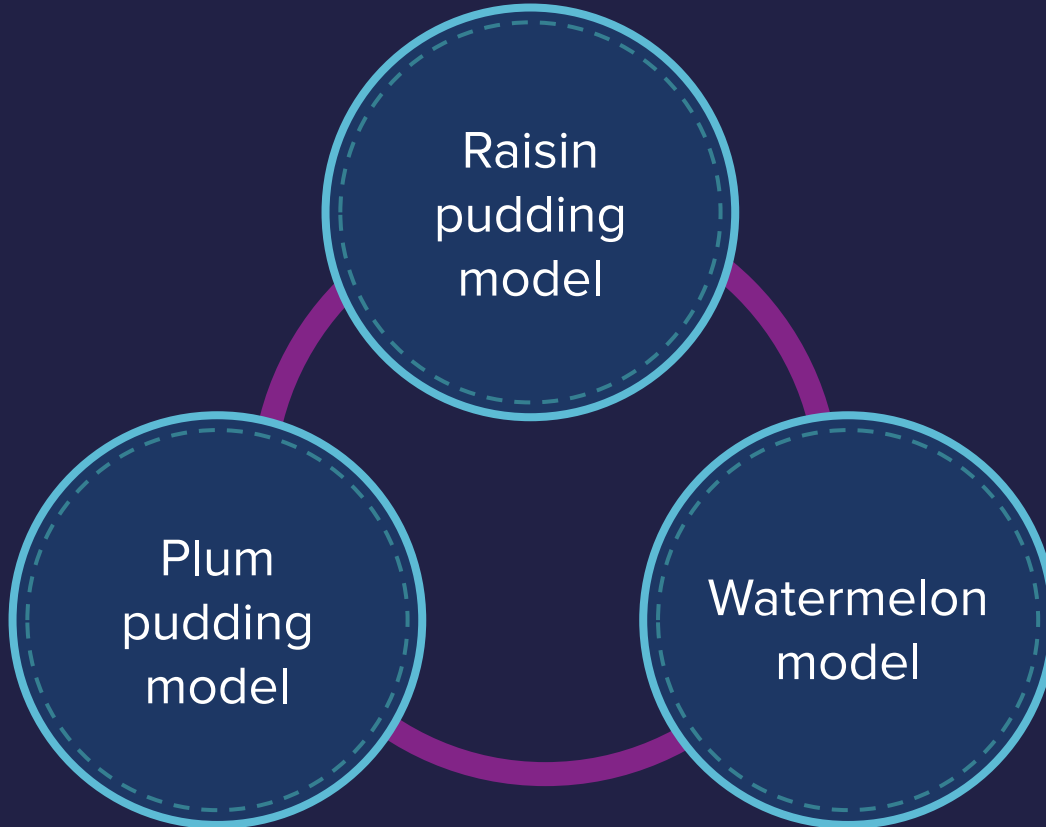
Mass of neutrons is slightly greater than that of protons

Bombarded a thin sheet of beryllium (${}^9_4\text{Be}$) with alpha particles (${}^4_2\text{He}^{2+}$)

Discovery of Neutrons



Thomson's Model



Thomson's Model

1. An atom has a spherical shape
(radius $\sim 10^{-10}$ m)

2. Positive charge is uniformly
distributed throughout the
sphere

3. Negatively charged electrons
are embedded in it like raisins in
a pudding

4. Mass of the atom is assumed to
be uniformly distributed all over it



Plum Pudding



Watermelon

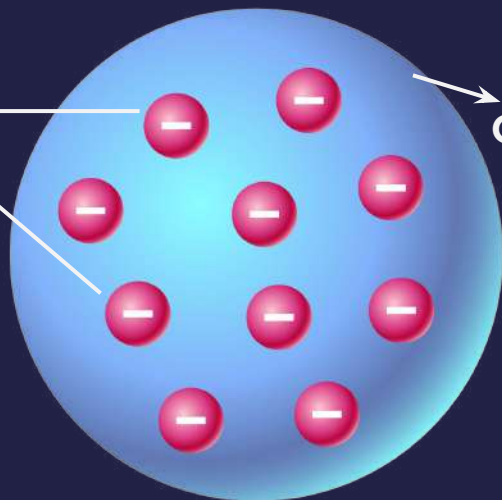
Thomson's Model

Electrons are embedded in an atom in such a way that the most stable electrostatic arrangement is achieved.

Explains the overall neutrality of an atom

Drawback:
Not consistent with the results of later experiments

**Negatively
Charged
Electrons**

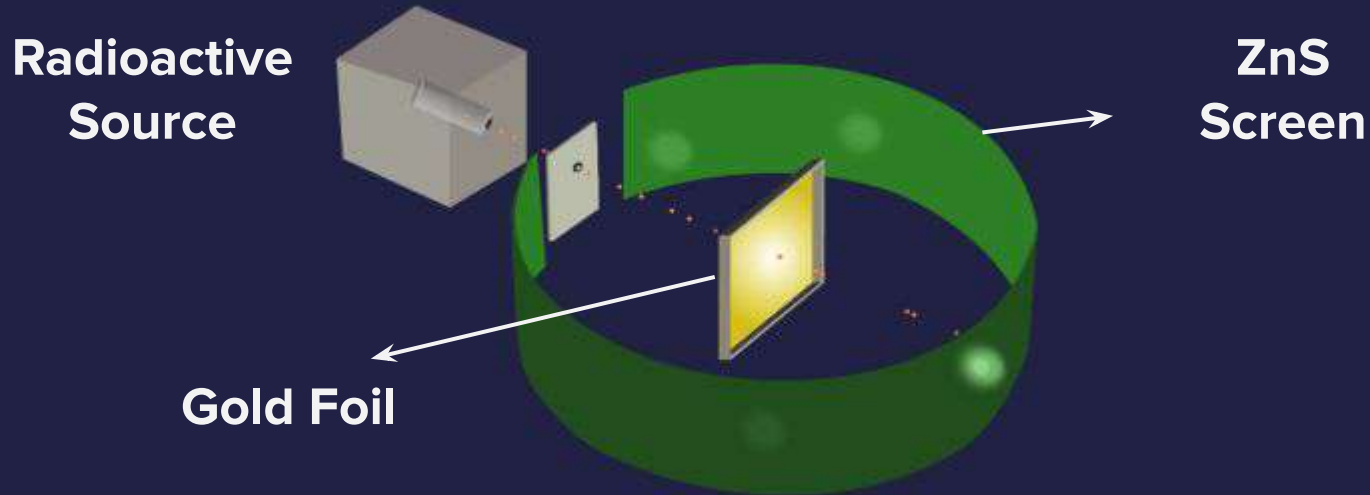


**Positively
Charged Matter**



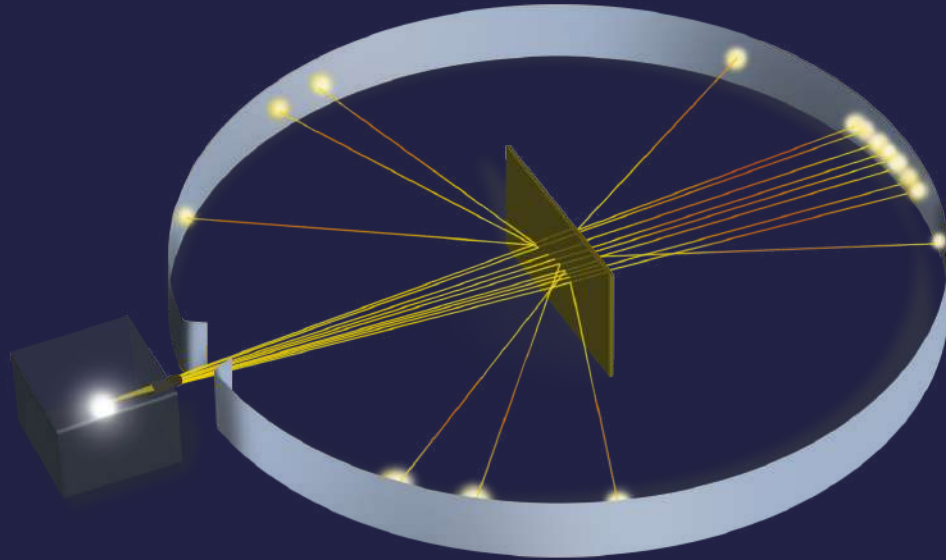
Rutherford's Experiment

A stream of high energy α -particles was directed at a thin gold foil (thickness ~ 100 nm)

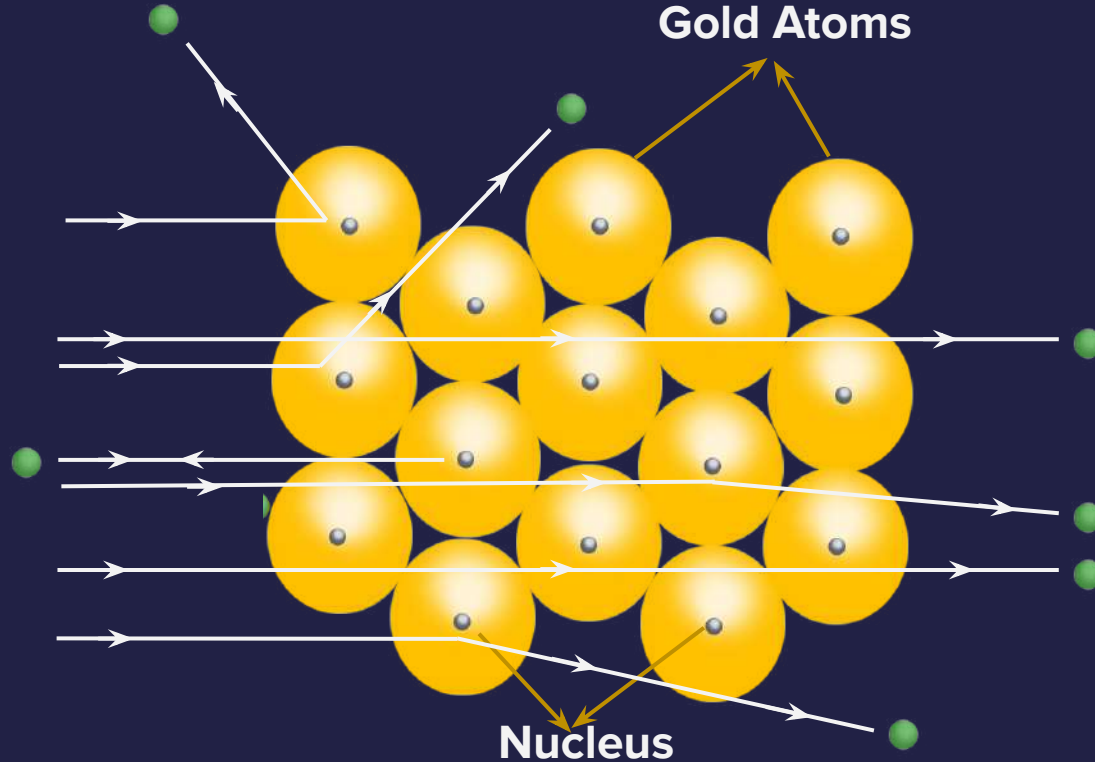


Observations of Rutherford's Experiment

When an α -particle strikes the screen, a glow was produced at that point on the screen



Observations of Rutherford's Experiment



Observations of Rutherford's Experiment

α -particles

1. Most of them passed undeflected

2. Very small fraction was deflected by large angles

3. Very few were deflected by 180° (~1 in 20,000)

4. Small fraction was deflected by small angles



Observation	Conclusion
Most α -particles passed through the foil without deflection.	Presence of large empty space in the atom.
Few α -particles were deflected by small angles.	Positive charge is concentrated in a very small region.
Very few α -particles (~1 of 20,000) deflected at 180° .	Small positively charged core at the centre.



Nucleus

Atom consists of a **small positively charged core** at the center which carries almost the entire mass of the atom

It has **negligible volume** compared to the volume of the atom.



Nucleus

Both, **protons and neutrons** present in the nucleus are collectively called **nucleons**.

$$R = R_0 A^{\frac{1}{3}}$$

Radius of the atom

$$\sim 10^{-10} \text{ m}$$

R = Radius of nucleus of an element

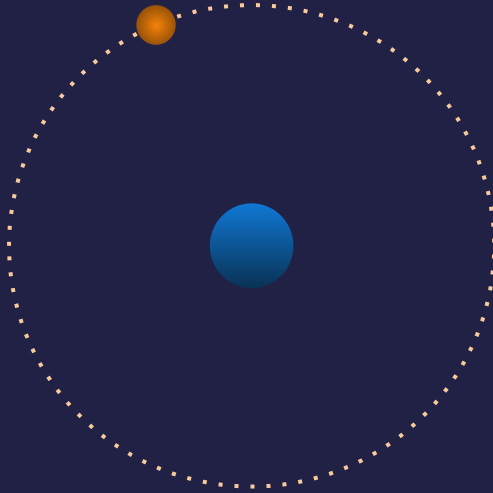
A = Mass number of element

$$\sim 10^{-15} \text{ m}$$

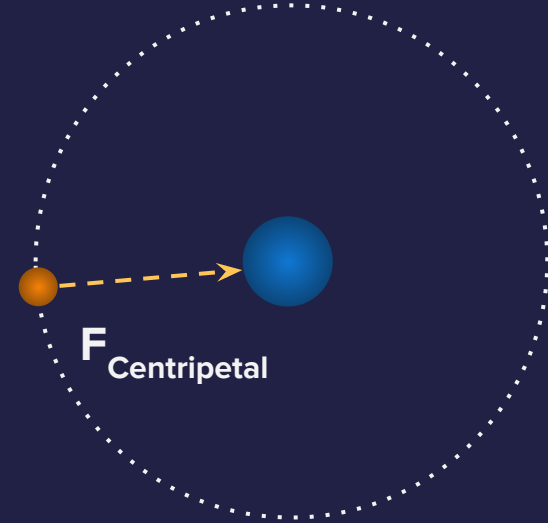
Radius of the nucleus

$$R_0 = 1.11 \times 10^{-15} \text{ m to } 1.44 \times 10^{-15} \text{ m}$$

Extranuclear part



Electrons and nucleus are held together by electrostatic forces of attraction.



Nucleus is surrounded by revolving electrons.

$F_{\text{Electrostatic}}$

=

$F_{\text{Centripetal}}$



Drawbacks of Rutherford's Model

It could not explain stability of the atom.

It could not explain line spectrum of the H atom.

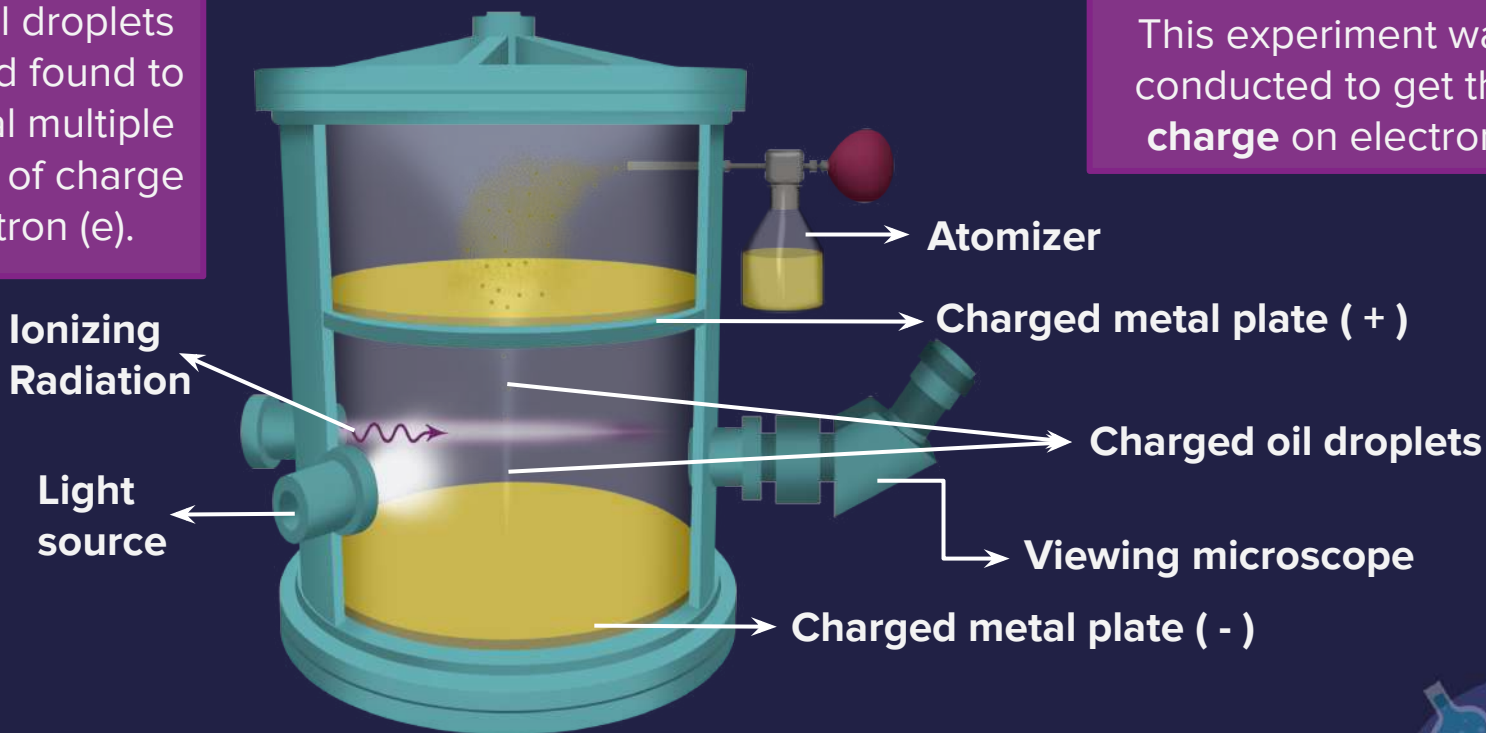
It could not explain the electronic structure of the atom.



R.A. Millikan's Oil drop experiment

Charge on oil droplets measured and found to be an integral multiple of magnitude of charge on an electron (e).

This experiment was conducted to get the **charge** on electron.



Charge on electron

$$- 1.602176 \times 10^{-19} \text{ C}$$



Mass of the electron

Thomson's e/m ratio

$$1.75882 \times 10^{11} \text{ C kg}^{-1}$$

Charge from
Millikan's experiment

$$- 1.602176 \times 10^{-19} \text{ C}$$

From **Thomson's experiment**, e/m ratio calculated and from **Oil drop experiment**, **charge** of electron calculated. Using the data from these two experiments, **mass of the electron** was determined.

Subatomic Particles

Subatomic Particles	Mass (u)	Absolute Mass (kg)
---------------------	----------	--------------------

Electron	0.0005	9.1×10^{-31}
----------	--------	-----------------------

Proton	1.007	1.6722×10^{-27}
--------	-------	--------------------------

Neutron	1.008	1.6749×10^{-27}
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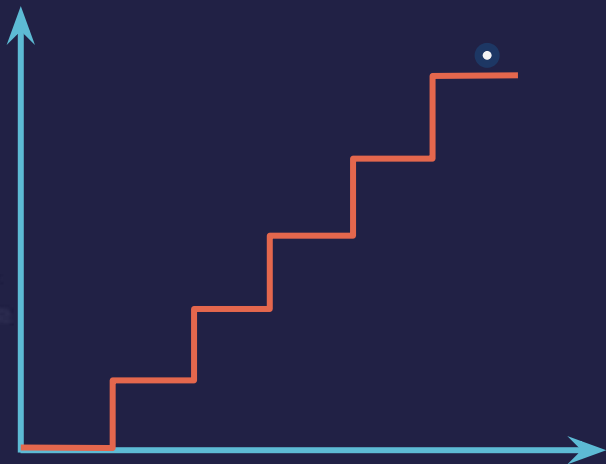
Subatomic Particles	Relative Charge	Absolute Charge (C)
---------------------	-----------------	---------------------

Electron	-1	-1.602×10^{-19}
----------	----	--------------------------

Proton	+1	1.602×10^{-19}
--------	----	-------------------------

Neutron	0	0
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Quantization of Charge



$$q = n(e)$$

$$q = n (1.6 \times 10^{-19} \text{ C})$$

$$q = n (4.8 \times 10^{-10} \text{ esu})$$

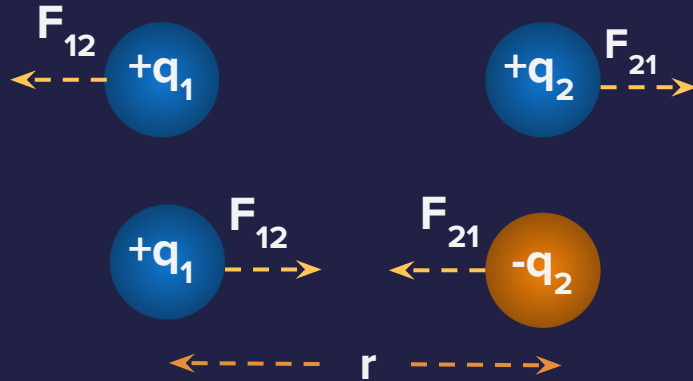
$$n = 1, 2, 3 \dots$$

The charge can't have continuous range of values but only take values in multiple of charge on one electron. The magnitude of charge on an electron is the smallest unit and denoted as "e". Thus charge on an electron is -e and on a proton, it is +e.

Electrostatic Force

$$F_{12} = F_{21} = K \frac{q_1 q_2}{r^2}$$

$$K = \frac{1}{4\pi\epsilon_0} = 9 \times 10^9 \frac{\text{Nm}^2}{\text{C}^2}$$



$$\epsilon_0 = 8.854 \times 10^{-12} \frac{\text{C}}{\text{Vm}}$$

ϵ_0 = Permittivity of vacuum



Potential Energy

$$\text{P.E.} = q \times V$$

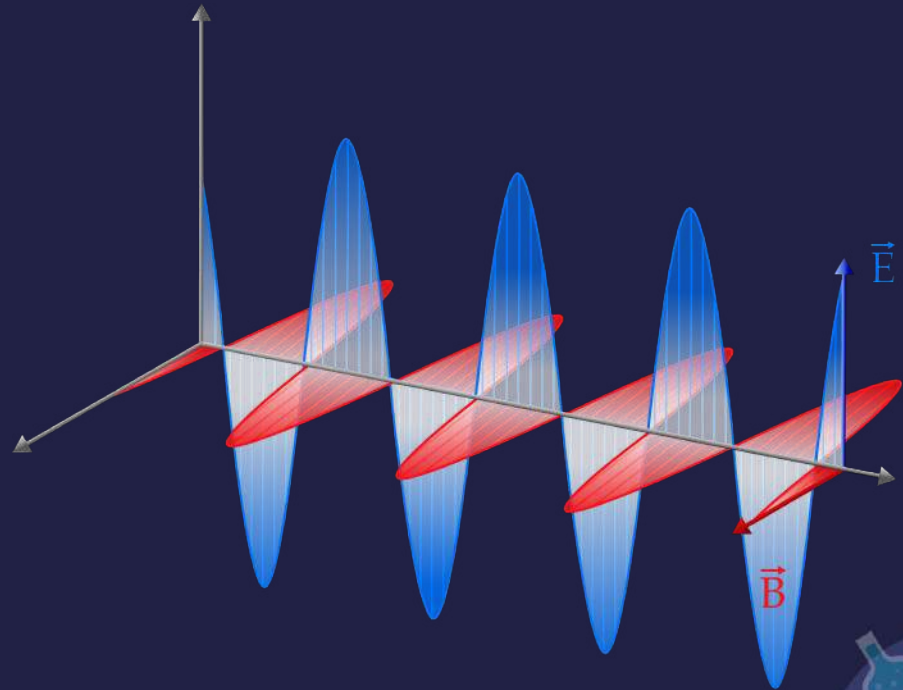
q = Charge of the particle
V = Potential of surface

$$\text{P.E.} = \frac{1}{4\pi\epsilon_0} \frac{q_1 q_2}{r}$$

$$\text{P.E.} = K \frac{q_1 q_2}{r}$$

Electromagnetic Waves

Oscillating
Electric &
Magnetic field





Properties of Electromagnetic Waves

Electric & magnetic field
oscillate perpendicular to each other

Both oscillate perpendicular to the
direction of propagation of wave

Do not require any medium for
propagation

Can travel in vacuum

$c = 3 \times 10^8 \text{ ms}^{-1}$ (in vacuum)

Propagate at a constant speed i.e. with
the speed of light (c)



Characteristics of Electromagnetic waves



Wavelength

Frequency

Velocity

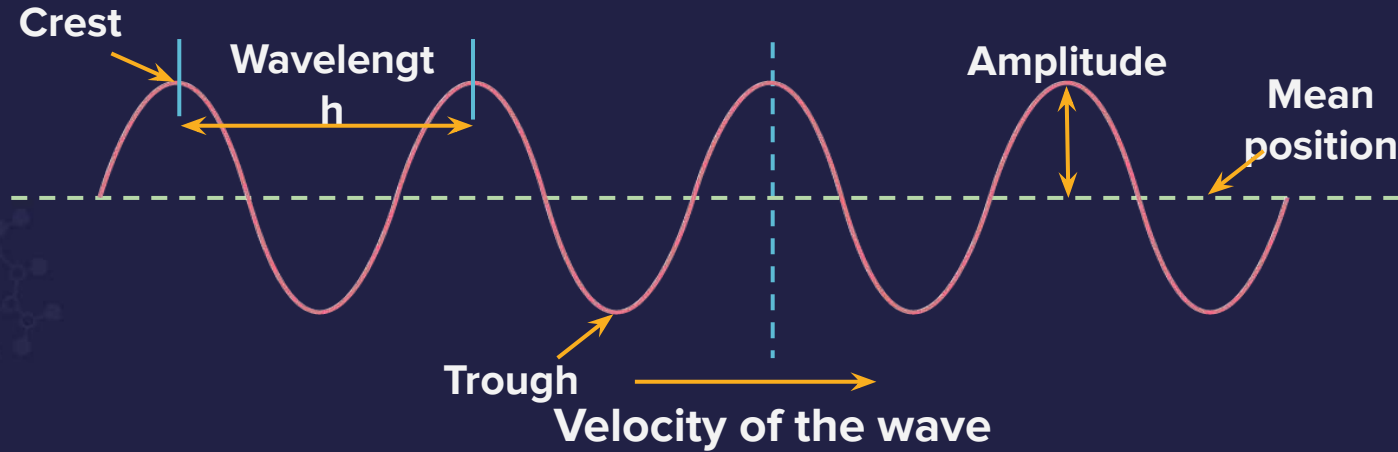
Time Period

Wavenumber

Amplitude



Characteristics of Electromagnetic waves



Frequency: Number of times a wave oscillate from crest to trough per second

Characteristics of Electromagnetic waves

Wavelength (λ)

Distance between two consecutive crests or troughs

SI unit : m

Frequency (ν)

Number of waves passing a given point in one second
SI unit : Hertz (Hz), s^{-1}

Related to time period as:

ν

=

$\frac{1}{T}$

Characteristics of Electromagnetic waves

Velocity (c or v)

Distance travelled by a wave in
one second SI unit : ms^{-1}

Related to frequency (ν) &
wavelength (λ) as:

c

=

$\nu \lambda$

Characteristics of Electromagnetic waves

Time Period (T)

Time taken to
complete one oscillation

SI unit : s

Wavenumber (ν)

Number of waves per unit
length
SI unit : m^{-1}

Amplitude (A)

Height of the crest or the
depth of the trough from the
mean position
SI unit : m

Characteristics of Electromagnetic waves

Consists of radiations
having
different wavelength or
frequency

$$\bar{\nu}$$

$$=$$

$$\frac{1}{\lambda}$$

$$\nu$$

$$=$$

$$c \bar{\nu}$$

$$\nu$$

$$=$$

$$\frac{1}{T}$$



Electromagnetic Spectrum

Electromagnetic radiations are arranged in the order of

Decreasing
frequency

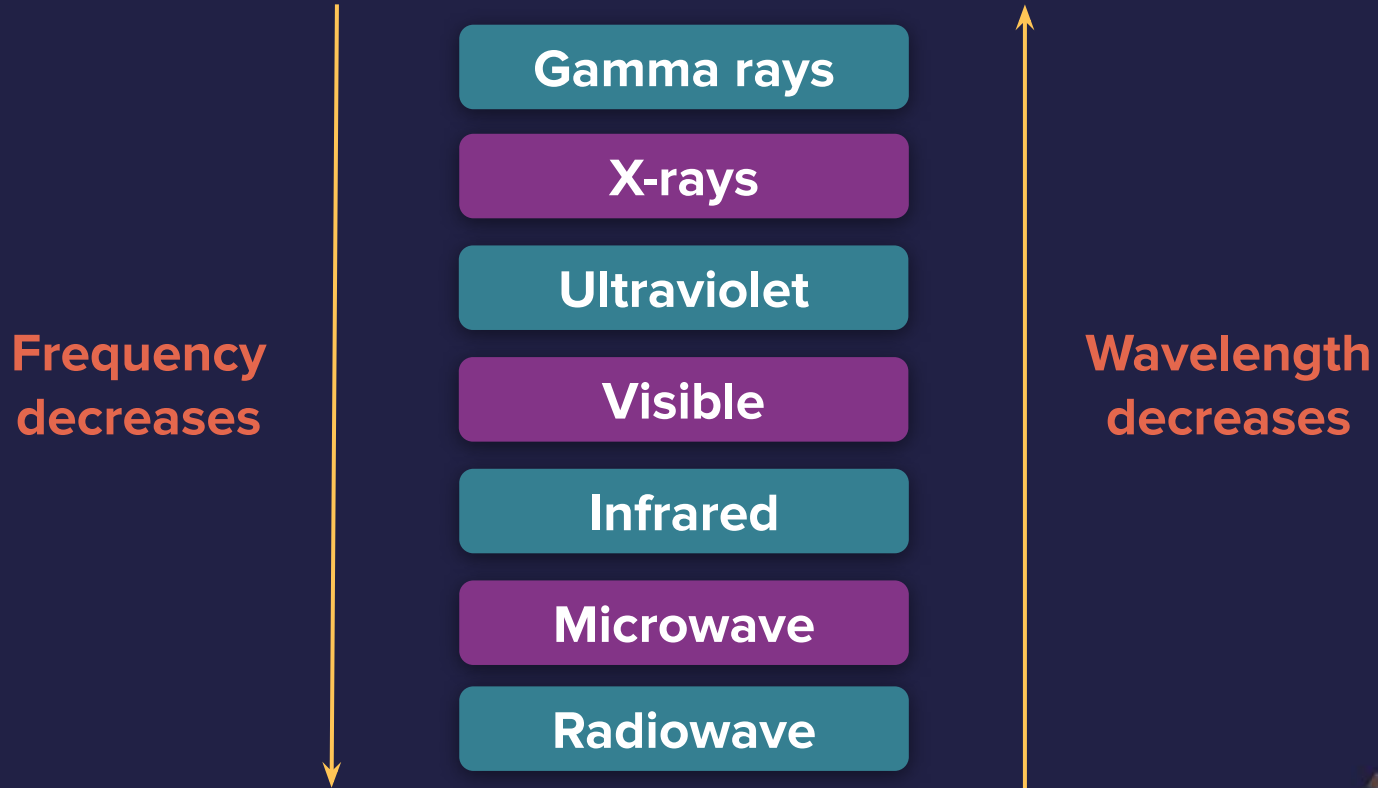
or

Increasing
wavelength

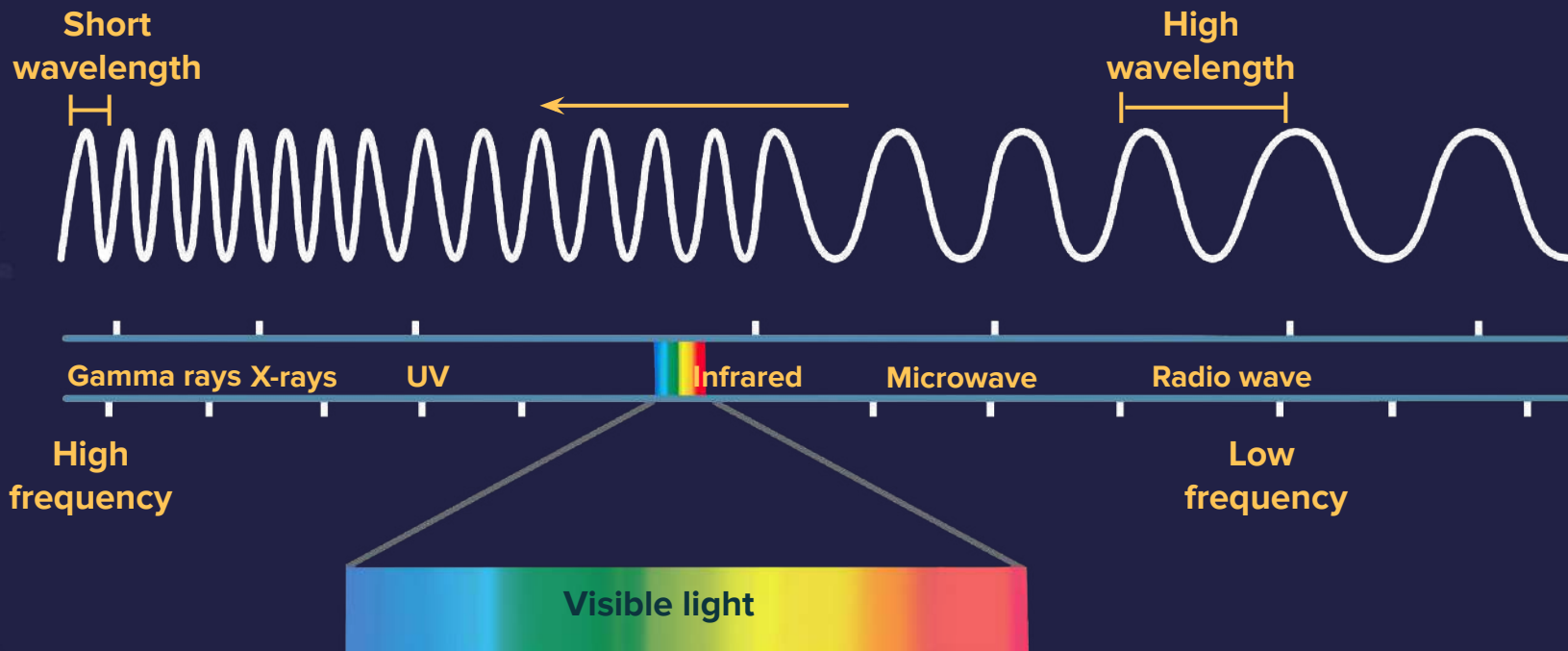




Electromagnetic Spectrum



Electromagnetic Spectrum



EM Radiation: Wave or Particle?

Wave nature of the EM radiation explains

Diffraction

Interference

EM Radiation: Wave or Particle?

Electromagnetic wave theory could not explain

Black-body radiation

Photoelectric effect

Variation of heat capacity of
solids with temperature

Line spectrum of Hydrogen



Continuous vs Discrete

Mass

=

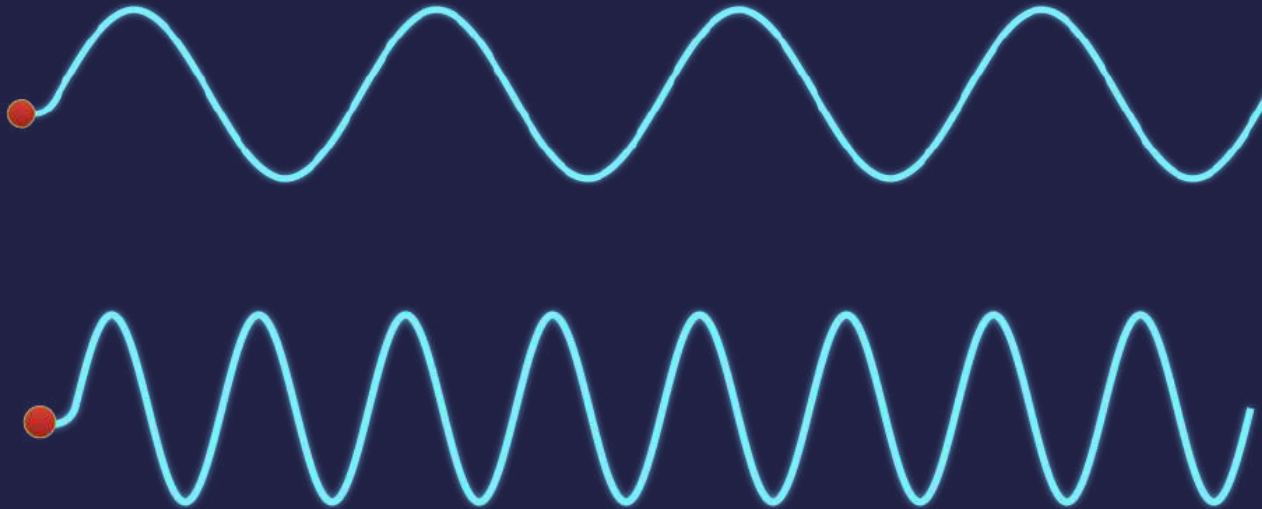
N (mass of 1 water molecule)

Where $N \in +\mathbb{I}$

It seems that mass of water (or any other matter) can take any values (suppose we can go till 30 decimal points) and so we can say that mass has continuous range of values. But on microscopic level, we can observe that mass of water is always an integral multiple of 1 molecule of water. i.e., mass is quantized or we can say that quantization is a property of matter.



Back to EM waves





What is a black body?

Idealized system

Absorbs & emits all frequencies

**Absorbs regardless of the angle
of incidence**

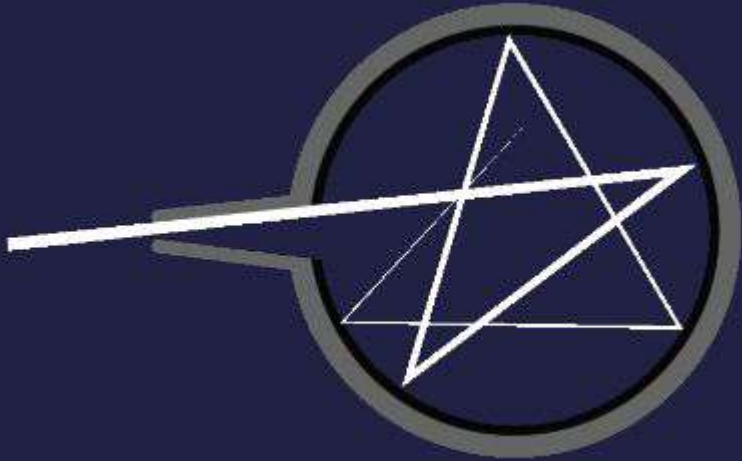


Why the name, Black Body?

Visually Black body

vs

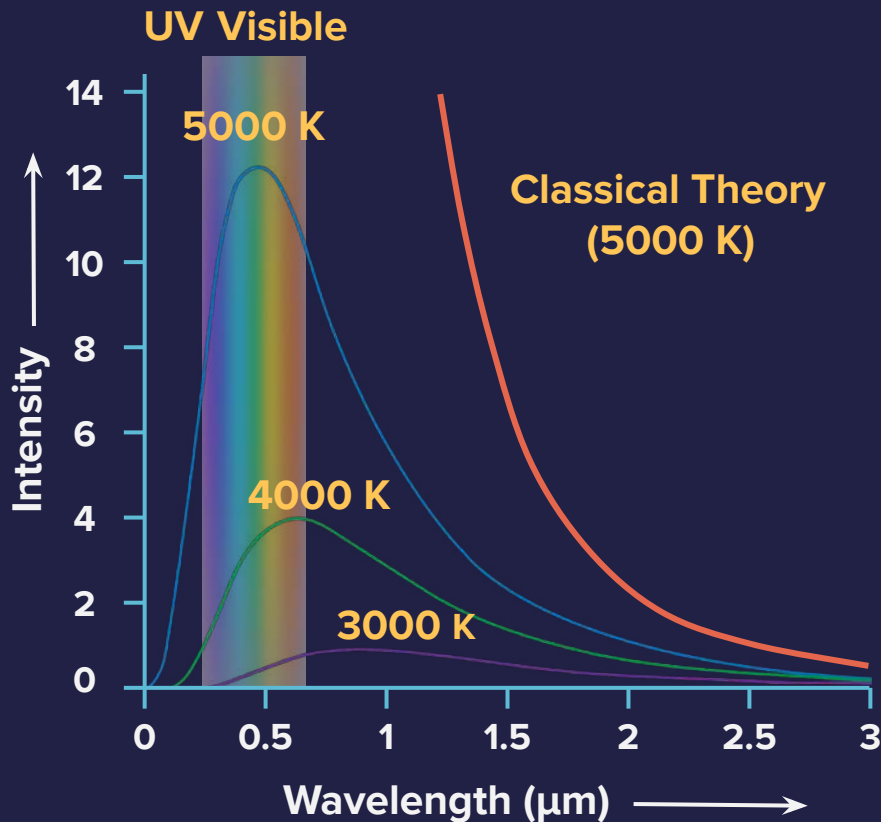
Radiatively Black
Body



A true black body appears black because it is not reflecting any electromagnetic radiation.

However, everything you see to be black can not be called as blackbody because there could be radiation coming out which is not in the visible range.

Wavelength-Intensity relationship



This graph shows intensity as a function of wavelengths emitted from a black body. It shows how bright it is at what wavelength. It shows quantization nature of energy and hence favours particle nature of light.



Particle Nature of Radiation

Planck's quantum theory explains

Quantisation
of Energy

Variation of
intensity with
wavelength





Planck's Quantum theory

The smallest packet or bundle of energy (quantum of radiation) is called a **photon**.

This is the smallest quantity of energy that can be emitted or absorbed in the form of EM radiation.



Quantum theory of Radiation

Energy (E) of a photon is proportional to its frequency (ν)

 E \propto $\nu_{\text{Radiation}}$ E $=$ $nh\nu$ E $=$ $h\nu$ $=$ $h \frac{c}{\lambda}$

n = number of photons
= 0, 1, 2, 3,

h = Planck's constant
= $6.626 \times 10^{-34} \text{ Js}$

One electron volt (eV)

Energy gained by an electron when
it is accelerated from rest through
a potential difference of 1 V

Important Conversions

1 eV

=

$1.6 \times 10^{-19} \text{ J}$

E (eV)

=

$\frac{12,400}{\lambda (\text{\AA})}$

$E \left(\frac{\text{kJ}}{\text{mole}} \right)$

=

$E \left(\frac{\text{eV}}{\text{particle}} \right) \times 96.48$



Photoelectric Effect

Phenomenon of
electrons ejection

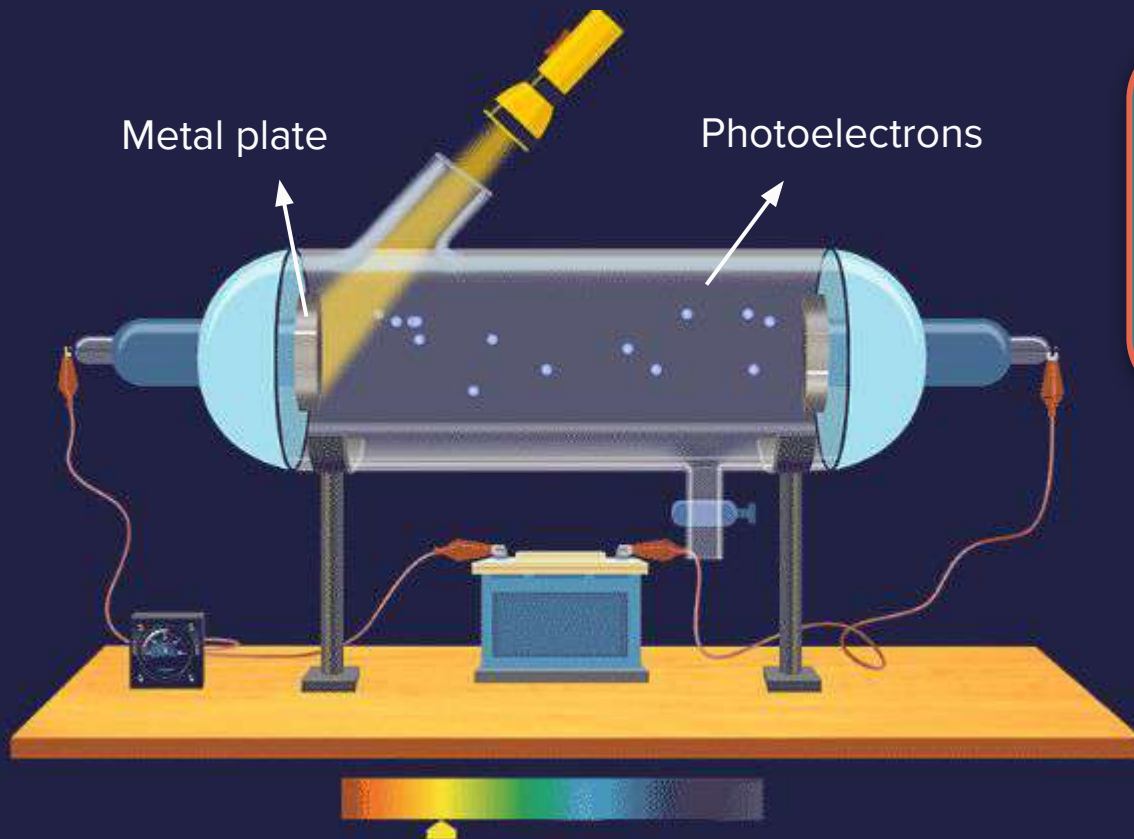
When a radiation of sufficient
frequency falls on the metal
surface

Photoelectrons

Electrons are ejected with the
aid of light



Photoelectric Effect



When radiation of sufficient energy falls on the metal plate, there starts emission of electrons called **photoelectrons**.



Observations

Electrons are ejected as soon as the beam of light of sufficient frequency strikes the metal surface

Instant transfer of energy to the electron when a photon of sufficient frequency strikes the metal atom



Threshold frequency (ν_0)

Minimum frequency
required to eject a
photoelectron from a
metal surface

Each metal has a
characteristic
threshold frequency

Observations



Number of electrons ejected

\propto

Intensity of light

or

Brightness of light



Observations

No electron is ejected,
regardless of the intensity of light

$$\nu_{\text{incident}} < \nu_0$$

$$\nu_{\text{incident}} > \nu_0$$

Even at low light intensities,
electrons are ejected immediately



Particle nature of light

One photon is absorbed by only one electron in a single interaction. Not more than one photon can be absorbed by an electron.

If intense beam of light is used, large number of photons are available and large number of electrons are ejected. This observation shows particle nature of light.



Observations

When

$$\nu_{\text{incident}} > \nu_0$$

K.E._{Ejected electron}

\propto

ν_{Incident}

Energy
possessed by
the photon ↑

Transfer of
energy to the
electron ↑

K.E. of the
ejected
electron ↑

Photoelectric Effect

0

\leq

K.E._{Ejected electrons}

\leq

K.E._{Max}

K.E. is **independent** of
the intensity of radiation

Striking photon's
energy

$=$

$h\nu$

Work function

$=$

ϕ



Work Function (ϕ)

ϕ

=

$h\nu_0$

$\phi = W_0 = \text{Work function}$

Minimum energy
required to eject
an electron from the
metal surface

Photoelectric Effect

$$E_{\text{Photon}} - \phi = \text{K.E.}_{\text{Max}}$$

From the Law of Energy Conservation

$$E_{\text{Incident}} = \phi + \text{K.E.}_{\text{Max}}$$

$$h\nu$$

$$=$$

$$h\nu_0$$

$$+$$

$$\frac{1}{2} m_e v_{\text{max}}^2$$

m_e = mass of the electron

v_{max} = maximum velocity of the electron

Photoelectric Effect

K.E. of the ejected electron is given as

K.E._{Max}

=

$h\nu$

-

$h\nu_0$

K.E._{Max}

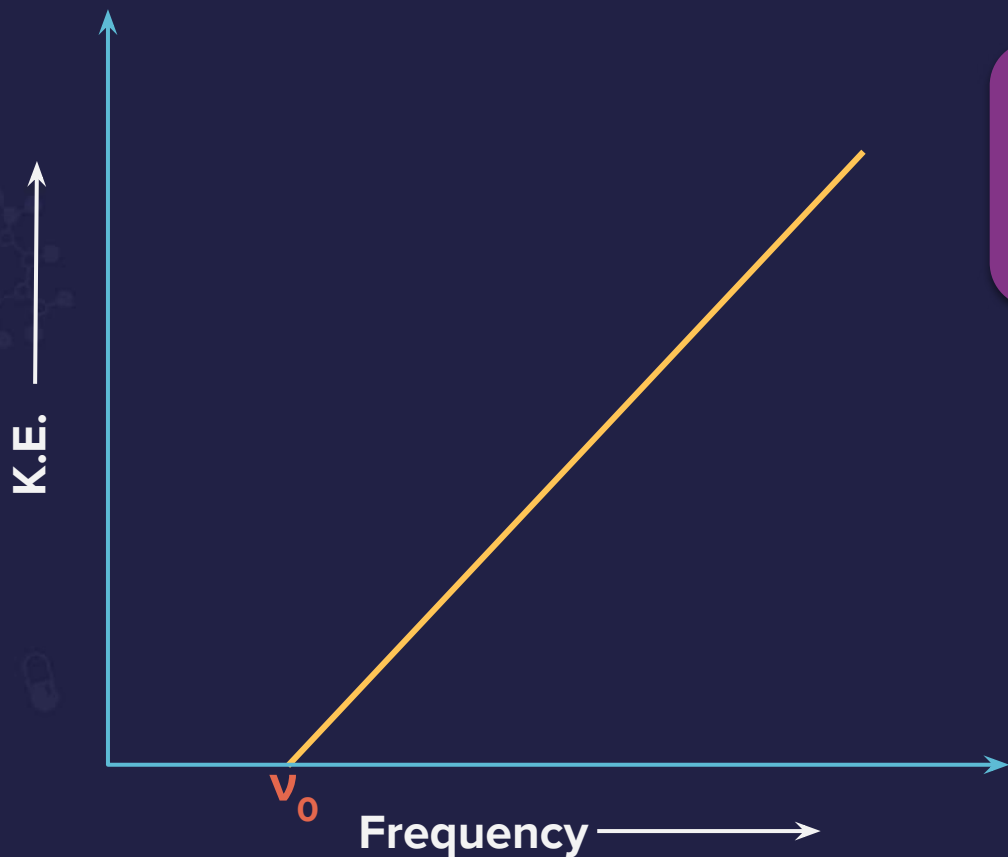
=

$h\frac{c}{\lambda}$

-

$h\frac{c}{\lambda_0}$

Plotting K.E. vs Frequency



From the plot of kinetic energy vs frequency, it shows linear variation according to the equation:

$$\text{K.E.}_{\text{Max}} = h\nu - h\nu_0$$

Bohr Atomic Model

Postulates

Stationary orbits

Concentric circular orbits around the nucleus

These orbits have fixed value of energy

Electrons revolve without radiating energy



Stationary
orbits

or

Energy states /
levels

Postulates

Quantization of **Angular momentum**



Angular momentum of the electron in these orbits is always an integral multiple of $\frac{h}{2\pi}$

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

$$n = 1, 2, 3...$$

h Planck's constant

m Mass of electron

v Velocity of electron

r Radius of orbit



Postulates

Electron can jump from lower to higher orbit by absorbing energy in the form of photon

Energy
Absorbed

=

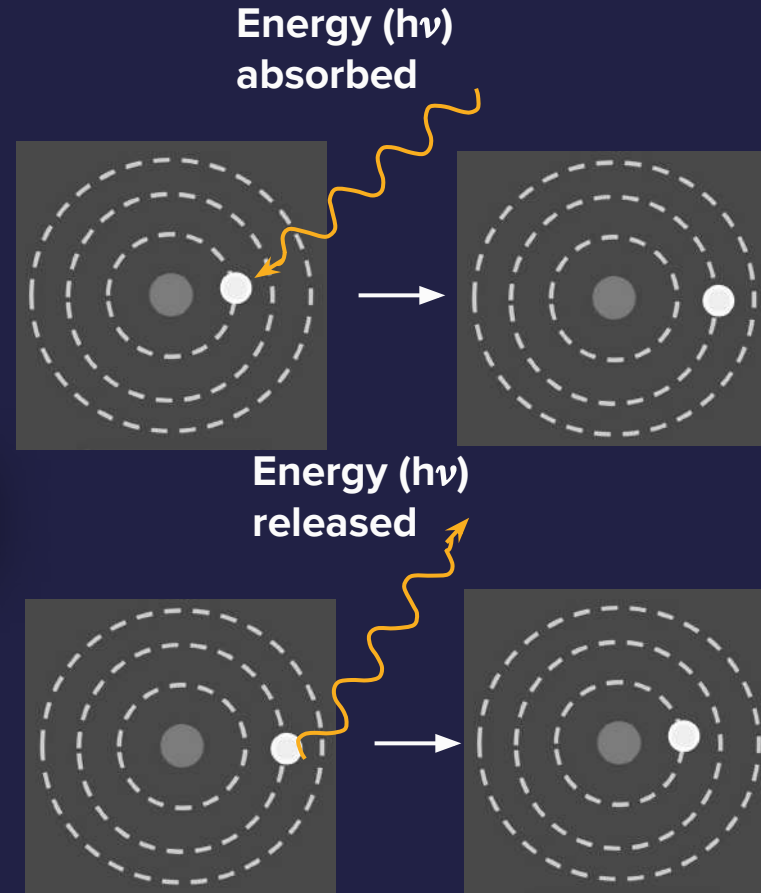
$$E_3 - E_2$$

Electrons can jump from higher to lower orbit by releasing energy in the form of photon

Energy
Released

=

$$E_2 - E_1$$



Postulates

Energy change does takes place in a discrete manner

 ΔE $=$ $E_{n_2} - E_{n_1}$ n_1

Initial energy state

 n_2

Final energy state

Bohr's Frequency Rule

Frequency (ν) of a **radiation absorbed**
or
emitted when a transition occurs

$$\nu = \frac{\Delta E}{h} = \frac{E_2 - E_1}{h}$$

E_1 = Energy of **lower energy state**

E_2 = Energy of **higher energy state**

Bohr's Atomic Theory

Applicable only
for **single**
electron species
like
 H , He^+ , Li^{2+} , Be^{3+}

Mathematical Analysis



Calculating

Radius of Bohr orbit

**Velocity of an electron
in Bohr orbit**

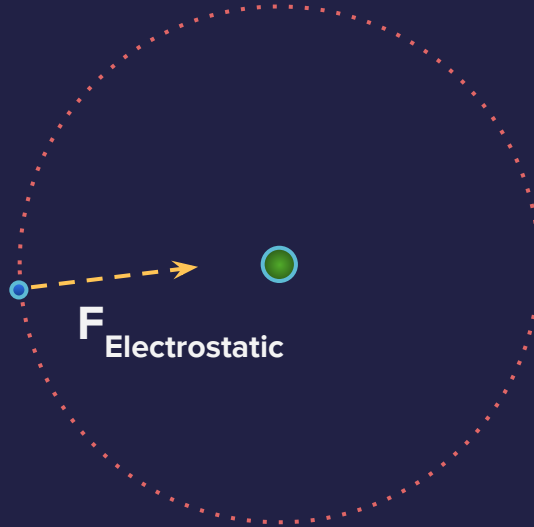
**Time period of an
electron in Bohr orbit**

**Frequency of an
electron in Bohr orbit**

**Energy of an electron
in Bohr orbit**



Postulate



Electron revolves in a circular orbit

**Required centripetal force is provided
by electrostatic force of attraction**



Calculating the radius of Bohr orbit

Equating both the forces,

$$F_{\text{Centripetal}} = F_{\text{Electrostatic}}$$

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

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

On rearranging,

$$v^2 = \frac{KZe^2}{mr} \rightarrow i$$



Calculating the radius of Bohr orbit

According to Bohr's Postulates,

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

$$v = \frac{nh}{2\pi rm}$$

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

→ ii

On comparing equation (i) and (ii),

$$\frac{KZe^2}{mr} = \frac{n^2 h^2}{4\pi^2 r^2 m^2}$$

$$r = \frac{n^2 h^2}{4\pi^2 m K Z e^2}$$





Calculating the radius of Bohr orbit

Putting the value of constants,

$$r_n = 0.529 \frac{n^2}{Z} \text{ \AA}$$

r_n = Radius of n^{th} Bohr orbit

n = Energy level

Z = Atomic number

$$r_n \propto n^2$$

$$r_n \propto \frac{1}{Z}$$

Calculation of velocity of an electron in Bohr orbit

Angular momentum of the electron revolving in the n^{th} orbit

v

$=$

$$\frac{nh}{2\pi r m}$$

i

mvr

$=$

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

r

$=$

$$\frac{n^2 h^2}{4\pi^2 m K Z e^2}$$

ii

Calculation of velocity of an electron in Bohr orbit

Putting equation (ii) in equation (i),

$$v = \frac{nh}{2\pi m} \times \frac{4\pi^2 m K Z e^2}{n^2 h^2}$$

$$v = \frac{2\pi K Z e^2}{nh}$$

$$v_n = 2.18 \times 10^6 \frac{Z}{n} \text{ ms}^{-1}$$

v_n = Velocity of the electron in n^{th} Bohr orbit

Relation between v_n , n and Z

 v_n \propto Z v_n \propto $\frac{1}{n}$

Time period of Revolution (T)

Time period of revolution of an electron in its orbit

T

=

$$\frac{\text{Circumference}}{\text{Velocity}}$$

=

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

T

=

$$1.5 \times 10^{-16} \frac{n^3}{Z^2} \text{ s}$$

T

\propto

$$\frac{n^3}{Z^2}$$

Frequency of Revolution (f)

Frequency of revolution of an electron in its orbit

$$f = \frac{1}{T} = \frac{v_n}{2\pi r_n}$$

Putting the value of constants, r_n & v_n

$$f = 6.6 \times 10^{15} \frac{Z^2}{n^3} \text{ Hz}$$

$$f \propto \frac{Z^2}{n^3}$$

Calculation of Energy of an electron

Total energy (T.E.) of an electron revolving in a particular orbit

$$\text{T.E.} = \text{K.E.} + \text{P.E.}$$

$$\text{K.E.} = \frac{1}{2} mv^2$$

K.E. Kinetic energy

$$\text{P.E.} = - \frac{KZe^2}{r}$$

P.E. Potential energy

$$\text{T.E.} = \frac{mv^2}{2} + - \frac{KZe^2}{r}$$

Calculation of Energy of an electron

Centripetal force = Electrostatic force

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

$$\text{K.E.} = \frac{mv^2}{2} = \frac{KZe^2}{2r}$$

Calculation of Energy of an electron

$$\text{T.E.} = \text{K.E.} + \text{P.E.}$$

$$\text{T.E.} = \frac{KZe^2}{2r} + -\frac{KZe^2}{r} = -\frac{KZe^2}{2r}$$

$$\text{T.E.} = -\text{K.E.} = \frac{1}{2} \text{P.E.}$$

Calculation of Energy of an electron

$$\text{T.E.} = - \frac{KZe^2}{2r}$$

Substituting the value of 'r' in the equation of T.E.

$$\text{T.E.} = - \frac{KZe^2}{2} \times \frac{4\pi^2Ze^2mK}{n^2h^2} = - \frac{2\pi^2Z^2e^4mK^2}{n^2h^2}$$

$$\text{T.E.} = - \frac{2\pi^2me^4K^2}{h^2} \frac{Z^2}{n^2}$$

Calculation of Energy of an electron

Putting the value of constants we get:

T.E.

=

E_n

=

$$- 13.6 \left[\frac{Z^2}{n^2} \right] \text{eV/atom}$$

Negative sign of T.E. shows attraction between electrons & nucleus.

Electron in an atom is more stable than a free electron

Energy of an electron

$$E_n \propto -\frac{Z^2}{n^2}$$

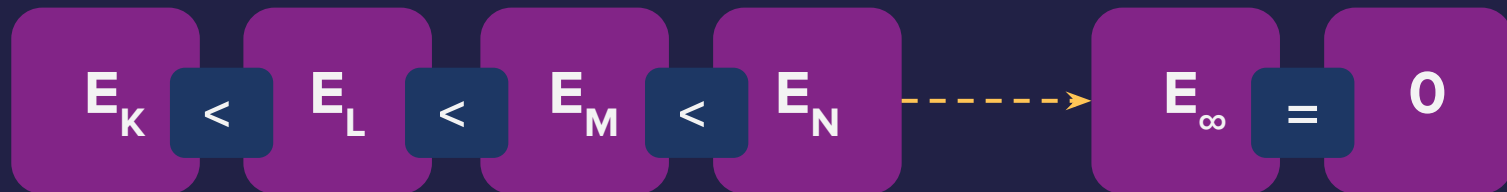
$Z \uparrow$

$E_n \downarrow$

$n \uparrow$

$E_n \uparrow$

Energy of an electron



Distance of electron
from the nucleus



Energy



Energy of an electron



Negative sign of T.E.

Attraction between
Electrons & Nucleus

Negative sign of T.E.

Electron in an atom is more
stable than a free electron



Energy of an electron

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

$$E_n = -2.18 \times 10^{-11} \frac{Z^2}{n^2} \text{ erg/atom}$$

$$E_n = -313.6 \frac{Z^2}{n^2} \text{ kcal/mol}$$

$$E_n = -2.18 \times 10^{-11} \frac{Z^2}{n^2} \text{ erg/atom}$$

$$E_n = -313.6 \frac{Z^2}{n^2} \text{ kcal/mol}$$

Energy of an electron

At

n

=

∞

T.E.

=

0

P.E.

=

0

K.E.

=

0

Energy Difference

$$\Delta E$$

$$=$$

$$E_{n_2}$$

$$-$$

$$E_{n_1}$$

$$\Delta E \left(\frac{\text{eV}}{\text{atom}} \right)$$

$$=$$

$$\left(-13.6 \frac{Z^2}{n_2^2} \right)$$

$$-$$

$$\left(-13.6 \frac{Z^2}{n_1^2} \right)$$

$$\Delta E$$

$$=$$

$$13.6 Z^2 \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right) \frac{\text{eV}}{\text{atom}}$$

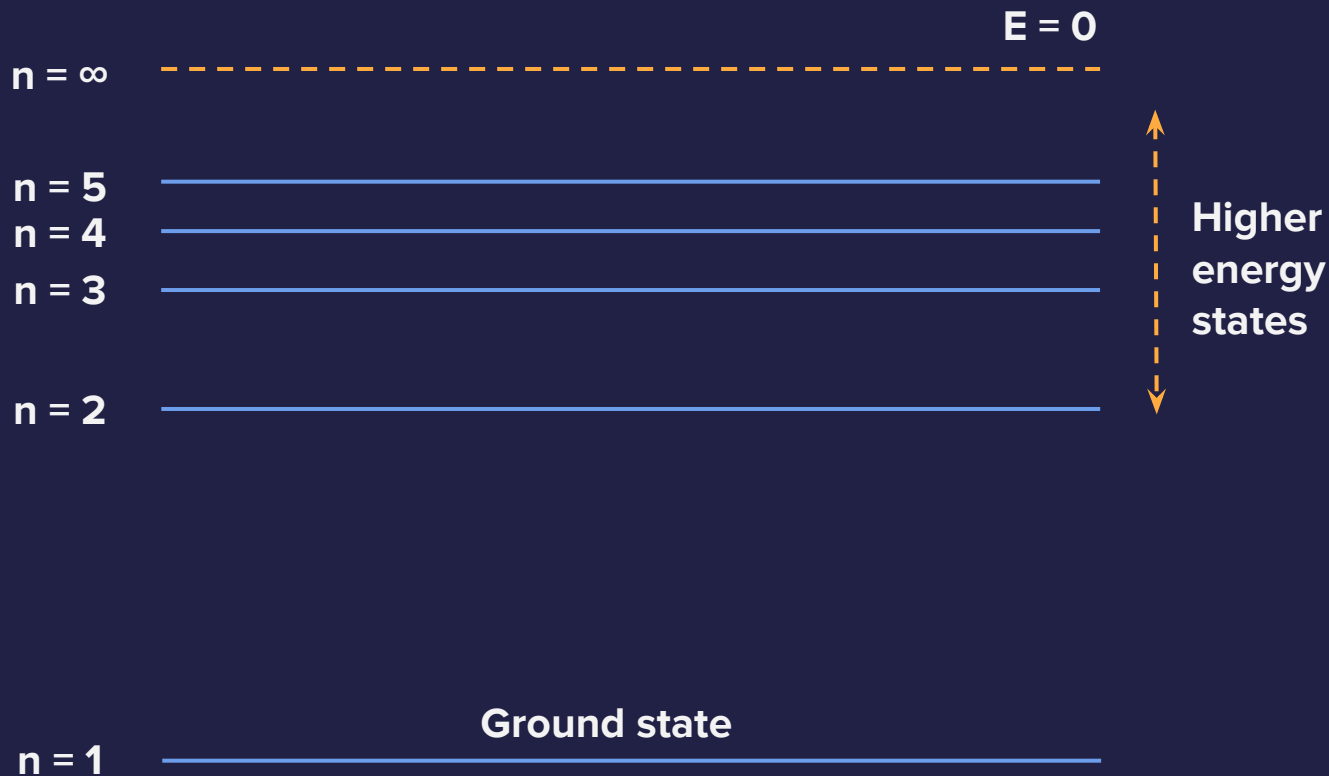
$$\Delta E$$

$$=$$

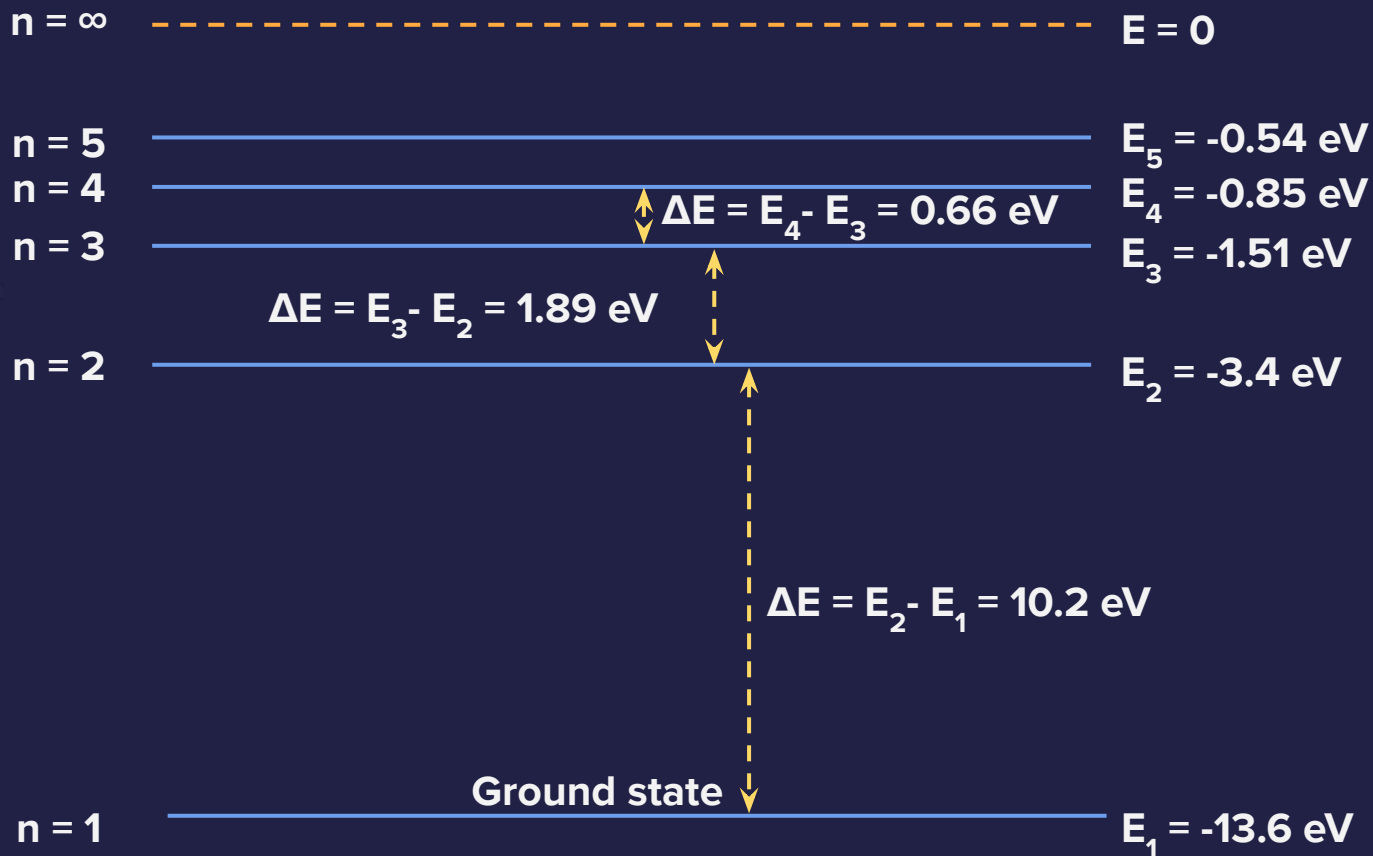
$$2.18 \times 10^{-18} Z^2 \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right) \frac{\text{J}}{\text{atom}}$$

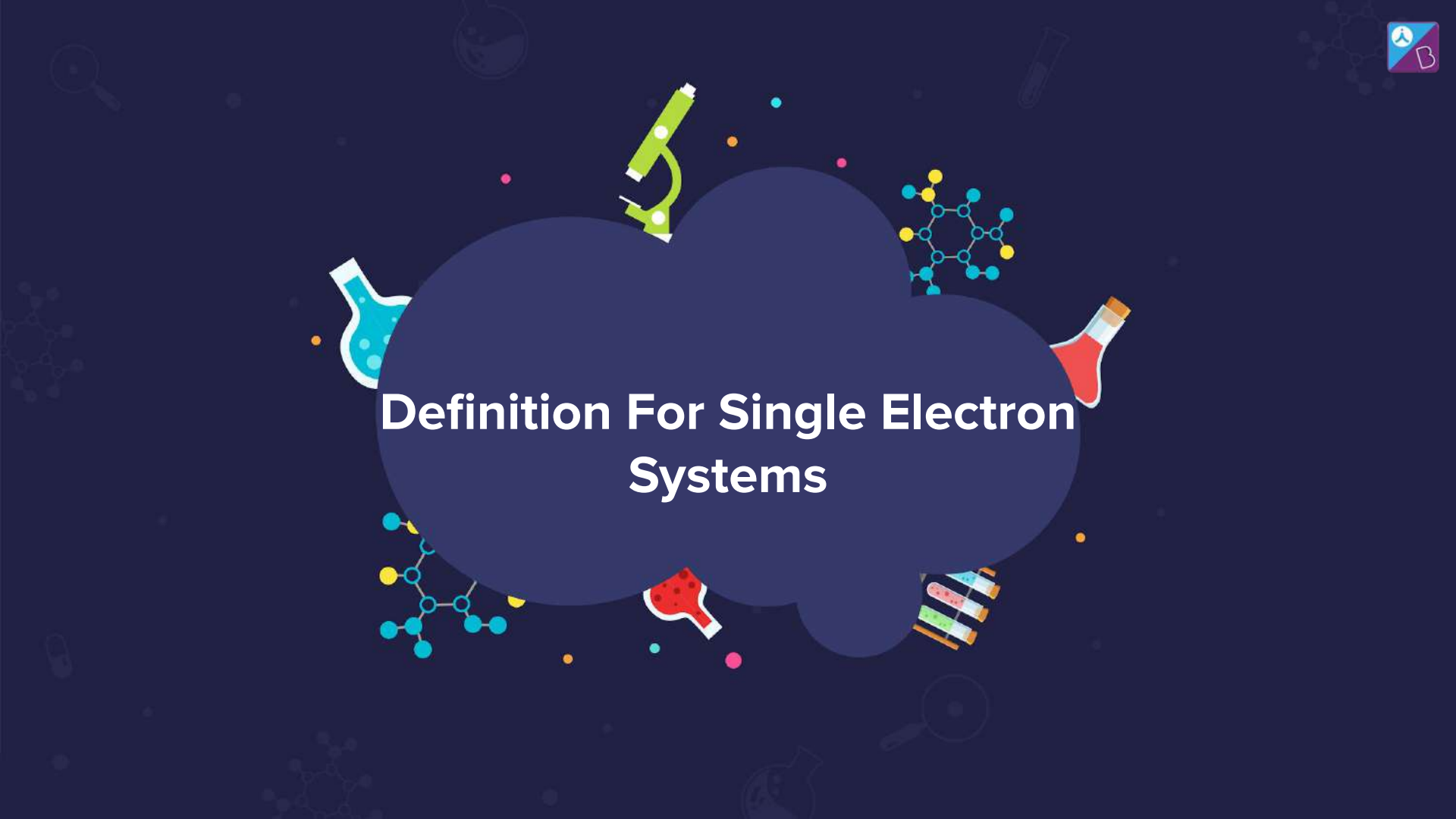


Energy level diagram



Energy level diagram



The background is a dark navy blue. In the center is a large, dark blue, irregular cloud-like shape. Surrounding this central shape are various colorful icons: a green microscope at the top, a blue and white flask on the left, a red and white flask on the right, a molecular structure at the bottom left, a test tube rack at the bottom right, and several small colored dots (orange, pink, blue) scattered around. Faint, larger-scale icons like a magnifying glass, a beaker, and a molecular structure are also visible in the background.

Definition For Single Electron Systems

Ground state (G.S.)

Lowest energy state of any atom or ion

$$n = 1$$

G.S. energy of H-atom

$$-13.6 \text{ eV}$$

G.S. energy of He^+ ion

$$-54.4 \text{ eV}$$



Excited state

States of atom or ion other than the ground state

$$n \neq 1$$

$$n = 2$$

First excited state

$$n = 3$$

Second excited state

⋮

$$n = m + 1$$

m^{th} excited state



Ionisation energy (I.E.)

Minimum energy required
to remove an electron

from
 $n = 1$ to $n = \infty$

ΔE

=

$$13.6 Z^2 \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right) \frac{\text{eV}}{\text{atom}}$$

Putting $n_2 = \infty$ & $n_1 = 1$

ΔE

=

$$13.6 Z^2 \frac{\text{eV}}{\text{atom}}$$



Ionisation energy (I.E.)

$$\text{I.E.}_\text{H} = 13.6 \text{ eV}$$

$$\text{I.E.}_{\text{He}^+} = 54.4 \text{ eV}$$

$$\text{I.E.}_{\text{Li}^{2+}} = 122.4 \text{ eV}$$

Ionisation potential (I.P.)

Potential difference through which a free electron must be accelerated from rest

such that its **K.E. = I.E.**

$$\text{I.P.} = 13.6 Z^2 \text{ V}$$

$$\text{I.P.}_H = 13.6 \text{ V}$$

$$\text{I.P.}_{\text{He}^+} = 54.4 \text{ V}$$

Excitation Energy

Energy required to
move an electron
from $n = 1$ to
any other state

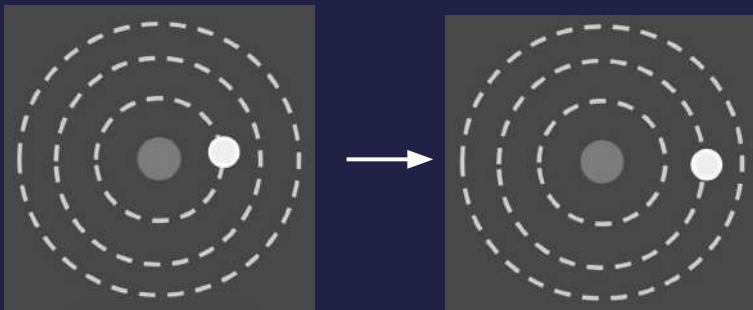
For H atom
 $n = 1$ to $n = 2$

Excitation
energy of
 2^{nd} state

10.2 eV

Excitation
energy of
 1^{st} E.S.

1^{st}
excitation
energy

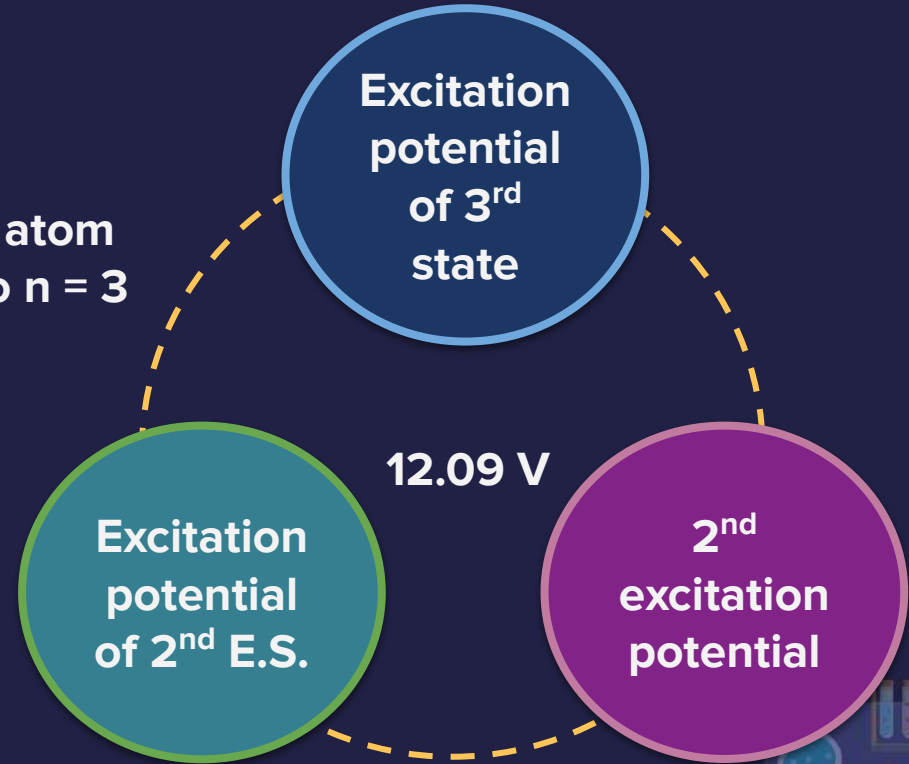


Excitation potential

Potential difference through which an electron must be accelerated from rest such that its

K.E. = Excitation energy

For H atom
 $n = 1$ to $n = 3$



Binding or Separation energy

Energy required to
move an electron

From
any state to $n = \infty$

B.E._{Ground state}

=

I.E._{Atom or Ion}



Summary

Ground State

$n = 1$

Excited State

$n > 1$

Ionization Energy

From
 $n = 1$ to $n = \infty$

Binding Energy

From
any state to $n = \infty$

Excitation Energy

From $n = 1$ to
any other state



The background is a dark blue gradient. It is decorated with numerous circles of various sizes and colors, including shades of purple, teal, pink, and white. Some circles have thick borders. Faint molecular structures are visible in the background, particularly on the left and bottom right.

Spectroscopy

Spectrograph

Spectrogram

Spectrum



Spectroscopy

Branch of
science that
deals with the
study of
spectra





Spectrograph / Spectroscope



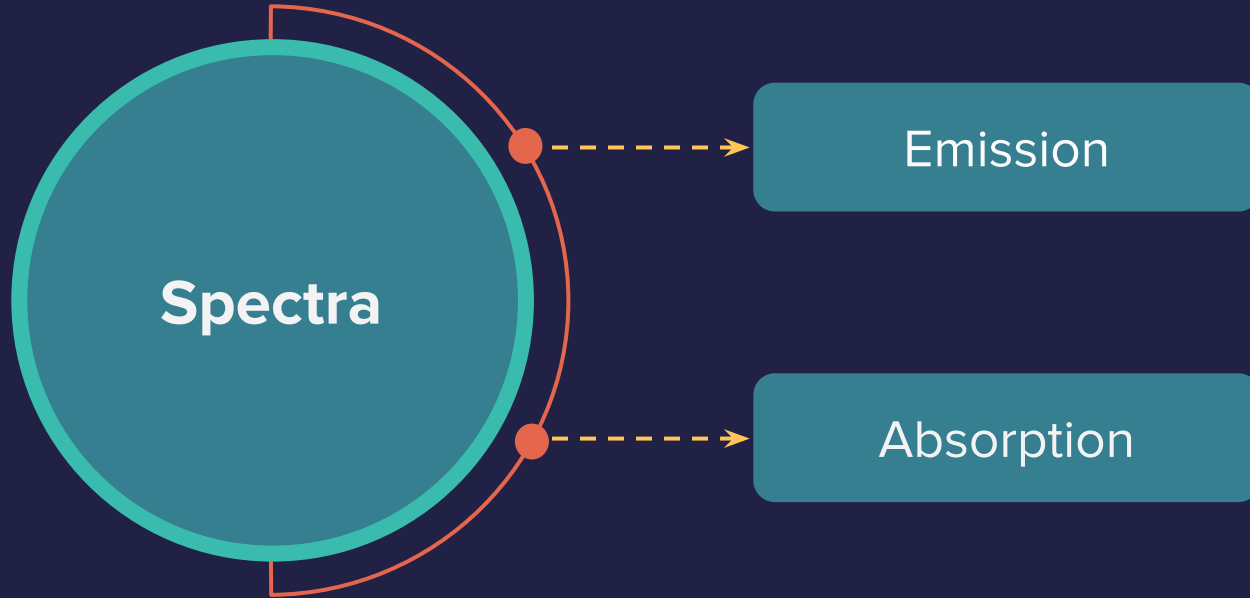
Instrument
used to
separate
radiation of
different
wavelengths



Spectrogram

**Spectrum of
the given
radiation**

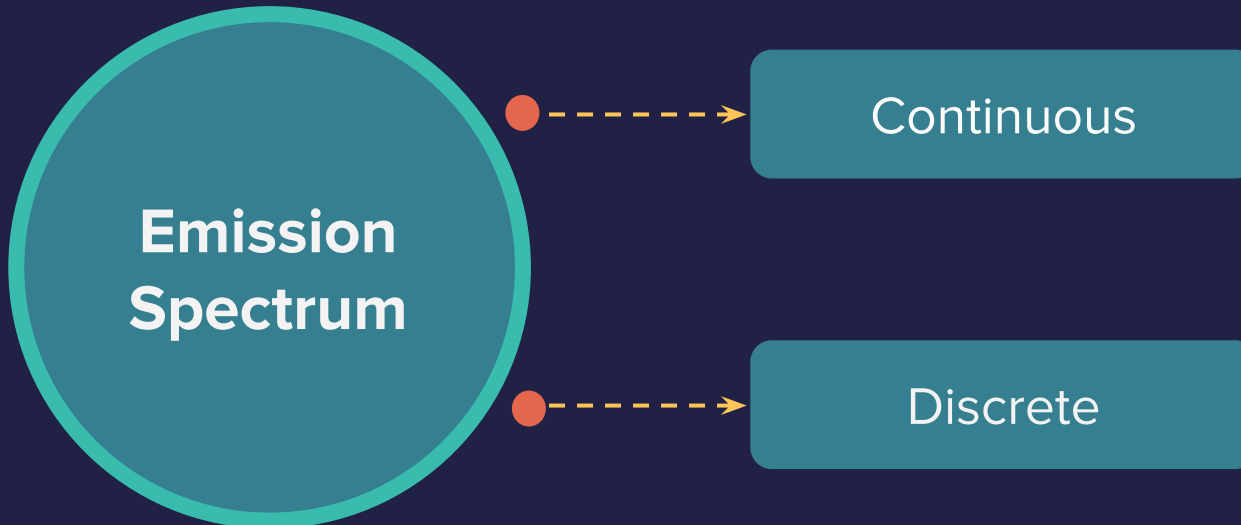
Classification: Based on Origin





Emission Spectrum

Spectrum of radiation emitted by a substance

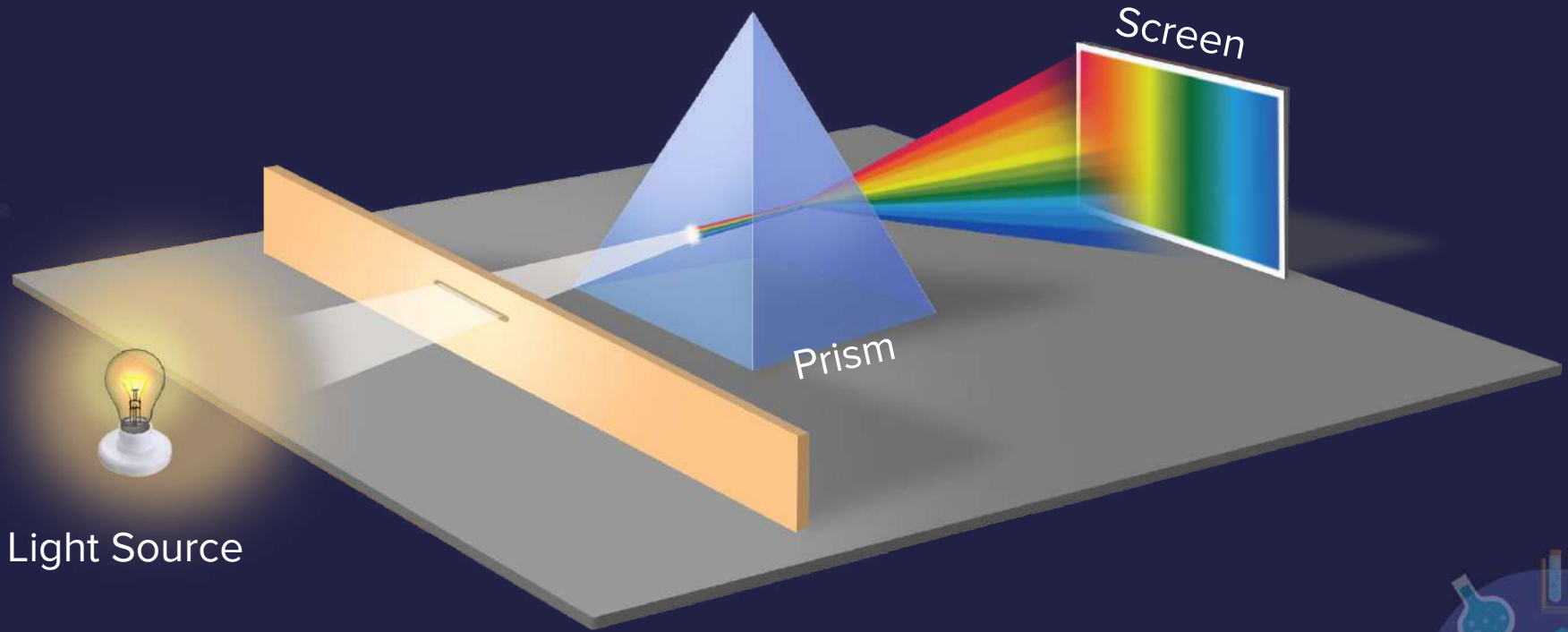


Continuous Spectrum

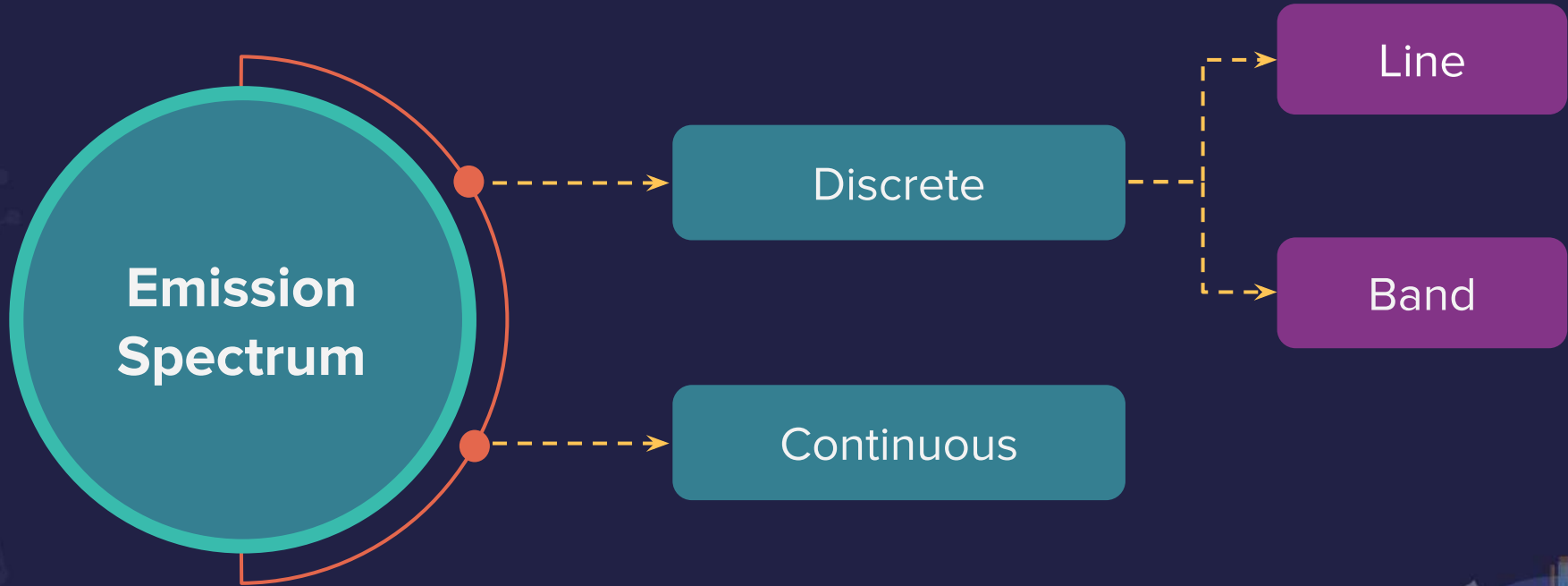
Continuous distribution of colours (VIBGYOR)
such that each colour merges into the next one



Continuous Spectrum

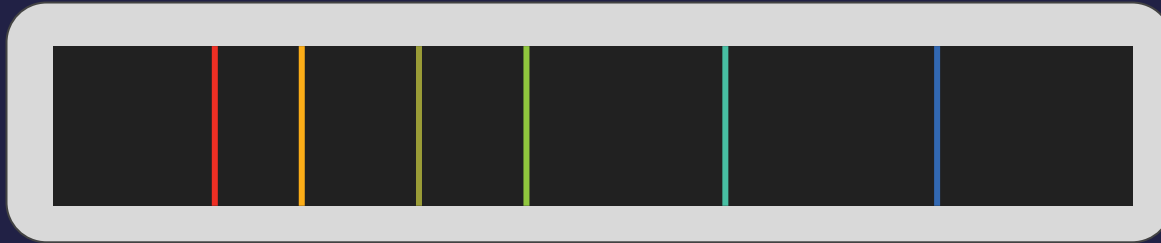


Classification: Based on Nature



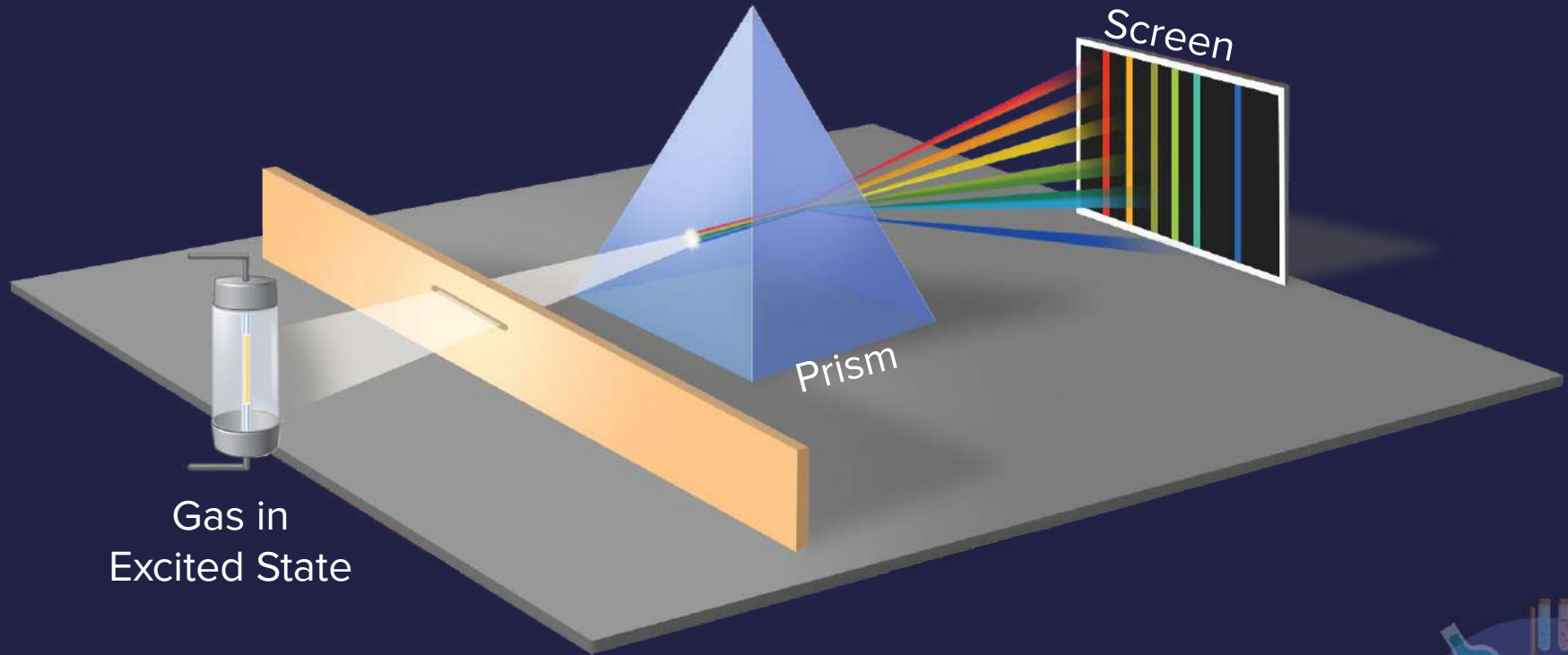
Line Spectrum

Ordered arrangement of lines of a particular wavelength separated by dark space



Line spectrum

Emission Spectra





Application of Line Spectrum

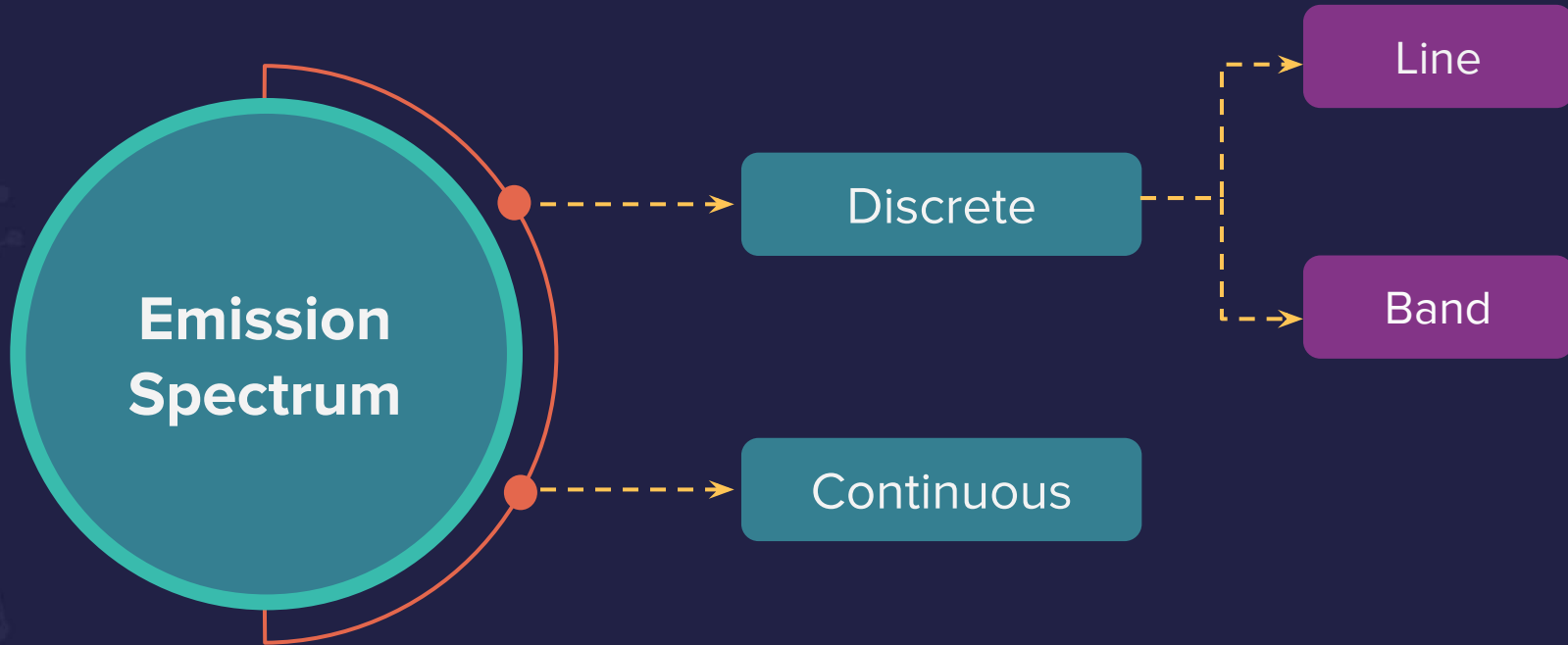
Each element has a unique
line spectrum



Identification of unknown atoms



Classification: Based on Nature



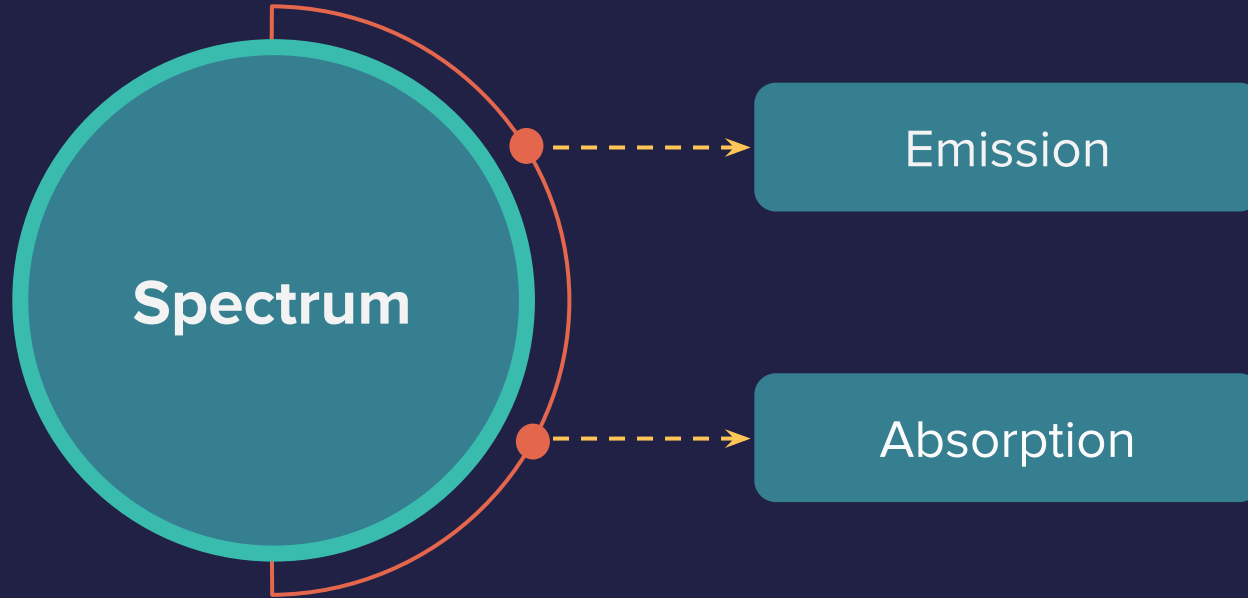
Band Spectrum

Continuous bands separated by
some dark space

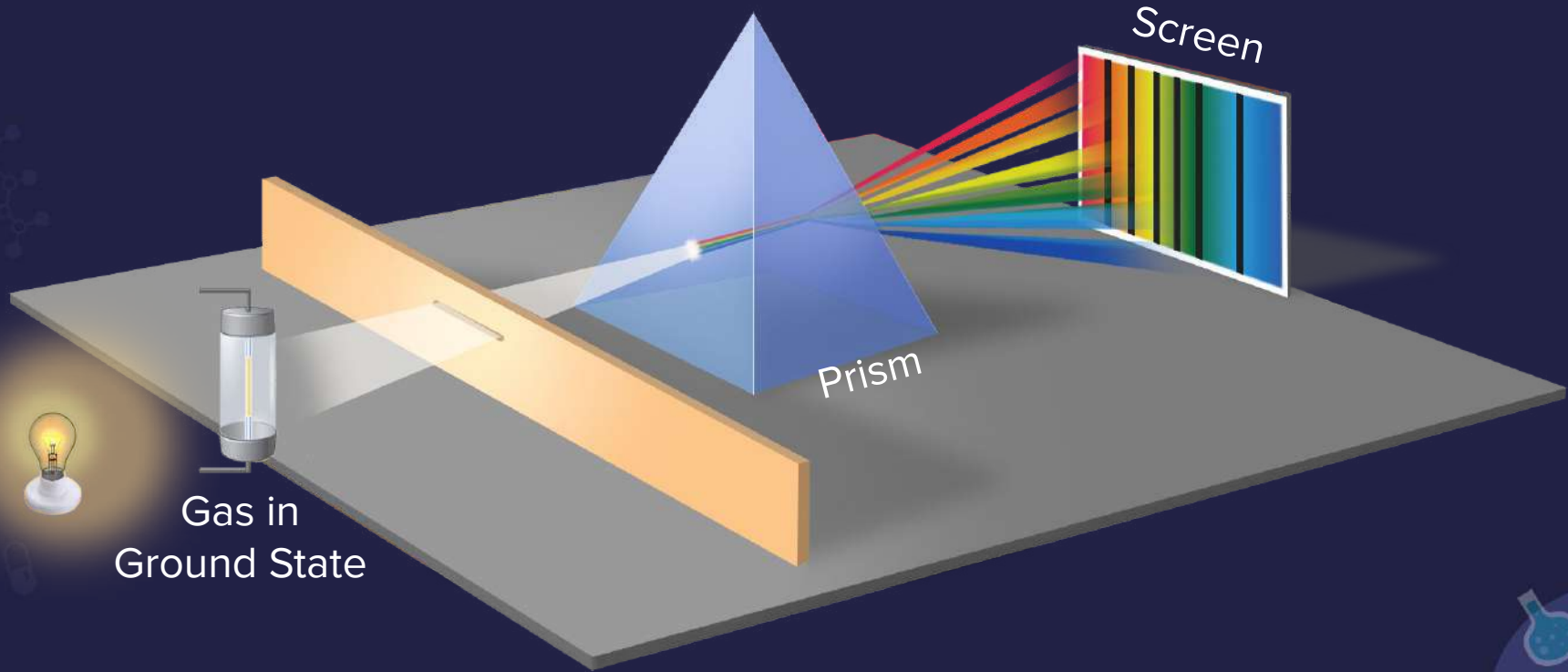


Molecular spectrum

Classification : Based on Origin



Absorption Spectrum



Absorption Spectrum

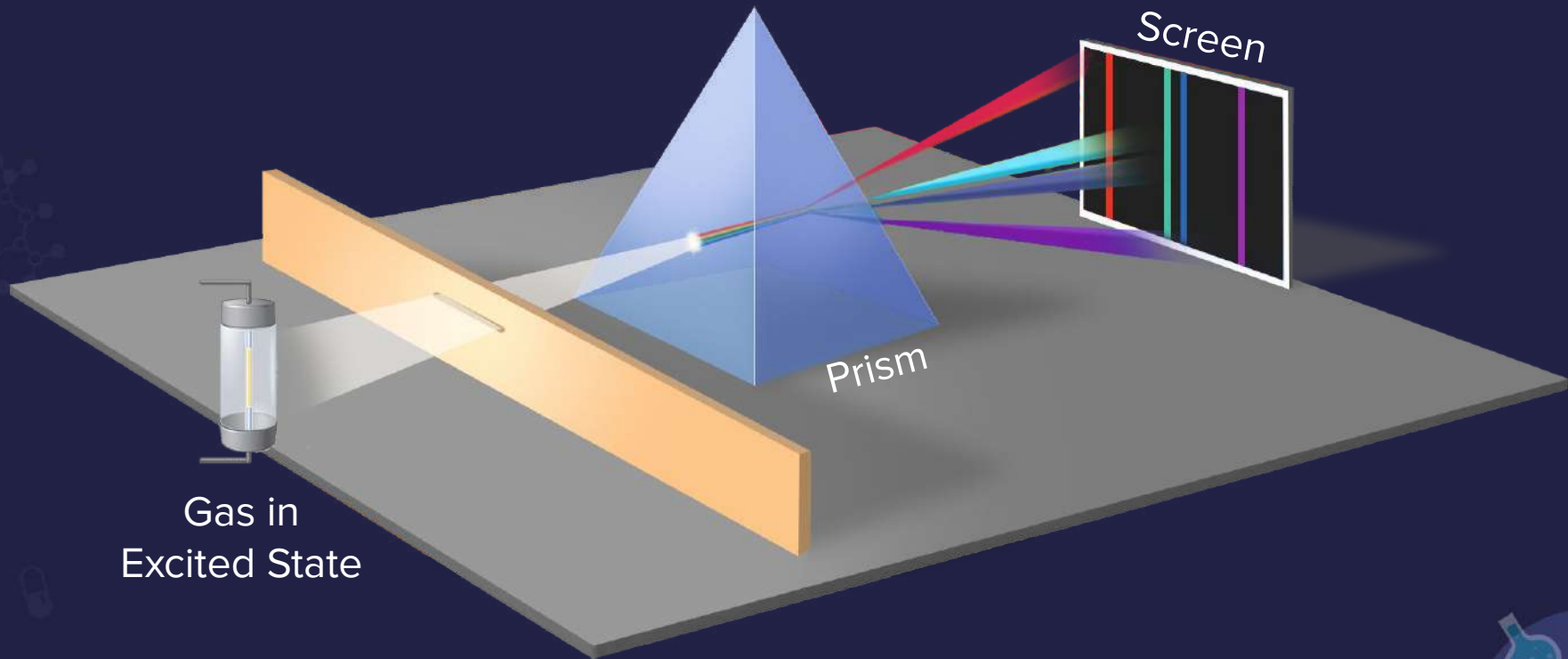
Some dark lines in the continuous spectrum



Represent absorbed radiations



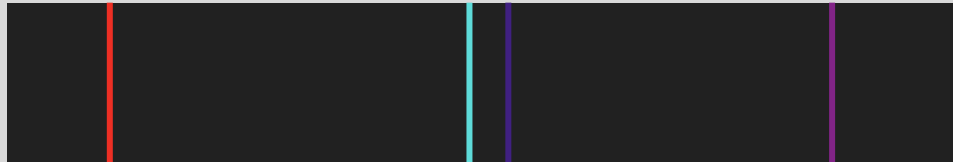
Emission Spectrum of Hydrogen



Line Spectrum of Hydrogen

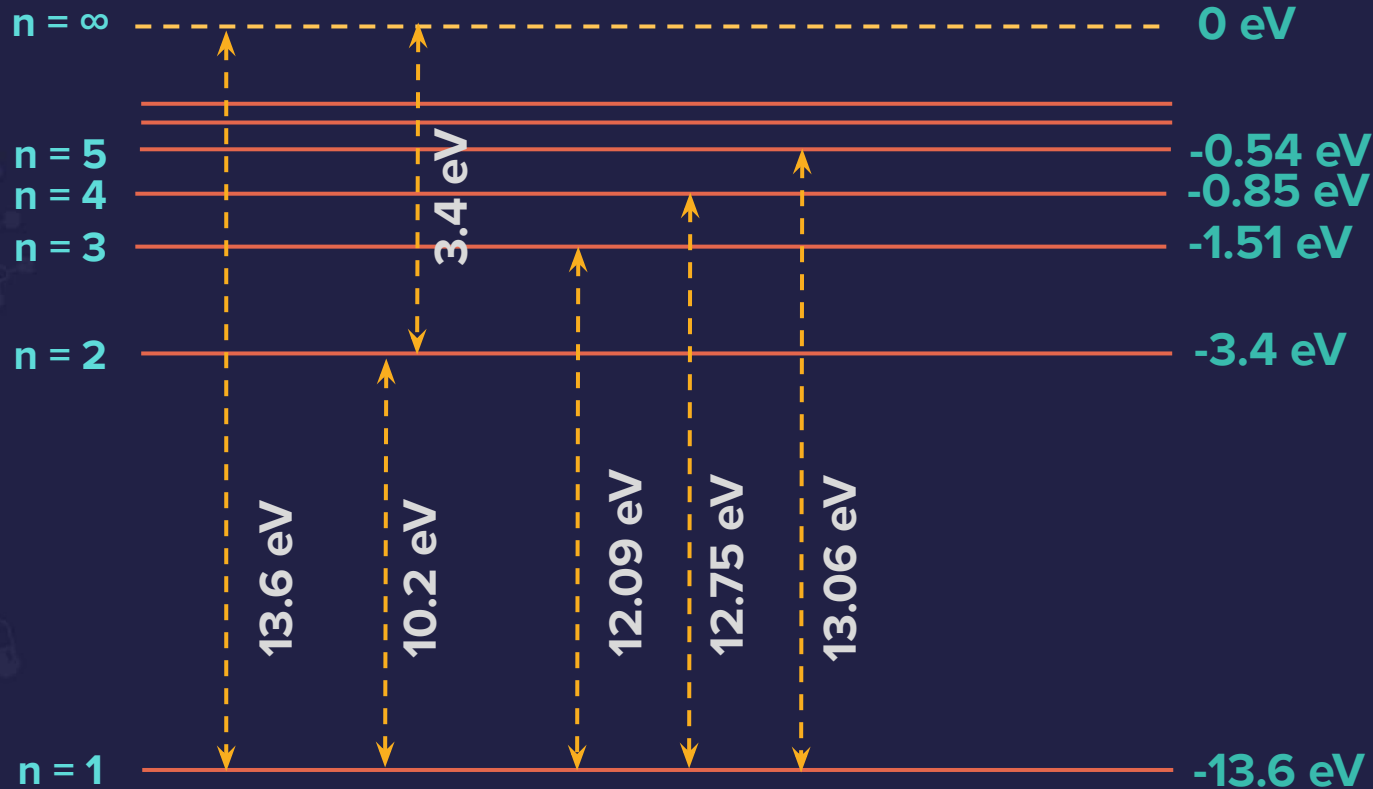
Emission Spectral Lines/
De-Excitation Series

Due to de-excitation of electron
from higher to lower orbit





Energy Level Diagram for H atom



Rydberg's Formula

Electron makes transition from n_2 to n_1

$$\Delta E = \frac{hc}{\lambda} = 2.18 \times 10^{-18} Z^2 \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right) \frac{\text{J}}{\text{atom}}$$

$$\frac{1}{\lambda} = \frac{2.18 \times 10^{-18} Z^2}{hc} \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right) \text{m}^{-1}$$



Rydberg's Formula

$$\frac{1}{\lambda} = 1.09678 \times 10^7 \times Z^2 \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right) \text{m}^{-1}$$

$$\frac{1}{\lambda} = 109678 \times Z^2 \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right) \text{cm}^{-1}$$

n_1

1, 2, 3, ...

n_2

$n_1 + 1, n_1 + 2, \dots$

R_H

Rydberg constant

R_H

=

$1.09678 \times 10^7 \text{ m}^{-1}$

≈

$1.1 \times 10^7 \text{ m}^{-1}$



Rydberg's Formula

For any atom

$$\frac{1}{\lambda}$$

=

$$R_H Z^2 \times \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$

n_1

1, 2, 3, ...

n_2

$n_1 + 1, n_1 + 2, \dots$

λ

=

$$\frac{912}{Z^2 \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right)} \text{ \AA}$$

Rydberg's Formula

For H atom

$$\frac{1}{\lambda} = R_H \times \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$

n_1

1, 2, 3, ...

n_2

$n_1 + 1, n_1 + 2, \dots$

Spectral series of H atom

Lyman

Balmer

Paschen

Brackett

Pfund

Humphrey



Lyman Series

For an electron present in H atom

1st spectral series.
Found in UV region
by Lyman

$$\frac{1}{\lambda} = R_H \times \left(\frac{1}{1^2} - \frac{1}{n_2^2} \right)$$

$n_1 = 1$ (Final state)

$n_2 = 2, 3, 4 \dots$
(Initial states, $n_2 > 1$)

Lyman Series

$$n_2 = \infty$$

1st line of
Lyman series (α line)

$$2 \rightarrow 1$$

Wavelength
of last line

=

$$\frac{n_1^2}{R_H}$$

2nd line of
Lyman series (β line)

$$3 \rightarrow 1$$

λ_{Lyman}

=

$$\frac{1}{R_H}$$

Last line of Lyman
series (Series limit)

$$\infty \rightarrow 1$$



Lyman Series



10.2 eV

\leq

$(\Delta E)_{\text{Lyman}}$

\leq

13.6 eV

$\frac{12400}{13.6} \text{ \AA}$

\leq

λ_{Lyman}

\leq

$\frac{12400}{10.2} \text{ \AA}$



Lyman Series

Longest
wavelength

=

λ_{longest} or λ_{max}

=

$$\frac{12400}{\Delta E_{\text{min}}} \text{ \AA}$$

Shortest
wavelength

=

$\lambda_{\text{shortest}}$ or λ_{min}

=

$$\frac{12400}{\Delta E_{\text{max}}} \text{ \AA}$$

Where,

E in eV



Lyman Series

1st spectral line

λ_{\max}

Last spectral line

λ_{\min}

Series limit

Limiting/last line of any spectral series

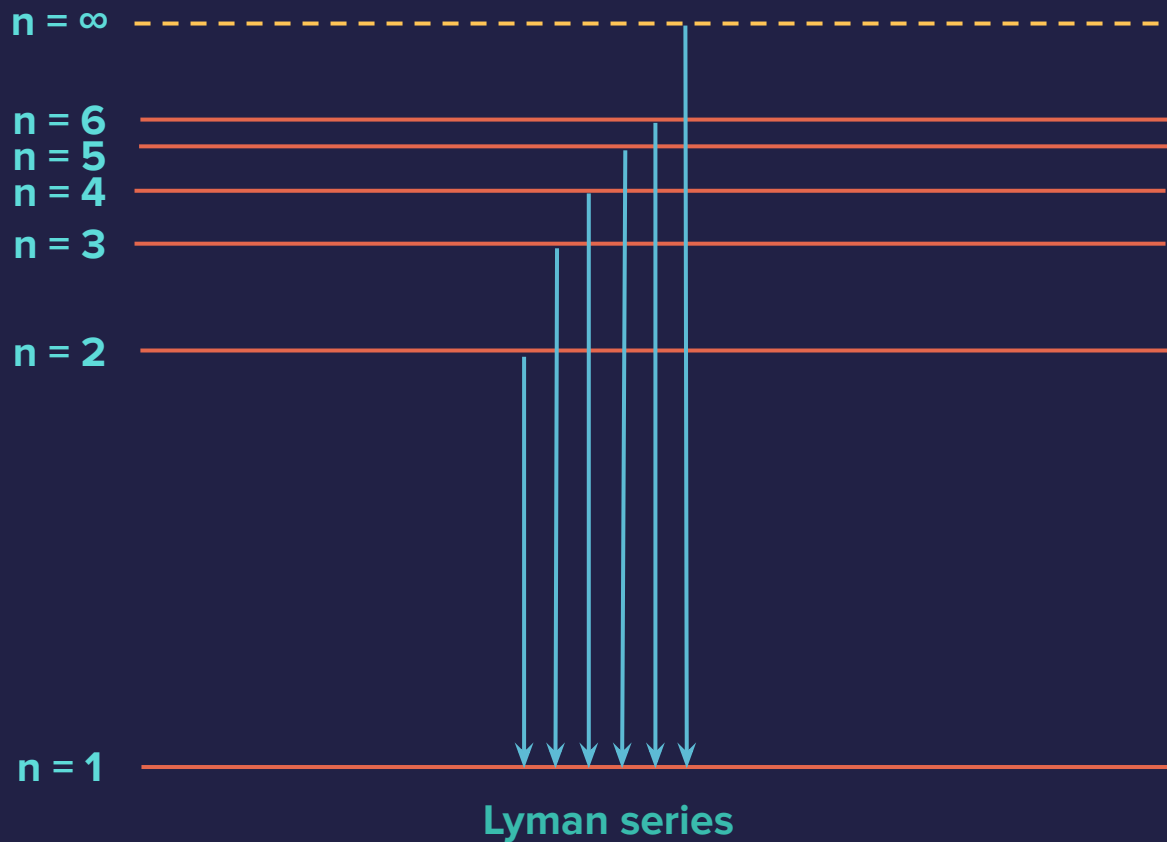
Since $n_2 = \infty$

$\bar{\nu}_{\text{last line}}$

=

R_H

Lyman Series





Balmer Series

2nd spectral series

Found in visible region by Balmer

For H atom

Only first 4 lines belongs to visible region

Rest belongs to UV region



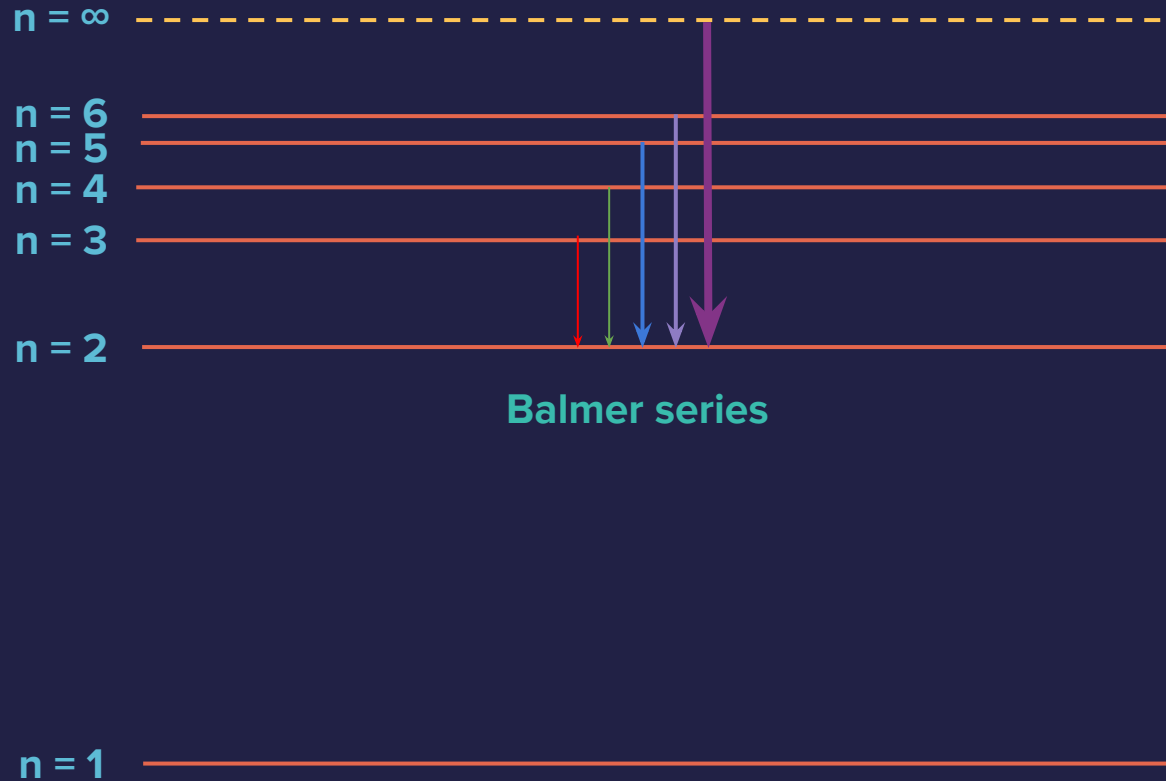
Balmer Series

$$\frac{1}{\lambda} = R_H \times \left(\frac{1}{2^2} - \frac{1}{n_2^2} \right)$$

$n_1 = 2$ (Final state)

$n_2 = 3, 4, 5 \dots$
(Initial states, $n_2 > 2$)

Balmer Series



Paschen Series

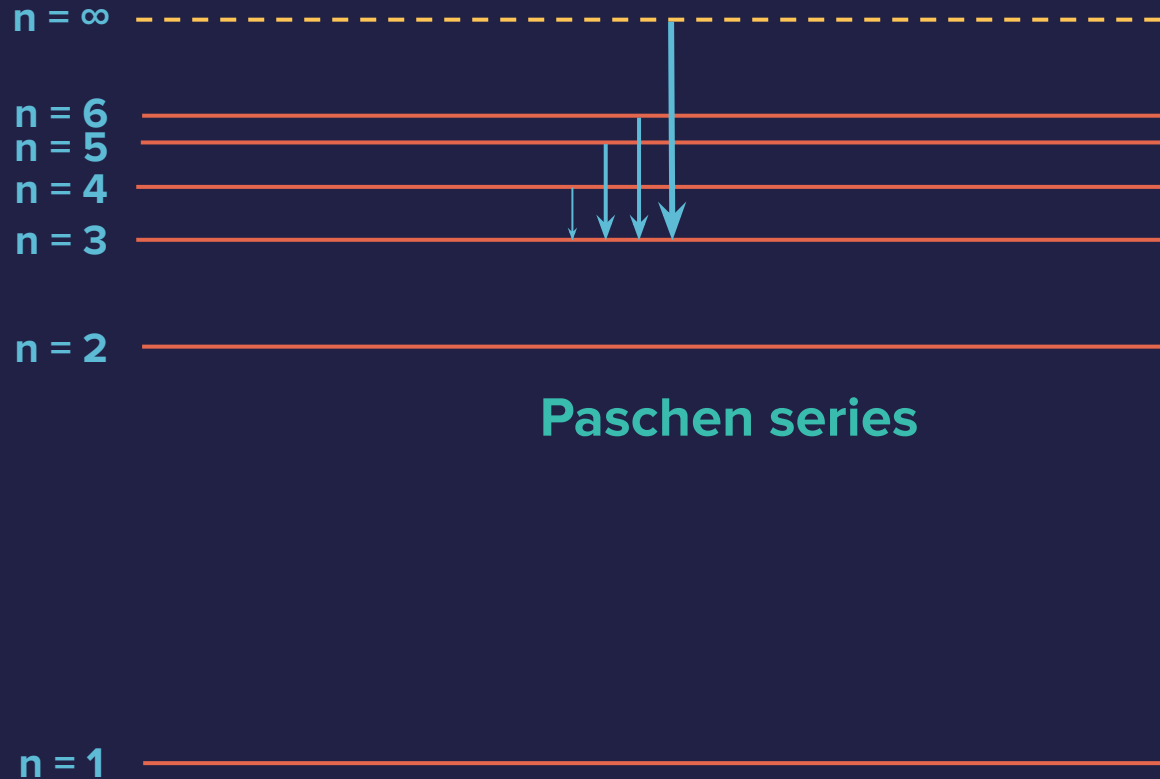
3rd spectral series; Found in IR region by Paschen

$$\frac{1}{\lambda} = R_H \times \left(\frac{1}{3^2} - \frac{1}{n_2^2} \right)$$

$n_1 = 3$ (Final state)

$n_2 = 4, 5, 6 \dots$
(Initial states, $n_2 > 3$)

Paschen Series



Paschen series



Brackett Series

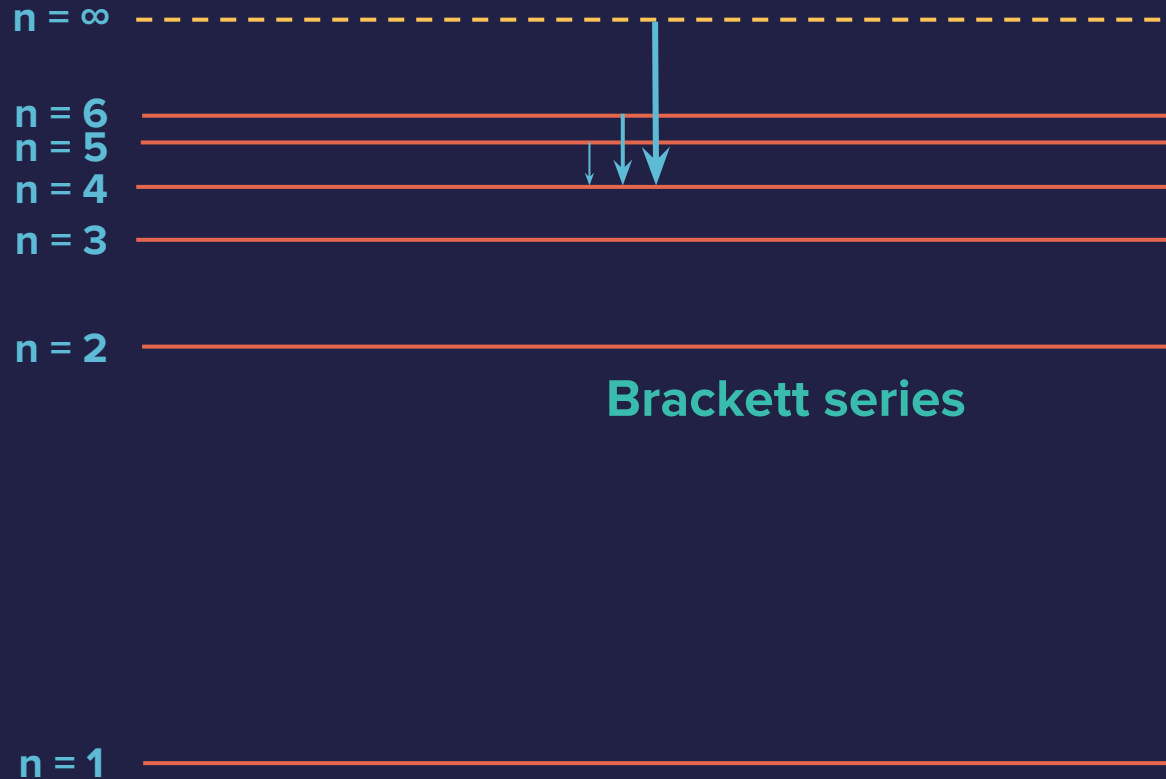
4th spectral series; Found in IR region by Brackett

$$\frac{1}{\lambda} = R_H \times \left(\frac{1}{4^2} - \frac{1}{n_2^2} \right)$$

$n_1 = 4$ (Final state)

$n_2 = 5, 6, 7 \dots$
(Initial states, $n_2 > 4$)

Brackett Series



Pfund Series

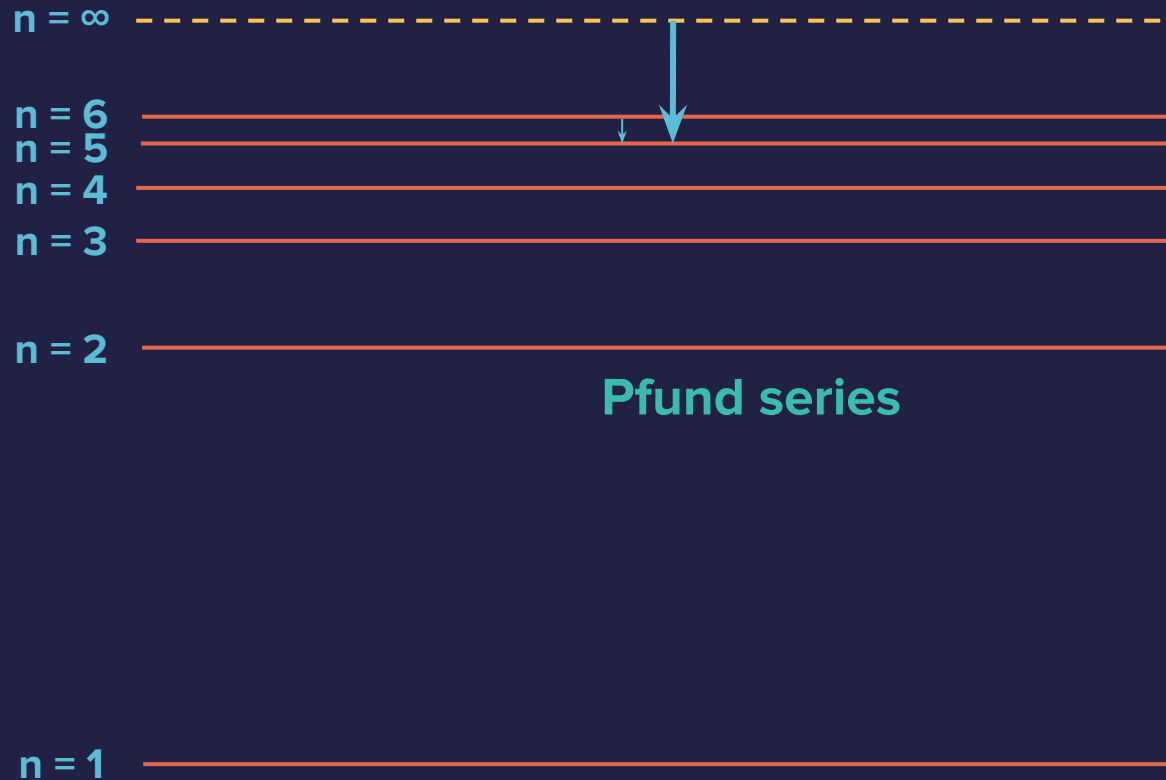
5th spectral series; Found in IR region by Pfund

$$\frac{1}{\lambda} = R_H \times \left(\frac{1}{5^2} - \frac{1}{n_2^2} \right)$$

$n_1 = 5$ (Final state)

$n_2 = 6, 7, 8 \dots$
(Initial states, $n_2 > 5$)

Pfund Series



Humphrey Series

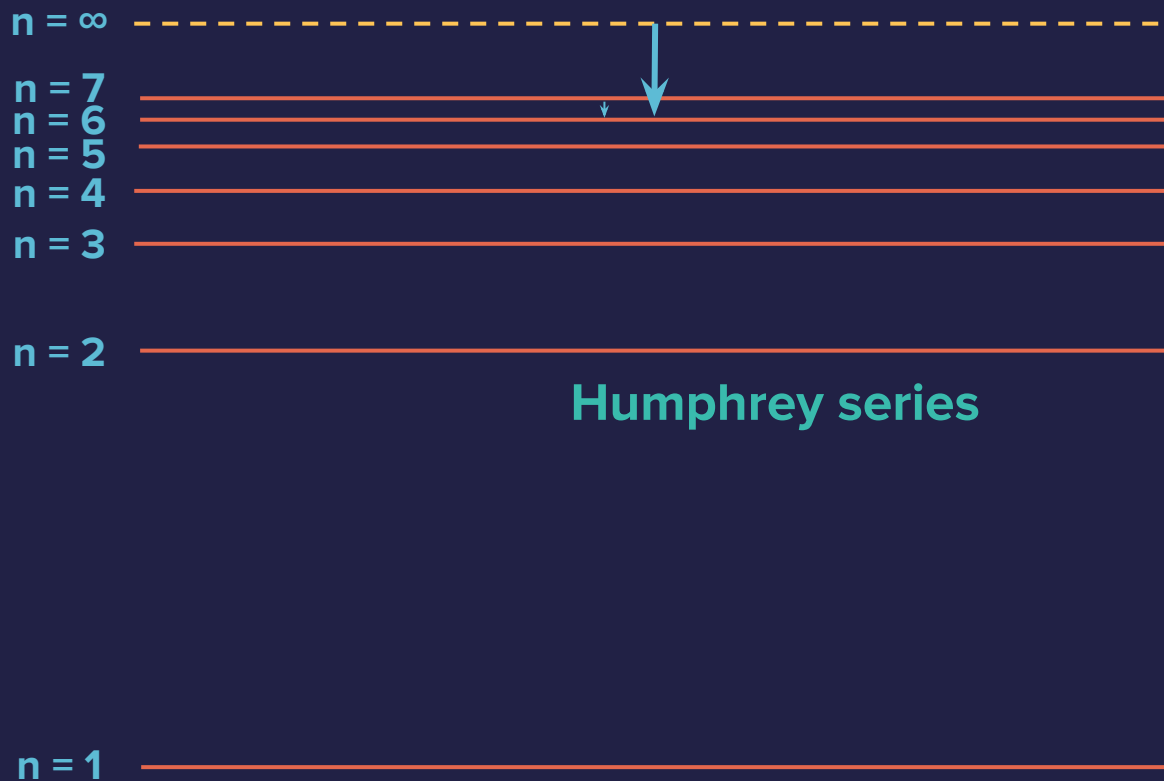
6th spectral series; Found in IR region by Humphrey

$$\frac{1}{\lambda} = R_H \times \left(\frac{1}{6^2} - \frac{1}{n_2^2} \right)$$

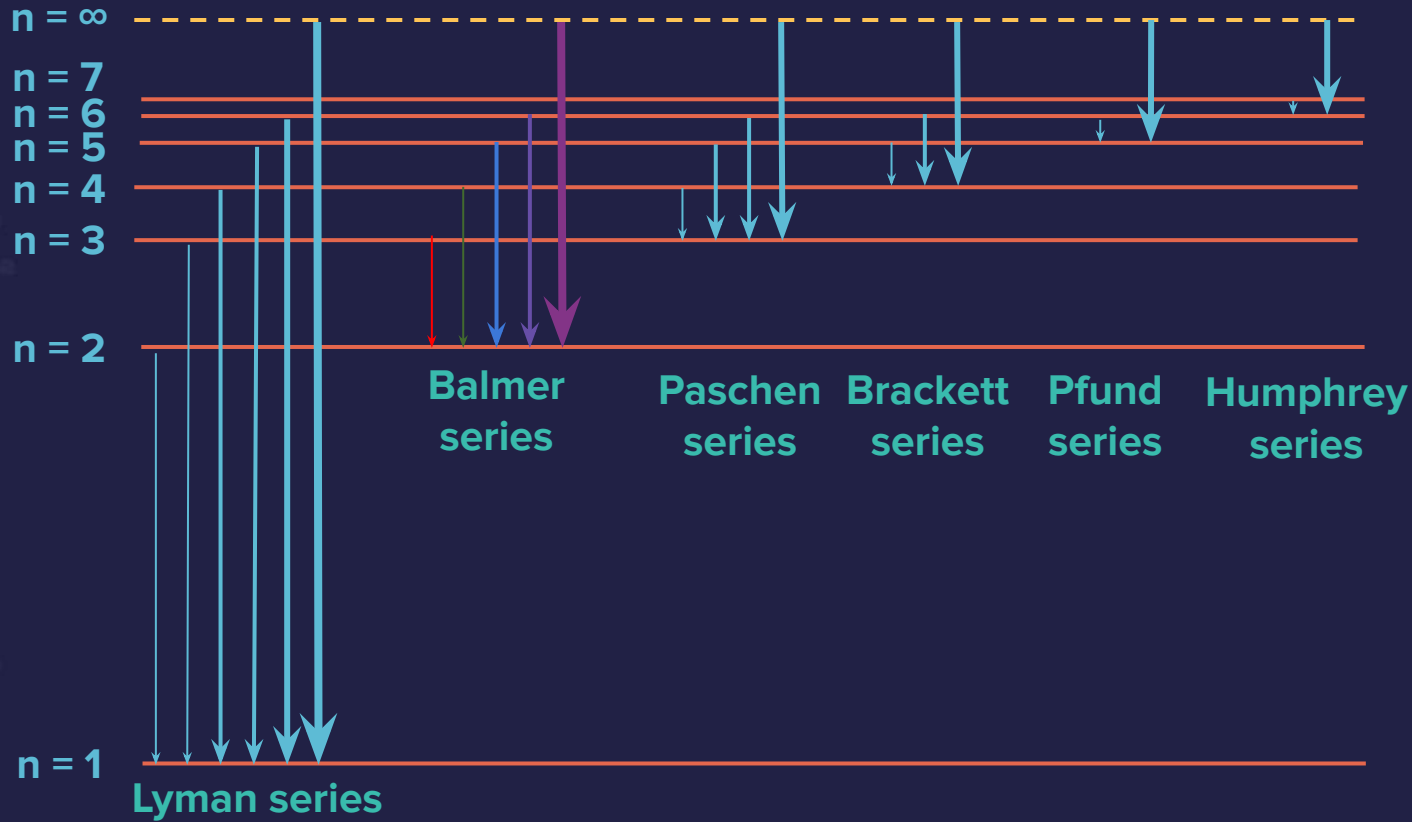
$n_1 = 6$ (Final state)

$n_2 = 7, 8, 9 \dots$
(Initial states, $n_2 > 6$)

Humphrey Series



Line Spectrum of Hydrogen





Maximum Number of Spectral Lines

Maximum number of lines

=

**Maximum number of different
types of photons**





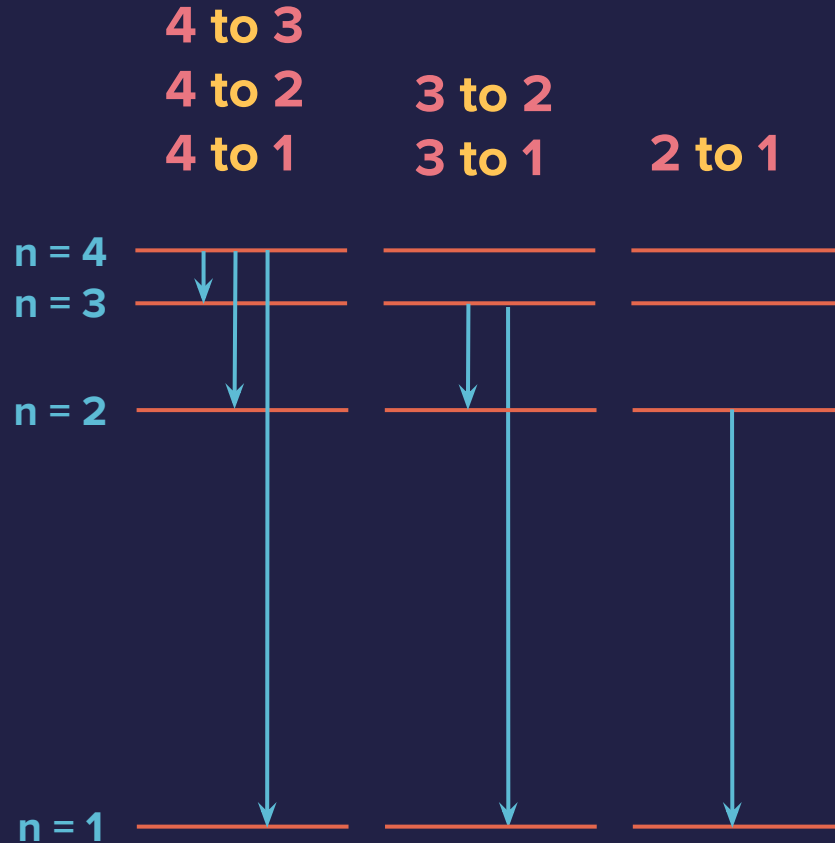
Maximum Number of Lines

Large sample

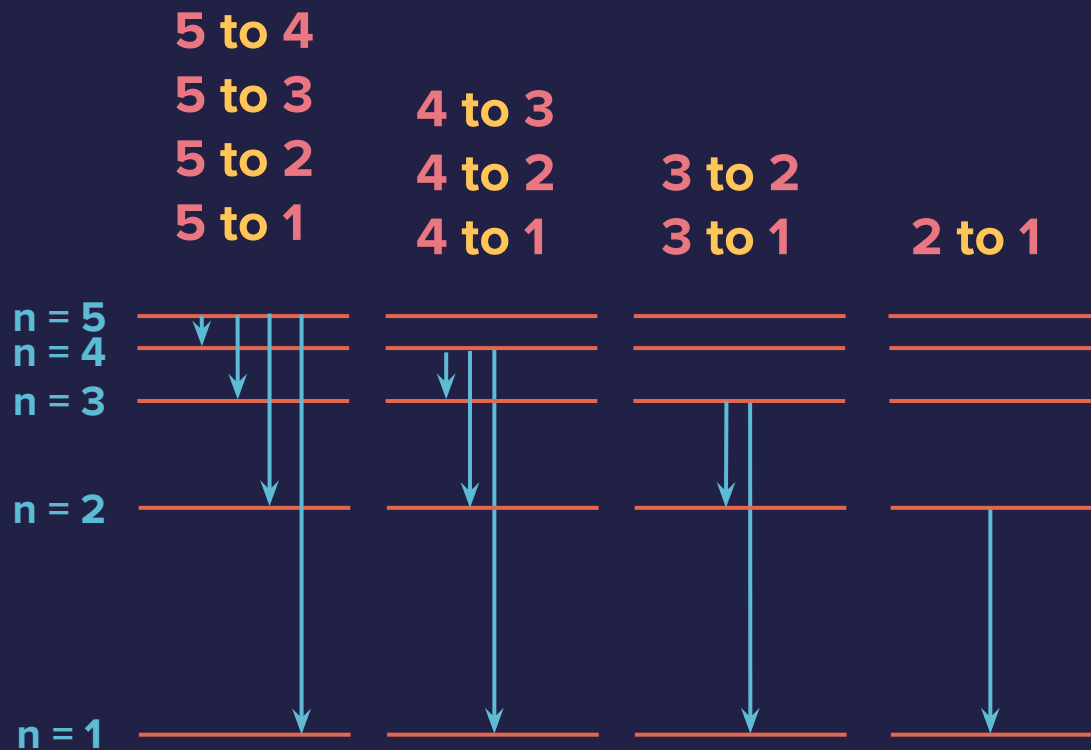
**Isolated
species**



Maximum Lines for the transition from 4 to 1



Maximum Lines for the transition from 5 to 1



Maximum Number of Lines

$$\text{Spectral Lines} = \frac{(n_H - n_L + 1)(n_H - n_L)}{2} = \frac{(\Delta n + 1)(\Delta n)}{2}$$

Δn

$$n_H - n_L$$

n_H

Higher energy level

n_L

Lower energy level

Maximum Number of Lines

For transition upto $n = 1$ or $n = n_{\text{Series}}$

In Lyman series
($n_{\text{Higher}} > 1$)

=

$$n_{\text{Higher}} - 1$$

For a particular series

In Balmer series
($n_{\text{Higher}} > 2$)

=

$$n_{\text{Higher}} - 2$$

Spectral lines

=

$$n_{\text{Higher}} - n_{\text{Series}}$$

In Paschen series
($n_{\text{Higher}} > 3$)

=

$$n_{\text{Higher}} - 3$$



Maximum Number of Lines

In Brackett series

$$(n_{\text{Higher}} > 4)$$

=

$$n_{\text{Higher}} - 4$$

In Pfund series

$$(n_{\text{Higher}} > 5)$$

=

$$n_{\text{Higher}} - 5$$

In Humphrey series

$$(n_{\text{Higher}} > 6)$$

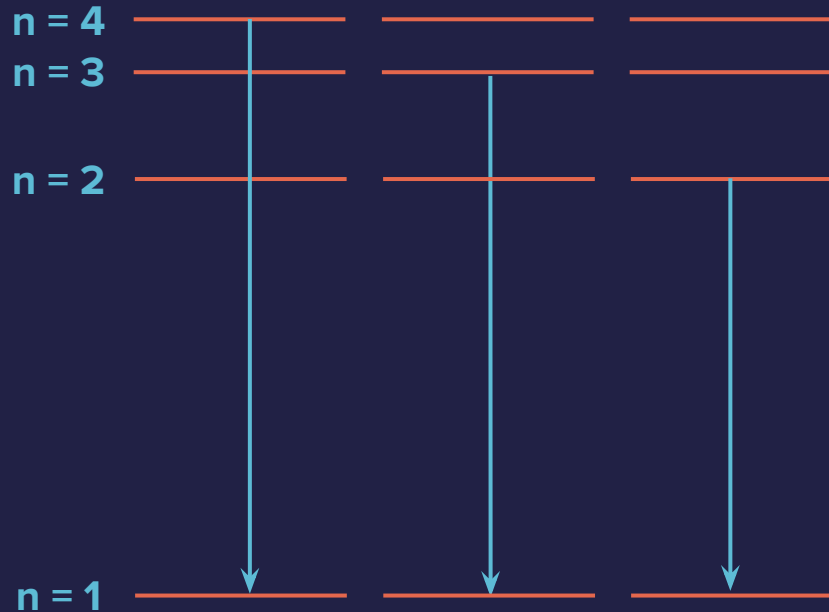
=

$$n_{\text{Higher}} - 6$$



Example

Number of spectral lines in Lyman series
from 4th shell $= n_H - 1 = 4 - 1 = 3$



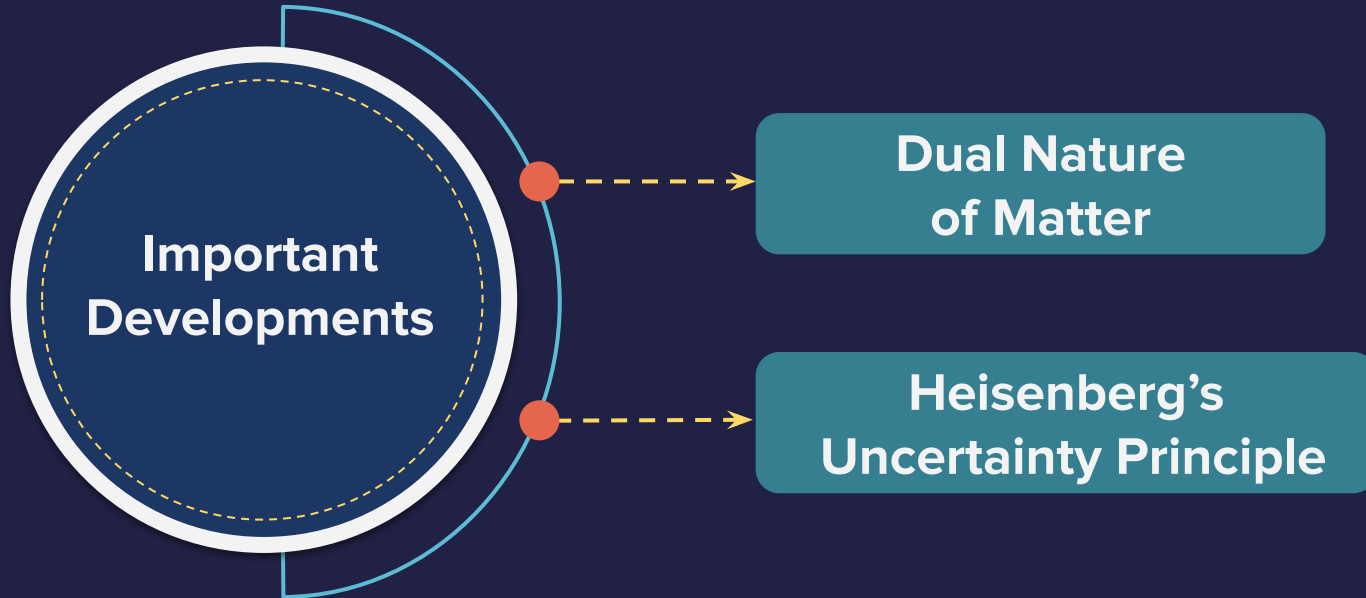
Example



The background is a dark blue gradient. In the center is a large, dark blue, irregular cloud-like shape. Surrounding this central shape are various colorful icons related to microbiology and science: a green microscope at the top, a blue and white Erlenmeyer flask with blue liquid on the left, a red and white Erlenmeyer flask with red liquid on the right, a molecular structure with blue and yellow spheres at the top right, a molecular structure with blue and yellow spheres at the bottom left, a red and white petri dish with red contents at the bottom, and a rack of test tubes with colored caps (blue, green, orange) at the bottom right. There are also several small, scattered colored dots (orange, pink, blue) throughout the scene.

Isolated species

Pathway to Quantum Mechanical Model



Dual Nature of Matter

de Broglie proposed that **particle** has dual nature

**Particle
nature**

**Wave
nature**

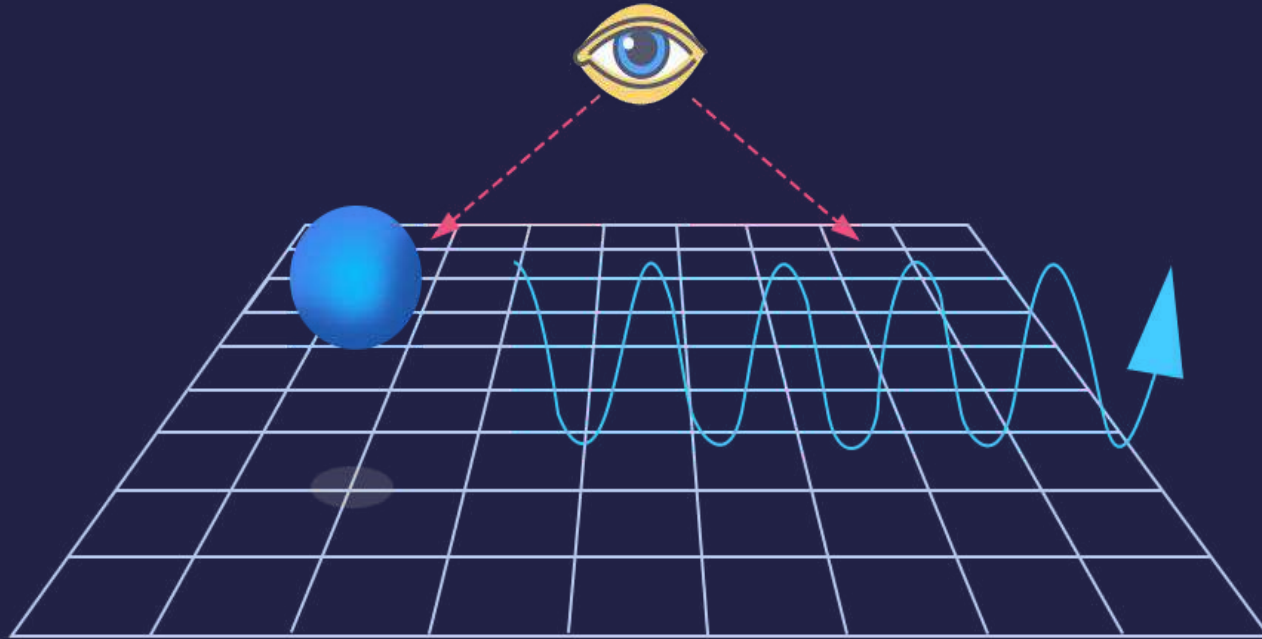
Einstein suggested that **light** has dual nature i.e.,
particle nature as well as wave nature.



Louis de Broglie



de Broglie Hypothesis





Matter Wave

$$\lambda = \frac{h}{p}$$

Wave
associated with
**moving
particles**



de Broglie Hypothesis



Planck's equation

E

$=$

$$\frac{hc}{\lambda}$$

Einstein's Mass
Energy relationship

E

$=$

$$mc^2$$



de Broglie Hypothesis

Equating both

$$\frac{hc}{\lambda}$$

=

$$mc^2$$

For photon

$$\lambda$$

=

$$\frac{h}{mc}$$

By same analogy, de Broglie proposed

For matter

$$\lambda$$

=

$$\frac{h}{mv}$$

de Broglie Wavelength (λ)

$$\lambda = \frac{h}{mv} = \frac{h}{p}$$

p

**Momentum
of particle**

v

**Velocity
of particle**

m

**Mass
of particle**

h

**Planck's
constant**

Davisson and Germer's Experiment

Experimental verification of
de Broglie's prediction



It was observed that an **electron beam** undergoes **diffraction**

Wavelength of a ball & an electron!

de Broglie wavelength: $\lambda = \frac{h}{mv}$

Cricket ball

$$m = 150 \text{ g}$$

$$v = 25 \text{ m s}^{-1}$$

$$\lambda = \frac{6.626 \times 10^{-34}}{(150 \times 10^{-3}) \times 25}$$

$$\lambda = 1.767 \times 10^{-34} \text{ m}$$

λ is **insignificant**.

Electron

$$m = 9.1 \times 10^{-31} \text{ kg}$$

$$v = 2 \times 10^3 \text{ m s}^{-1}$$

$$\lambda = \frac{6.626 \times 10^{-34}}{(9.1 \times 10^{-31}) \times 2 \times 10^3}$$

$$\lambda = 0.364 \times 10^{-6} \text{ m}$$

$$= 364 \text{ nm}$$

λ is **significant**.

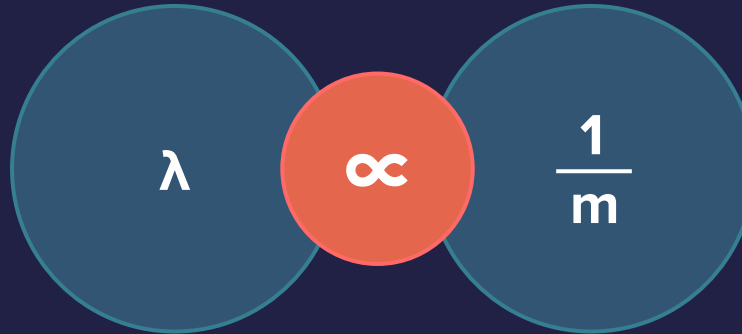


Matter Waves

Wave nature
can't be detected
for macroscopic object

λ small

Due to
larger mass



de Broglie's Equation & Kinetic Energy

$$\text{K.E.} = \frac{1}{2}mv^2$$

Multiplying both sides by m & rearranging

$$m^2v^2$$

$$=$$

$$2 \text{ K.E.} \times m$$

$$mv$$

$$=$$

$$\sqrt{2 \text{ K.E.} \times m}$$

de Broglie's Equation & Kinetic Energy

de Broglie
equation

$$\lambda = \frac{h}{mv} = \frac{h}{p}$$

Since

$$mv = \sqrt{2 \text{ K.E.} \times m}$$

$$\lambda = \frac{h}{\sqrt{2 \text{ K.E.} \times m}}$$



de Broglie's Equation & Kinetic Energy

A charged particle accelerated from rest across a **potential difference of V**

$$| \text{K.E.} |$$

$$=$$

$$| q V |$$



$$mv$$

$$=$$

$$\sqrt{2m \times \text{K.E.}}$$



$$mv$$

$$=$$

$$\sqrt{2m \times q V}$$



de Broglie's Equation & Kinetic Energy

 λ
 $=$

$$\frac{h}{\sqrt{2m \times q V}}$$

 λ

Wavelength (m)

 q

Charge on a particle (C)

 m

Mass of charged particle (kg)

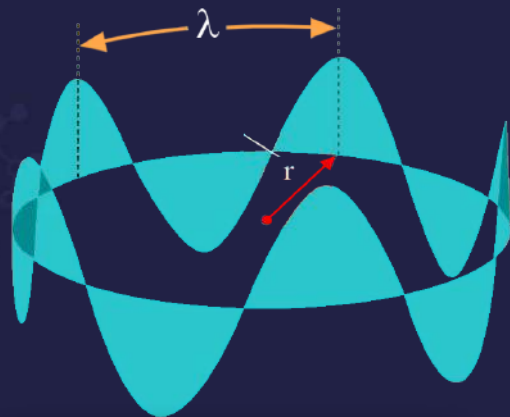
 h

Planck's constant (Js)



Electron as a Wave

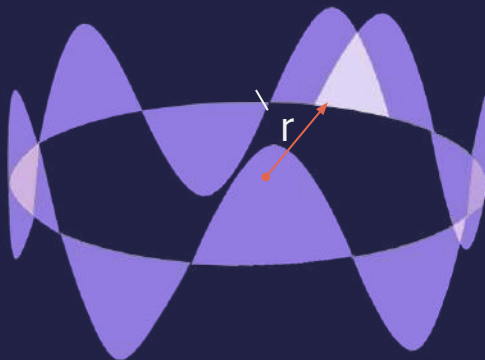
In phase



Electron exist

Circumference,
 $2\pi r = n\lambda$

Out of phase



Electron don't exist

Circumference,
 $2\pi r \neq n\lambda$

n = Number of waves made
in Bohr's orbit

An integral number of
complete wavelengths must
fit around the circumference
of the orbit.





Electron as a Wave

When electrons
are in phase,

$$2\pi r$$

$$=$$

$$\frac{nh}{mv}$$

Bohr's Postulate
verified

$$mvr$$

$$=$$

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

n = Energy level



Heisenberg's Uncertainty Principle (H.U.P.)



Werner Heisenberg

Exact **position** and
momentum of a
microscopic particle
cannot be determined
simultaneously



Heisenberg's Uncertainty Principle

$$\Delta x \cdot \Delta p$$

$$\geq$$

$$\frac{h}{4\pi}$$

$$\Delta x \cdot m \cdot \Delta v$$

$$\geq$$

$$\frac{h}{4\pi}$$

$$\Delta x$$

Uncertainty in
position

$$\Delta p$$

Uncertainty in
momentum

$$m$$

Mass of
particle

$$\Delta v$$

Uncertainty in
velocity



Principle of Optics



If a light (wavelength ' λ ') is used to locate the position of a particle, then

Minimum error in the position measurement (Δx)

=

$\pm \lambda$



Heisenberg's Uncertainty Principle

Since

Δx

=

λ

For accurate
position

$\Delta x \rightarrow 0$

$\lambda \rightarrow 0$

For a photon

E

=

$\frac{hc}{\lambda}$

$\lambda \rightarrow 0$

$E \rightarrow \infty$

Heisenberg's Uncertainty Principle

High energy photon
strikes particle

$$\Delta p \uparrow$$

Similarly

For accurate momentum

$$\Delta x \uparrow$$

Heisenberg's Uncertainty Principle

For an electron

$$\Delta x \cdot m \cdot \Delta v$$

$$\geq$$

$$\frac{h}{4\pi}$$

$$\Delta x \cdot \Delta v$$

$$=$$

$$\frac{6.626 \times 10^{-34} \text{ Js}}{4 \times 3.14 \times 9.1 \times 10^{-31} \text{ kg}}$$

$$\Delta x \cdot \Delta v$$

$$\approx$$

$$10^{-4} \text{ m}^2\text{s}^{-1}$$



Heisenberg's Uncertainty Principle

If $\Delta x = 10^{-8} \text{ m}$ then $\Delta v = 10^4 \text{ ms}^{-1}$

Position

High
accuracy

Δx is small

Velocity

Uncertain

Δv is large

If $\Delta v = 10^{-8} \text{ ms}^{-1}$ then $\Delta x = 10^4 \text{ m}$

Velocity

High
accuracy

Δv is small

Position

Uncertain

Δx is large

Conclusion:
Heisenberg's
uncertainty
principle is
meaningless for
bigger particles.





Significance of the Uncertainty Principle



1

Not an instrumental error,
rather conceptual error

2


Rules out the existence of
definite paths of electrons

3

Introduced concept of
probability of finding the
electrons

Precise statements of
position & momentum
of an electron replaced with
probability

Forms the basis of
**Quantum Mechanical Model
of atom**



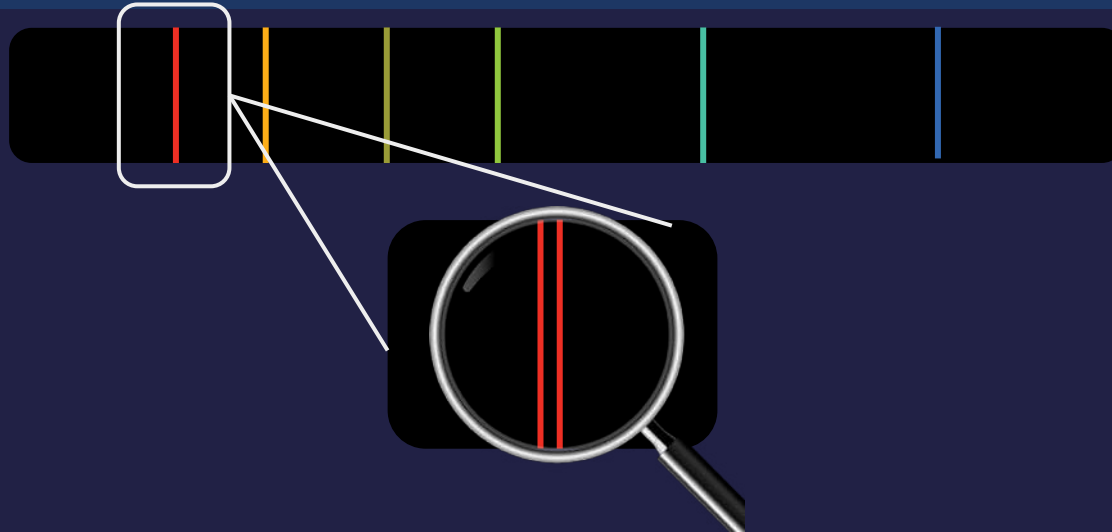
Limitations of Bohr Model

1

Could not explain the line spectra of atoms containing more than one electron

2

Could not explain the presence of doublet i.e. two closely spaced lines





Limitations of Bohr Model

3

Unable to explain the splitting of spectral lines in the presence of magnetic field (**Zeeman effect**) and electric field (**Stark effect**).

4

No conclusion was given for the principle of quantisation of angular momentum

5

Unable to explain de Broglie's concept & Heisenberg's Uncertainty Principle





Quantum Mechanical Model



Wavefunction

SWE is solved to get values of Ψ and their corresponding **energies**



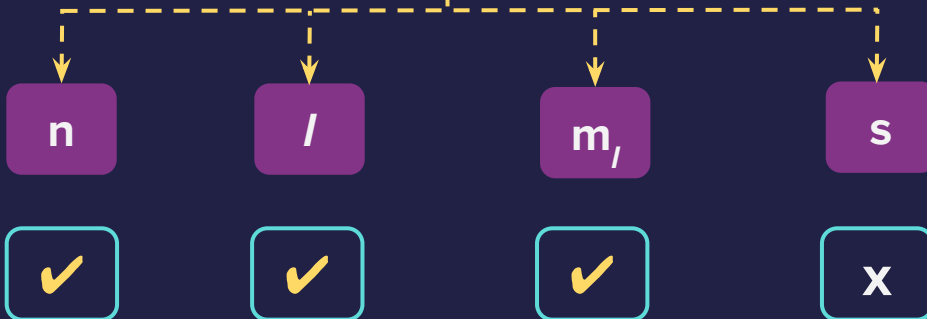
A function that contains all the **dynamical information** about a system



Schrodinger Wave Equation

Ψ corresponds to **atomic orbital**

Characterized by a **set of quantum numbers**





Quantum Numbers

Set of **four numbers** required to **define an electron** in an atom completely

1

Principal Quantum Number (n)

2

Azimuthal Quantum number (l)

3

Magnetic Quantum Number (m_l)

4

Spin Quantum Number (s)



Principal Quantum Number (n)



Proposed by
Niels Bohr

1

Designates the **shell** to which the electron belongs

2

Signifies energy level for **single electron species**

3

Accounts for the **main lines** in the atomic spectrum



Principal Quantum Number (n)

Describes the **size**
of electron wave
& the **total energy**
of the electron

$$n = 1, 2, 3...$$

Represented as K, L, M, N,...

Angular momentum in any
shell

=

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

Azimuthal Quantum Number (l)



Proposed by
Sommerfeld

1

Designates the **subshell** to which the electron belongs

2

Energy of the orbital in **multielectron species** (both n & l)

3

Accounts for the **fine lines** in atomic spectrum



Azimuthal Quantum Number (l)

Describes the **3-D shape** of the **orbital** or the electron cloud

Also known as

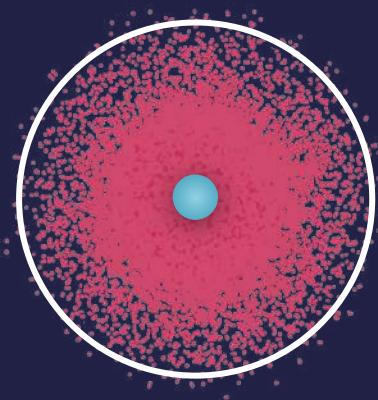
Subsidiary Quantum Number

Orbital Angular momentum Quantum Number

Boundary Surface Diagram

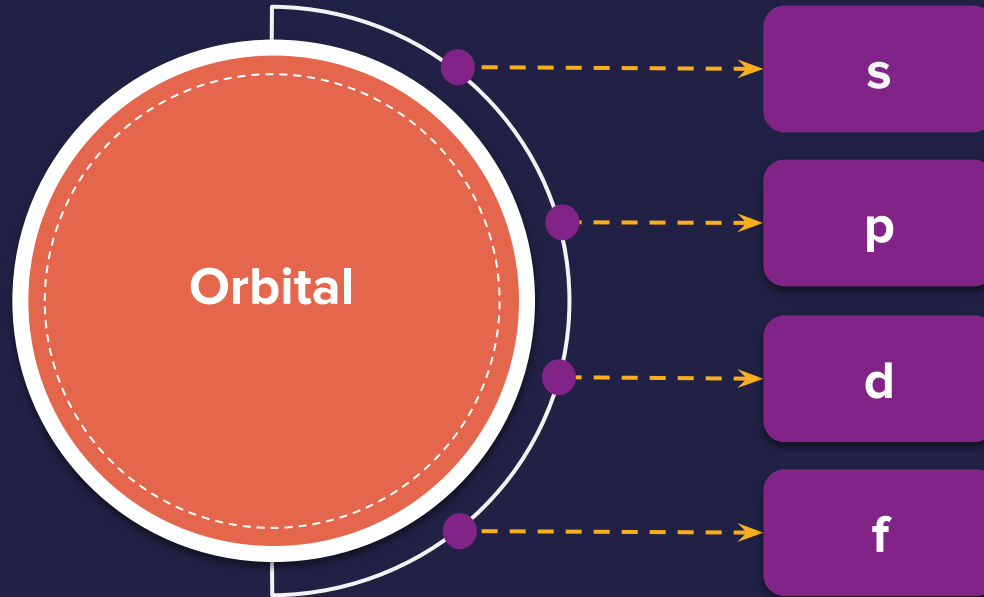
Encloses the 3D region where probability of finding electrons is maximum

Example



Shape : **Spherical**

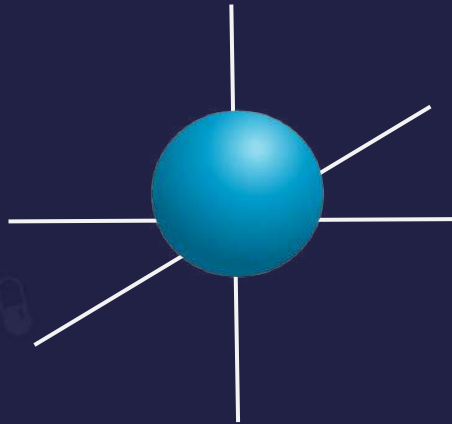
Classification of Orbitals



Shape of Orbitals

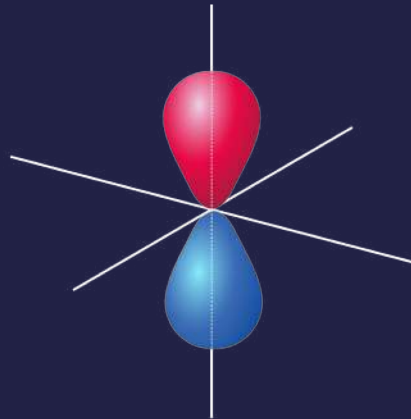
s - orbital

Shape : **Spherical**

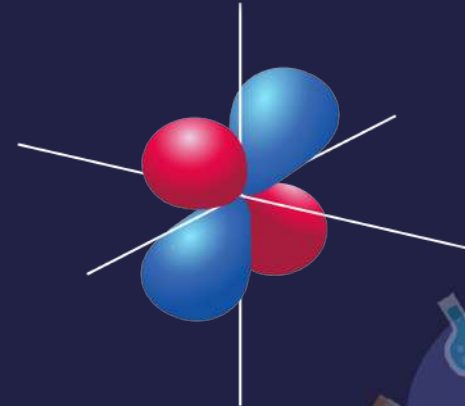


p - orbital

Shape : **Dumb bell**



Shape : **Double dumb bell**



Shapes of Orbitals

Orbital	Shape
s	Spherical
p	Dumb bell
d	Double dumb bell
f	Leaf like / Complicated



Subshell

Collection of
**similar shaped
orbitals** of same **n**.

Azimuthal Quantum Number (l)

For a given value of Principal Quantum Number (n)

l

$=$

0 to ($n - 1$)

Subshell

/	Subshell	Description
0	s	Sharp
1	p	Principal
2	d	Diffused
3	f	Fundamental
4	g	Generalised

Subshell Representations

Number of subshells in the n^{th} shell

n	/	Subshell notation
1	0	1s
2	0, 1	2s, 2p
3	0, 1, 2	3s, 3p, 3d
4	0, 1, 2, 3	4s, 4p, 4d, 4f

Azimuthal Quantum Number (l)

Orbital angular
momentum (L)

=

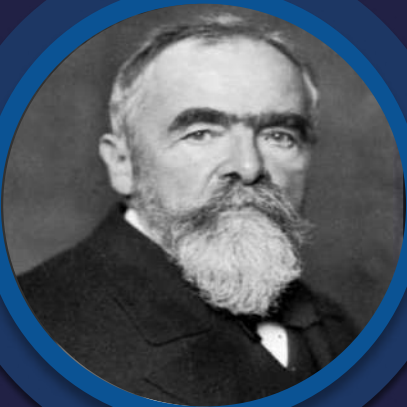
$$\sqrt{l(l+1)} \hbar$$

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

Subshell	Orbital angular momentum
s	0
p	$\sqrt{2} \hbar$
d	$\sqrt{6} \hbar$



Magnetic Quantum Number (m_l)



Proposed by
Linde

1

Designates the **orbital** to which the electron belongs

2

Describes the **orientation** of orbitals

3

Accounts for the **splitting of lines** of atomic spectrum in **magnetic field**



Magnetic Quantum Number (m_l)

Can have values from - / to + /
including **zero**



Each value corresponds to an **orbital**

For d
subshel,
 $l = 2$

$$m_l = -2, -1, 0, 1, 2$$



Magnetic Quantum Number (m_l)

Maximum number of orbitals in a subshell

=

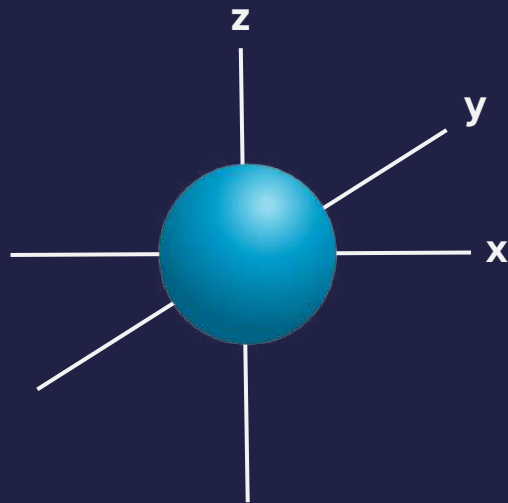
$$2l + 1$$

Subshell	Number of orbitals
s	1
p	3 (p_x, p_y, p_z)
d	5 ($d_{xy}, d_{yz}, d_{zx}, d_{x^2-y^2}, d_z^2$)
f	7



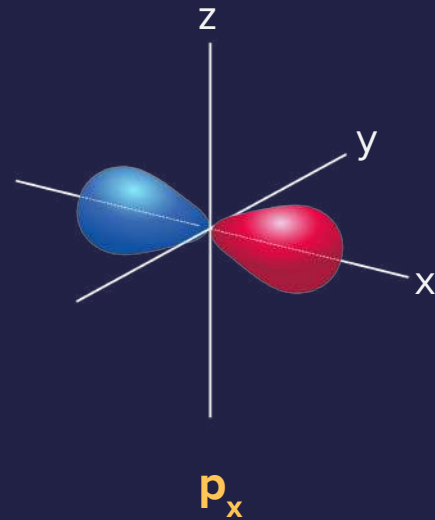
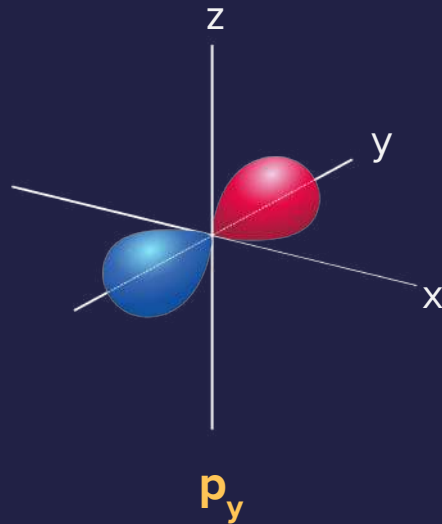
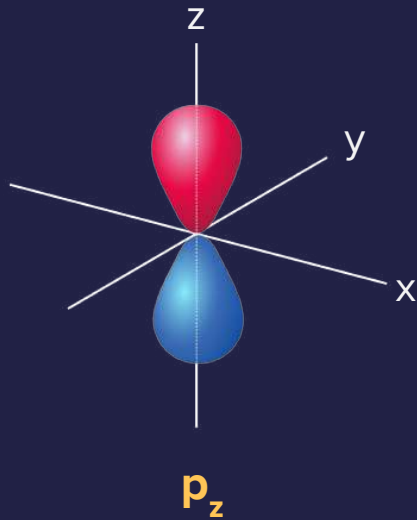
s - orbital

Shape : **Spherical**
Non-directional in nature

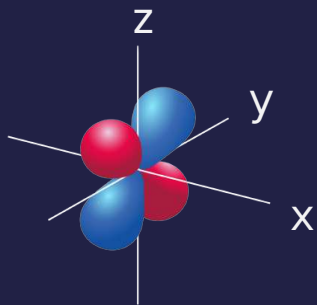


p - orbital

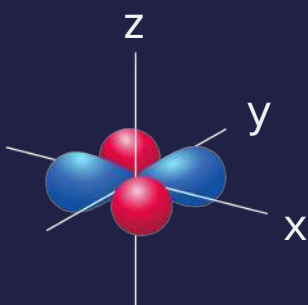
Shape : **Dumb bell**
Directional in nature



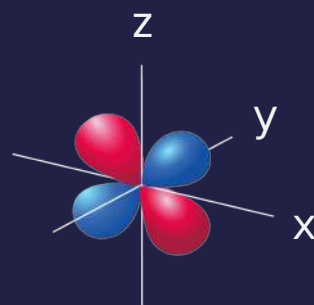
d - orbital



d_{yz}



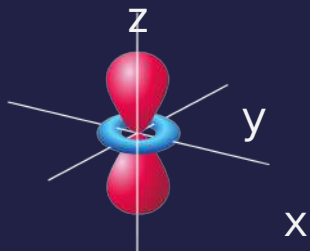
d_{xy}



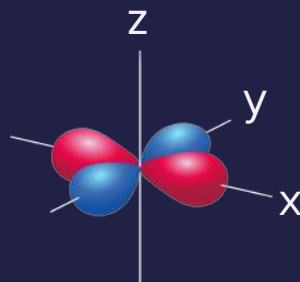
d_{xz}

**Non axial
d-orbitals**

Shape : **Dumb bell**
Directional in nature



d_{z^2}



$d_{x^2-y^2}$

**Axial
d-orbitals**



Remember!

An **orbitals** can accommodate maximum of **2 electrons**.

Maximum number of
electrons in a subshell

=

$$2 (2l + 1)$$

Subshell	s	p	d	f
<i>l</i>	0	1	2	3
Number of electrons	2	6	10	14

Spin Quantum Number (s or m_s)



Proposed by George Uhlenbeck (left)
and Samuel Goudsmit (Right)

Presence of **two closely spaced lines** in
atomic spectrum



Spin of an **electron**

$$s = +\frac{1}{2}$$

$$s = -\frac{1}{2}$$



Spin Quantum Number (s)

Spin magnetic
moment (μ)

=

$\sqrt{n(n+2)}$ B.M.

n = number of unpaired electron



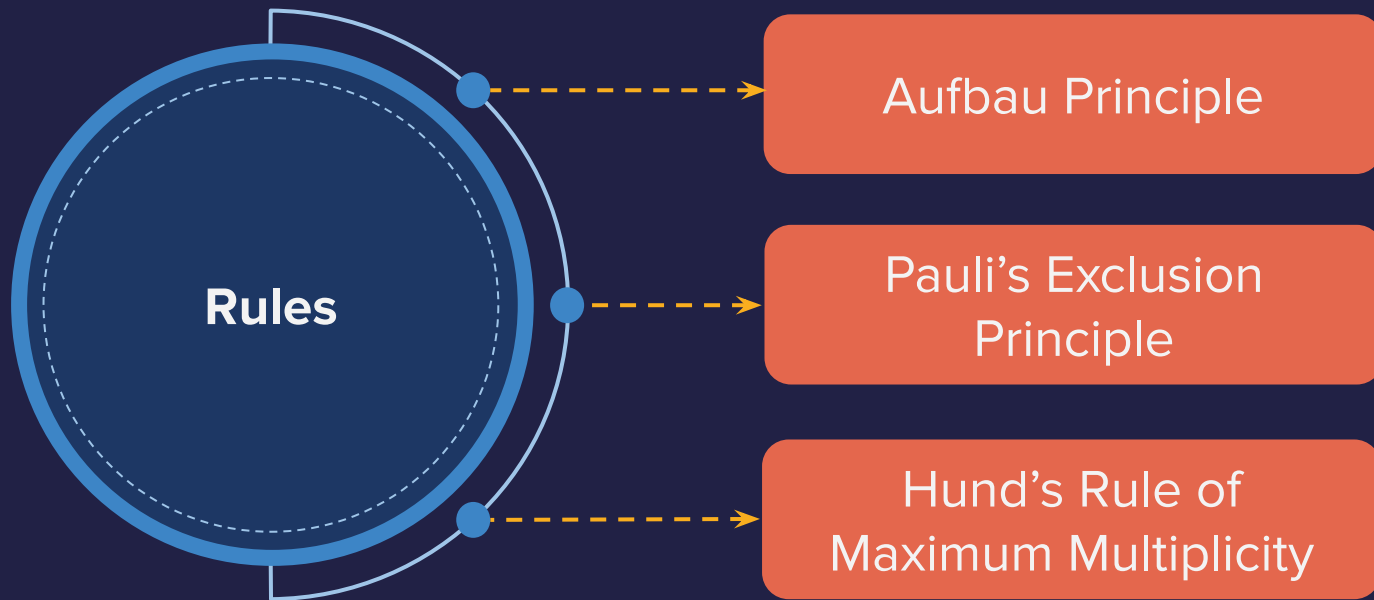
Orbit and Orbital

Orbit	Orbital
Well defined circular path around the nucleus where electrons revolve	3D region around the nucleus where electrons are most likely to be found
Maximum number of electrons in n^{th} orbit is $2n^2$	Cannot accommodate more than two electrons

Orbit and Orbital

Orbit	Orbital
Not in accordance with Heisenberg's Uncertainty Principle	In accordance with Heisenberg's Uncertainty Principle
Designated as K, L, M, N, ...	Designated as s, p, d, f, ...


Rules for Filling Electrons in Orbitals





Aufbau Principle

**Electrons are
filled in various
orbitals** in order of
their increasing
energies



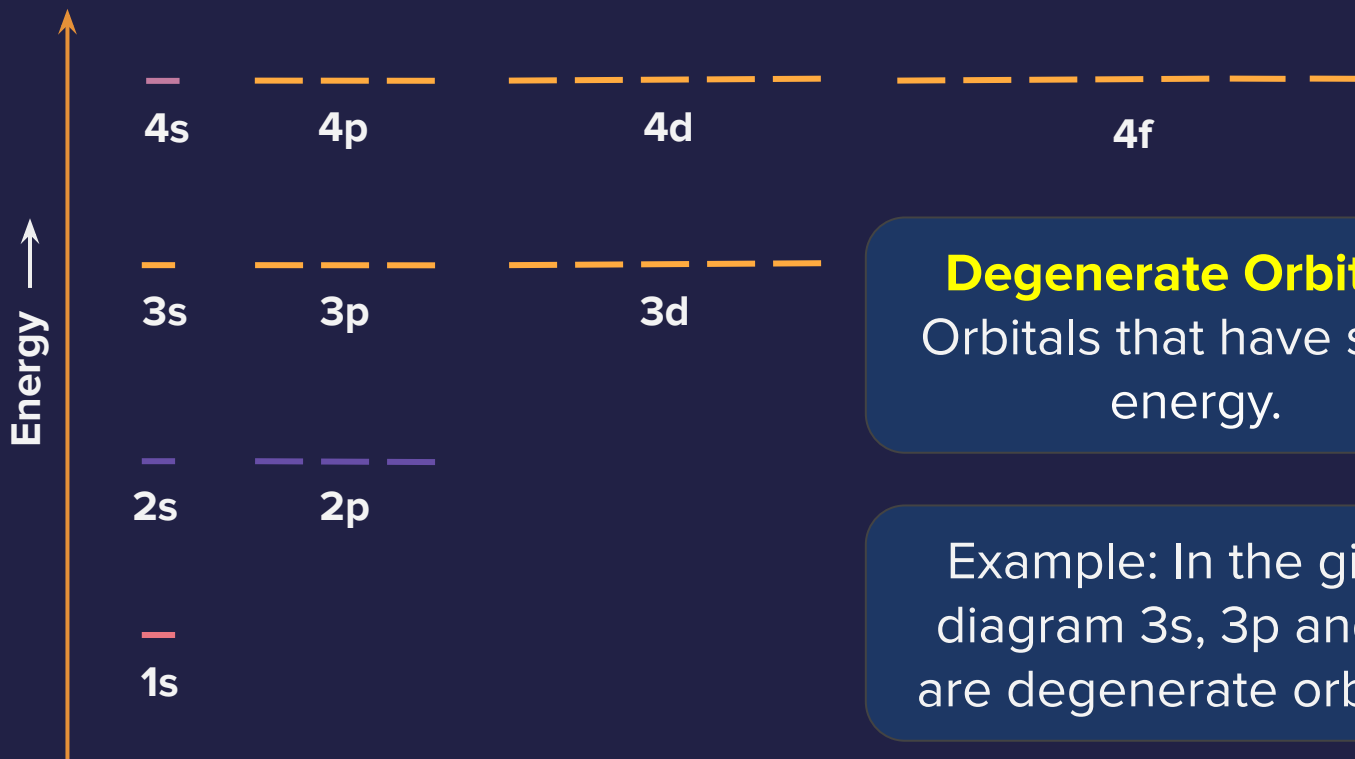
Energies of Subshells of H-like Species

Energy of **single electron species** depends only on the
Principal Quantum Number

$$1s < 2s = 2p < 3s = 3p = 3d < 4s = 4p = 4d = 4f < \dots$$

Order of
Energy

Energies of Subshells of H-like Species



Energy of Subshells of Multi-electron Species

Different subshells have different energy
which depends on:

**Principal Quantum
Number**

**Azimuthal
Quantum Number**

$(n + l)$ rule or Bohr-Bury's Rule

Lower value of
 $(n + l)$

Lower will be
energy of subshell

Two subshells with
same $(n + l)$ value

Subshell with **lower 'n'**
value has **lower energy**



Comparison of orbital energy

1s

<

2s

2s

<

2p

5p

>

4d

2p

<

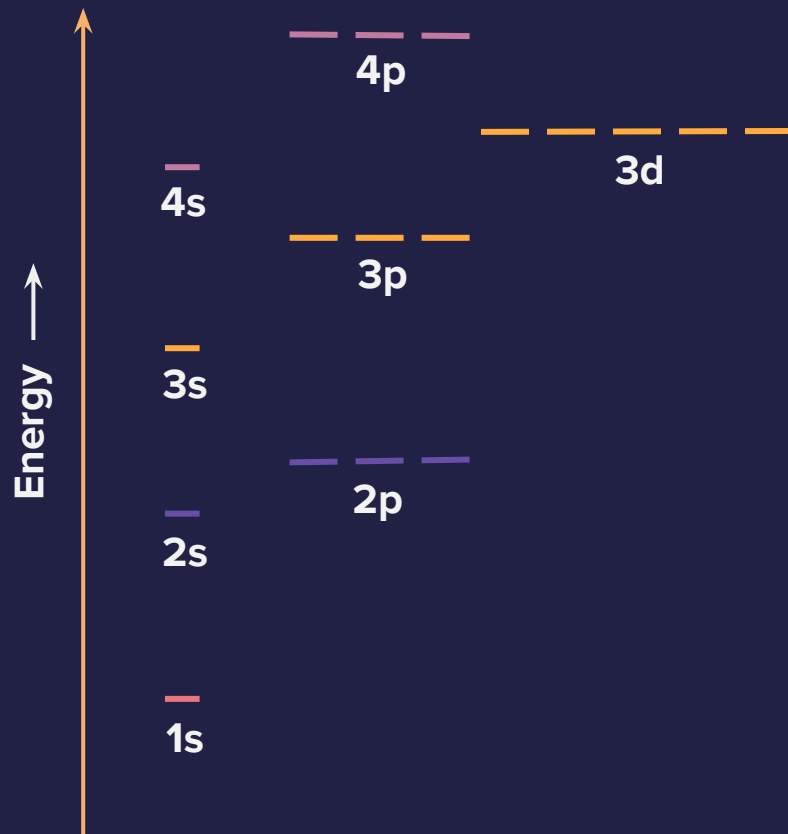
3p

3d

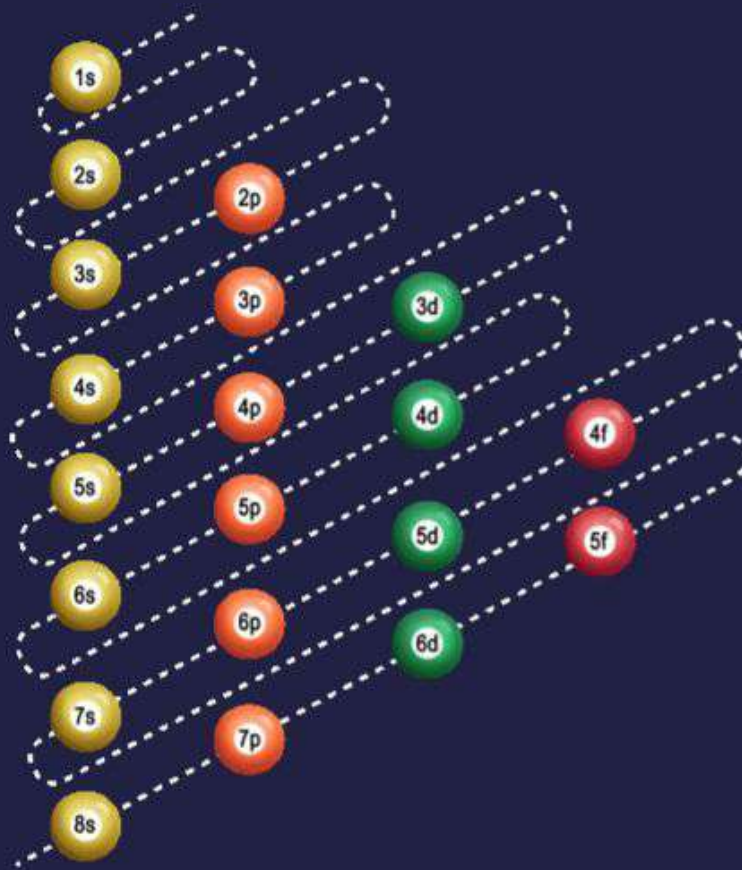
<

4p

Energies of Subshells of Multi electron Species



Energies of Subshells of Multi electron Species



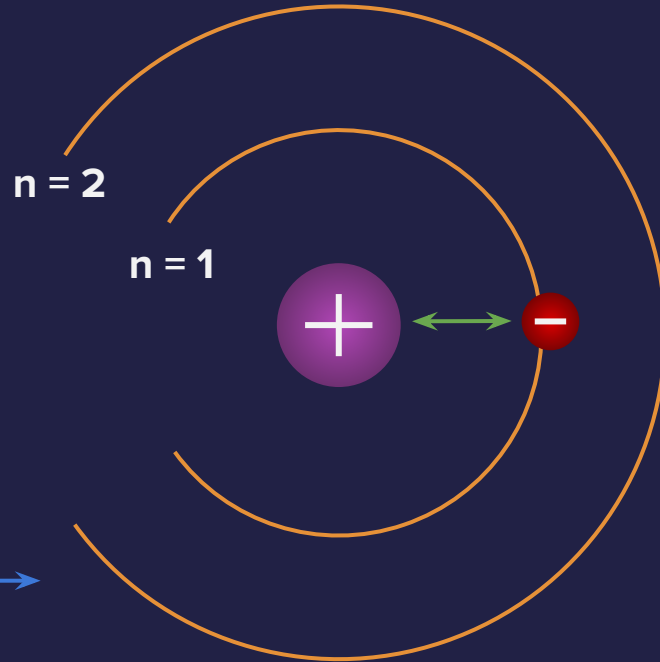
H-like v/s Multi-electron species



H-like species	Multi-electron species
Energy of a subshell depends on ' n ' only .	Energy of a subshell depends on (n + l) .
Only attractive forces are present between the nucleus and the electron .	Electrons experience attractive forces towards the nucleus as well as repulsive forces from other electrons .



One-electron species



Repulsion \longleftrightarrow

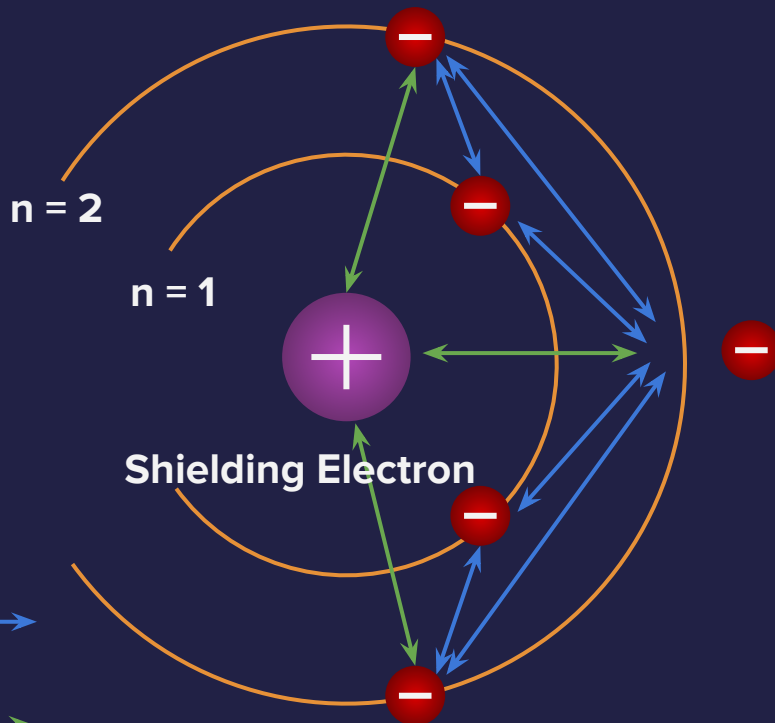
Attraction \longleftrightarrow



Multiple-electron species



Outer Electron



Repulsion \longleftrightarrow

Attraction \longleftrightarrow





Pauli's Exclusion Principle



Wolfgang Pauli

No two electrons
in an atom can
have **the same
set of all four
quantum
numbers**

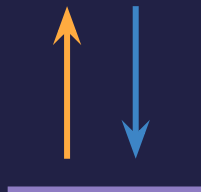
Pauli's Exclusion Principle



Restrict the **filling** of number of **electrons**
in an **orbitals**



Wrong



Right



Subshell electron capacity

s^2

↑↓

p^6

↑↓

↑↓

↑↓

d^{10}

↑↓

↑↓

↑↓

↑↓

↑↓

f^{14}

↑↓

↑↓

↑↓

↑↓

↑↓

↑↓

↑↓

Hund's Rule of Maximum Multiplicity



Friedrich Hund

Hund's Rule of Maximum Multiplicity

No **electron pairing** takes place
in
the orbitals in a subshell

Until each orbital is occupied
by **1 electron** with **parallel spin**

Hund's rule is an **empirical rule**

Determines the **lowest energy arrangement** of electrons

Why Maximum multiplicity?

Maximum spin of
an atom (S)

=

$$\frac{1}{2} \times n$$

Spin Multiplicity
(S.M.)

=

$$2S + 1$$

Spin Multiplicity
(S.M.) ↑



Stability ↑

Electrons with **parallel spins**

Repel each other

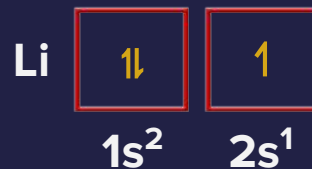
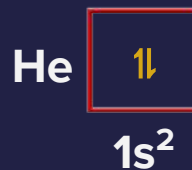
Have a **tendency to stay apart**

Atom **shrink** slightly

Electron-nucleus interaction is
improved

Electronic Configuration

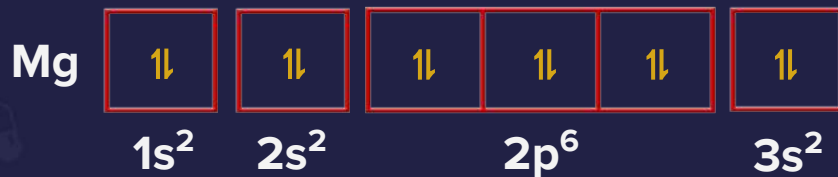
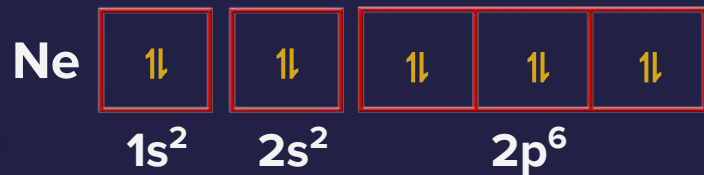
**Distribution
of electrons** in
orbitals of
an atom



Electronic Configuration of Various Elements

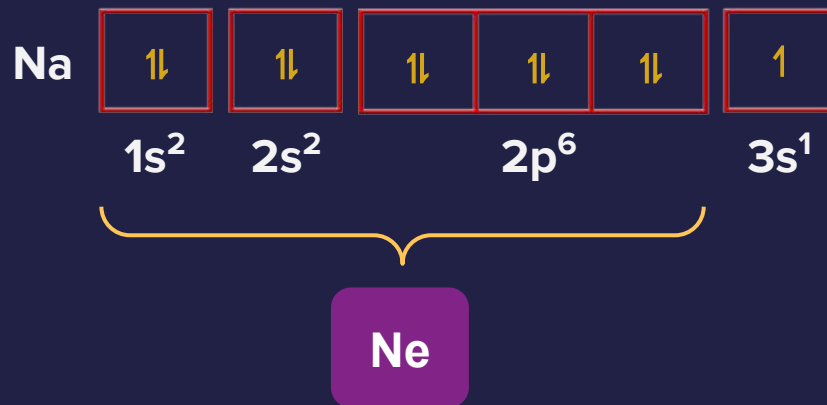


Electronic Configuration of Various Elements



Simplified Electronic Configuration

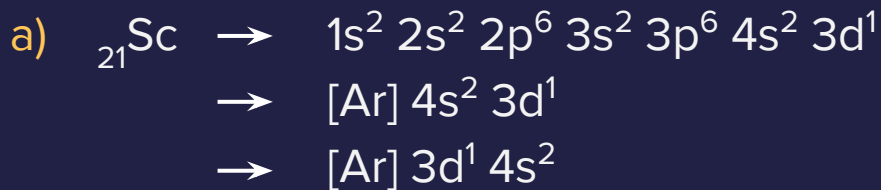
Configuration of Sodium:



Simplified configuration:



Electronic Configuration



Number of unpaired electrons

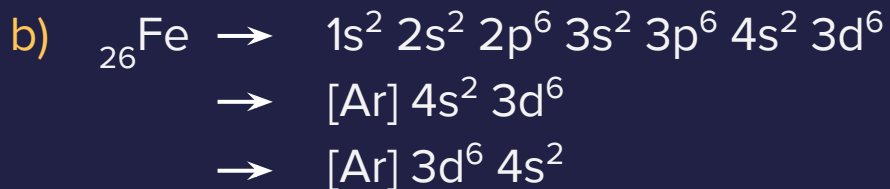
1

Total spin

$+\frac{1}{2}$ or $-\frac{1}{2}$



Electronic Configuration



Number of unpaired electrons

4

Total spin

$+\frac{4}{2}$ or $-\frac{4}{2}$

Exceptions

${}_{24}\text{Cr}$

$[\text{Ar}] 4s^2 3d^4$

Not
Correct

${}_{24}\text{Cr}$

$[\text{Ar}] 4s^1 3d^5$

Correct

52
Cr
24

d^5 is more stable than d^4 configuration



Exceptions

$_{29}\text{Cu}$

$[\text{Ar}] 4s^2 3d^9$

Not
Correct

$_{29}\text{Cu}$

$[\text{Ar}] 4s^1 3d^{10}$

Correct

$^{63}_{29}\text{Cu}$

d^{10} is more stable than d^9 configuration





Half-filled & Fully Filled Orbitals

Exactly **half filled** & **fully filled** orbitals make the configuration more stable

$p^3, p^6, d^5, d^{10}, f^7$ & f^{14} configurations are stable

Stability of **half filled** & **fully filled** orbitals

Symmetry

Exchange Energy



Symmetry

Symmetrical
distribution of
electrons

Symmetry
leads to
stability

Electrons in
the **same**
subshell

Equal
energy

Different
spatial
distribution

Consequently, their
shielding of one another is
relatively small

Electrons are more **strongly**
attracted by the nucleus

Have **less energy**
and more stability



Exchange Energy

Energy released when **two or more electrons** with the **same spin** in the **degenerate** orbitals

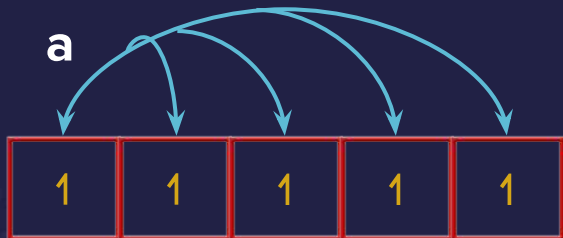


Tends to **exchange** their **positions**

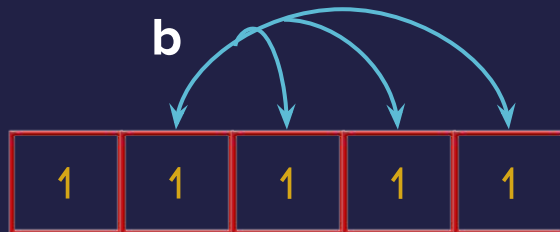
Number of exchanges that can take place is **maximum**

When subshell is either **half filled or fully filled.**

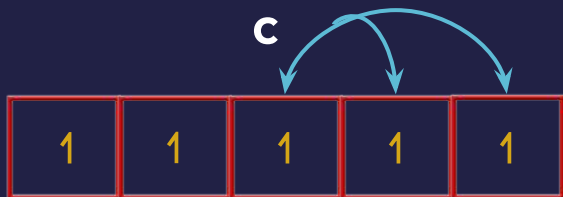
Exchange Energy



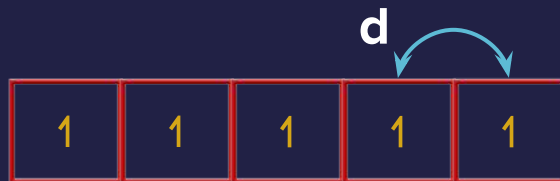
4 exchange by electron 'a'



3 exchange by electron 'b'



2 exchange by electron 'c'



1 exchange by electron 'd'



Electronic Configuration of Ions



Electronic Configuration of Cations

Formed by **removing outermost electron** from a **neutral atom**



Electronic Configuration of Cations

In **d-block** metals

electrons are **first removed**
from **ns** orbital, then from the
penultimate **(n-1)d** orbital

Examples

Fe: [Ar] 3d⁶ 4s² or



Fe²⁺: [Ar] 3d⁶ 4s⁰ or

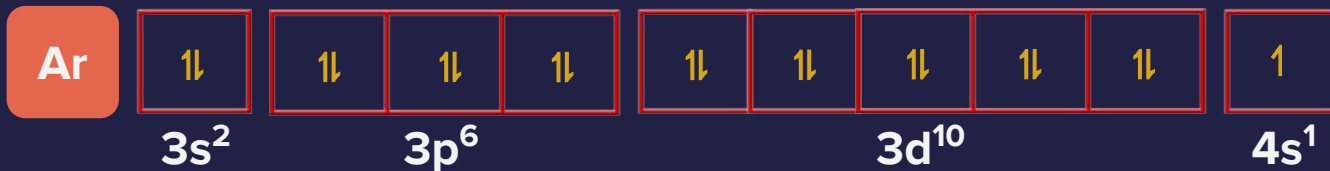


Fe³⁺: [Ar] 3d⁵ 4s⁰ or

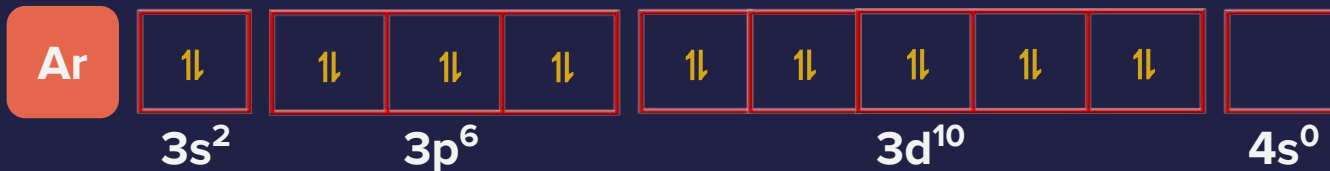


Examples

$_{29}\text{Cu}:$



$_{29}\text{Cu}^+:$



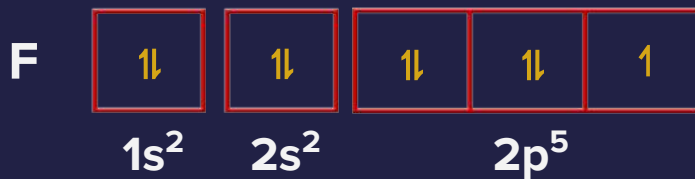
18 electrons

Pseudo inert gas configuration



Electronic Configuration of Anions

Formed by **adding electrons to a neutral atom** according to the 3 rules (**Pauli's, Aufbau & Hund's rule**)



Schrodinger Wave Equation (SWE)

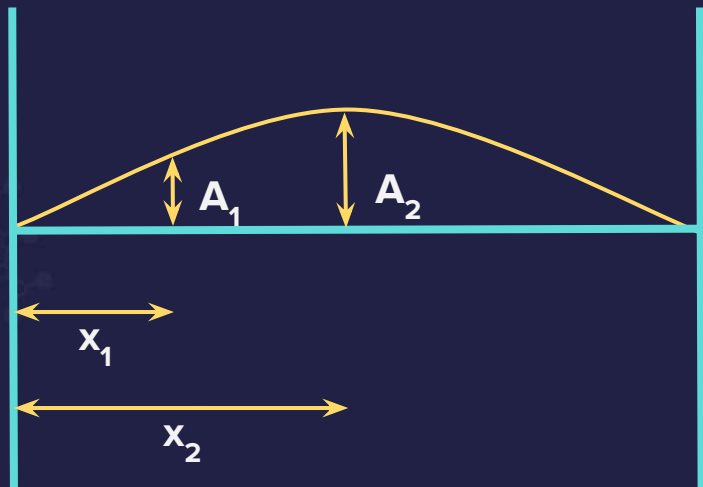


Based on the **dual nature of matter**

Describes the behavior of **electron**
around the nucleus



Wavefunction



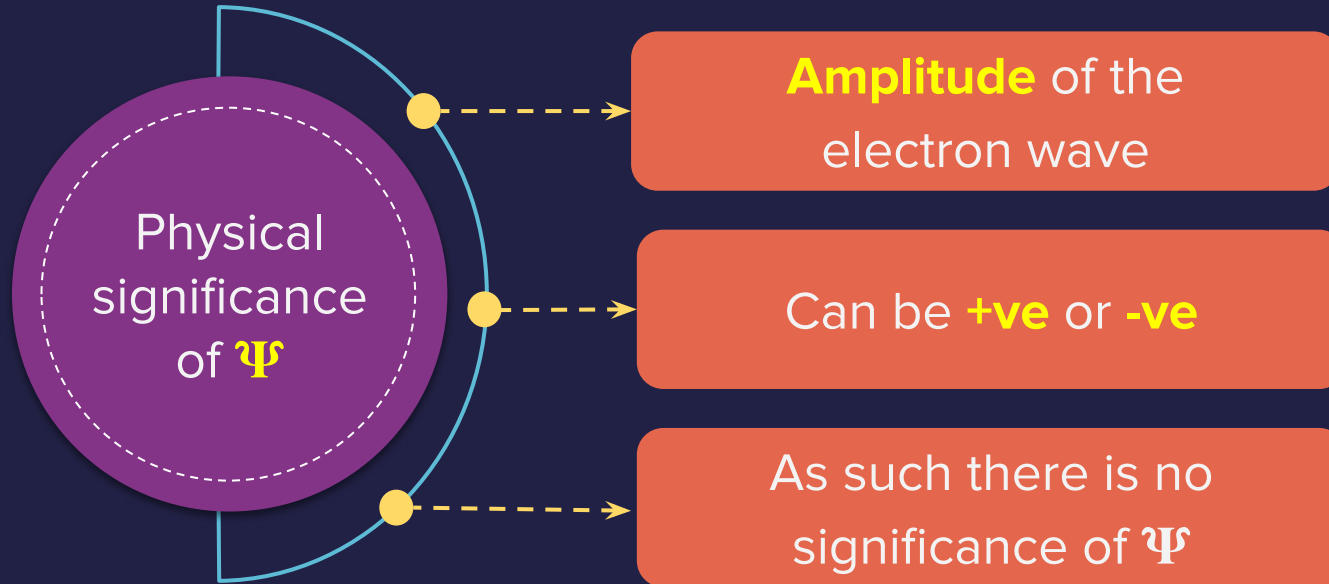
Ψ corresponds to the allowed solutions of SWE

Ψ contains all the information related to the **motion of an electron** in an atom

Amplitude of a standing wave is a function of x

Similarly, Ψ is a **function of coordinates**

Physical Significance of Ψ



Physical significance of Ψ^2

Maxwell's wave theory

Intensity of wave

\propto

Square of amplitude

Max Born suggested that

Ψ^2

Probability of finding an electron per unit volume or
probability density

Nodes

Region where the **probability density** is **zero** i.e.
where the **probability of finding** an **electron** is **zero**

Ψ or Ψ^2

=

0

Nodes





Radial Node

Spherical region
around nucleus

where probability of
finding an electron is
zero

Number of **radial nodes** in an **orbital**

=

$n - l - 1$





Angular Node

Plane or a surface
passing through the
nucleus

where probability of
finding an electron is
zero

Number of **angular nodes** in an **orbital**

=

/



Nodes

Total number
of nodes

=

Radial nodes
($n - l - 1$)

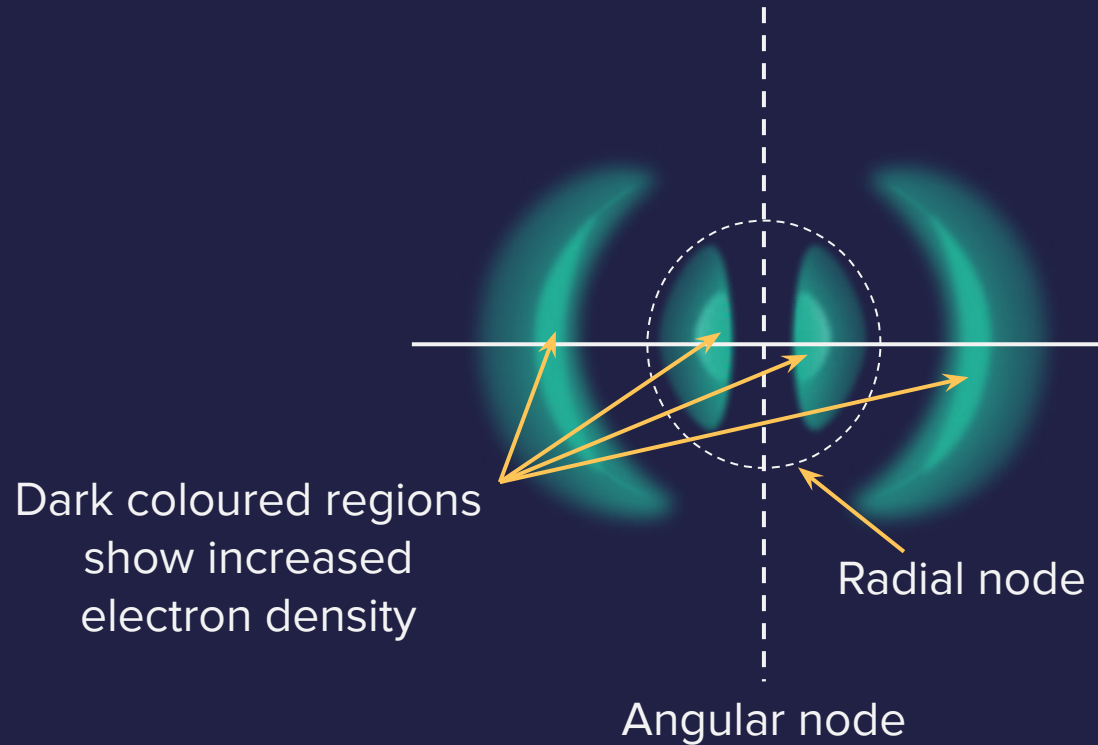
+

Angular nodes
(l)

=

$n - 1$

What are these radial and angular nodes?

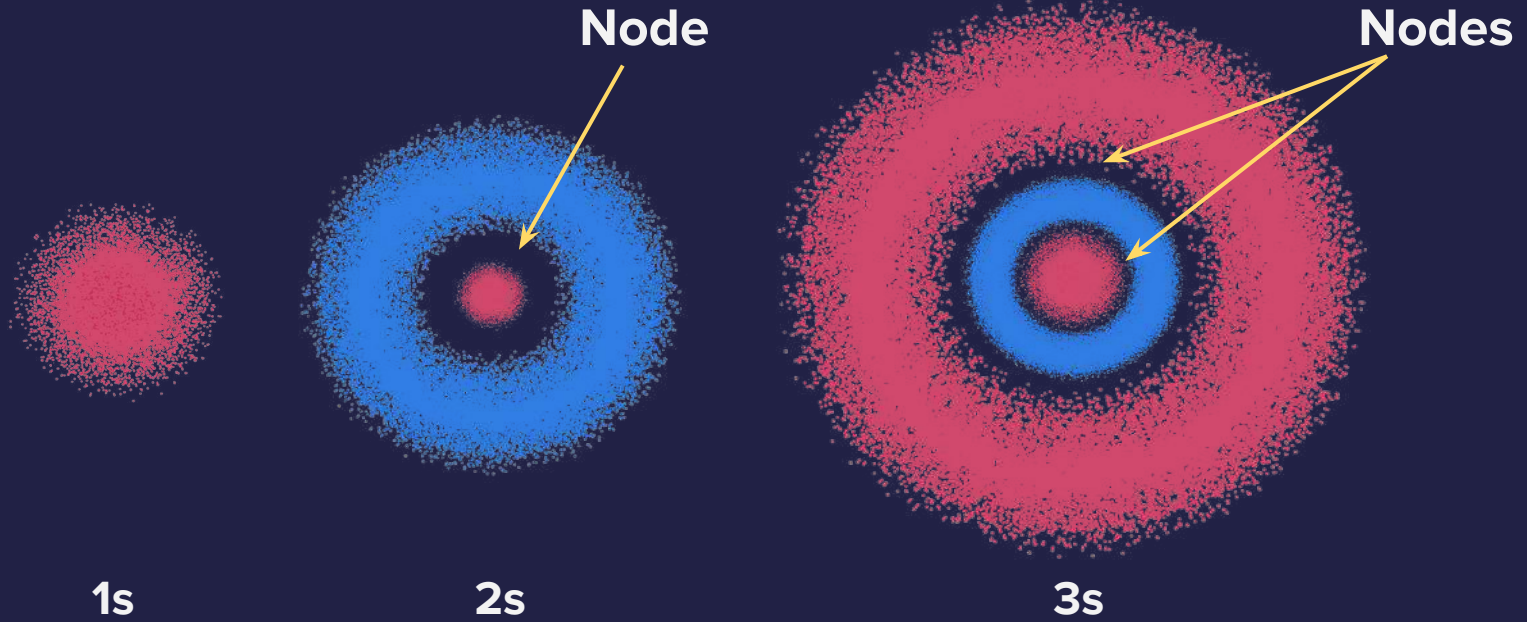




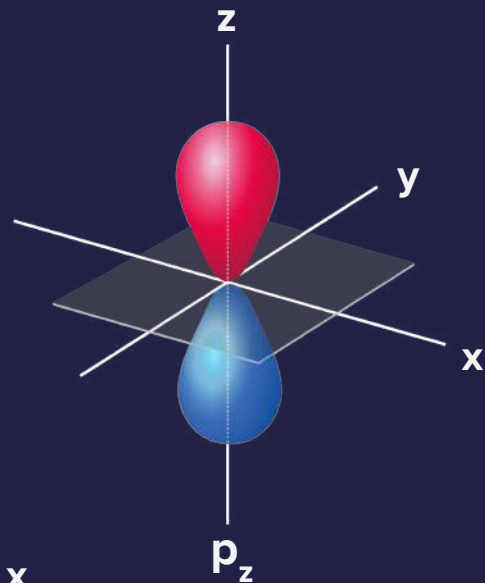
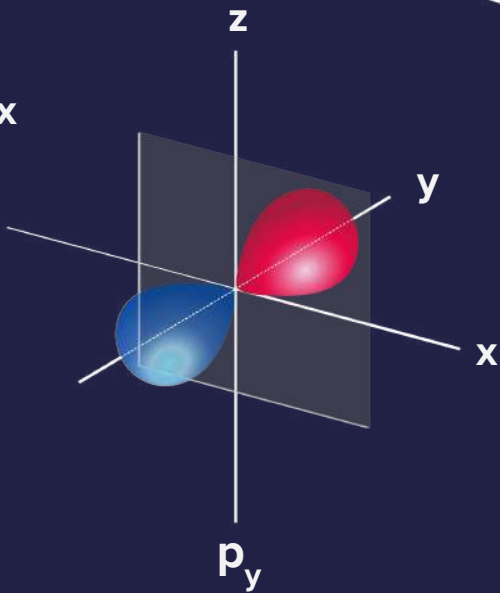
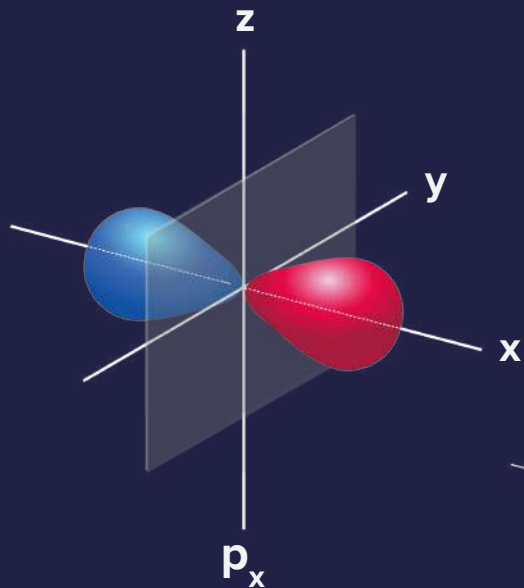
Radial Node vs Angular Node

Radial node	Angular node
Spherical regions where the probability of finding an electron is zero .	Flat planes or cones where the probability of finding an electron is zero .
Have fixed radii .	Have fixed angles .
Number of radial nodes is given by $(n - l - 1)$	Number of angular nodes is given by (l)

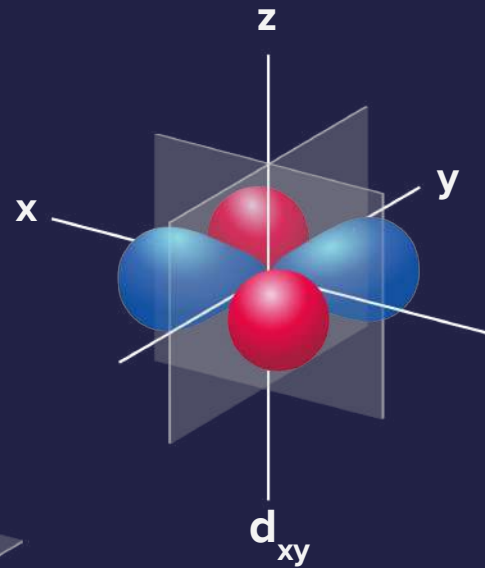
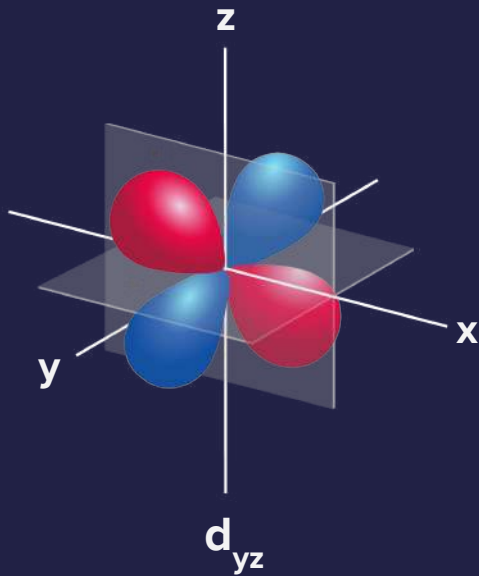
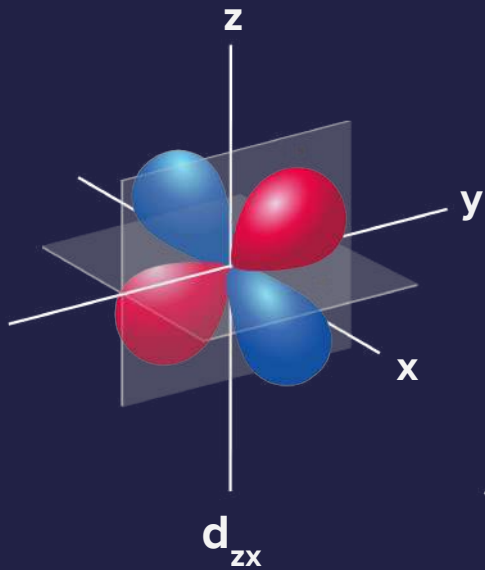
Nodes of 's' orbitals



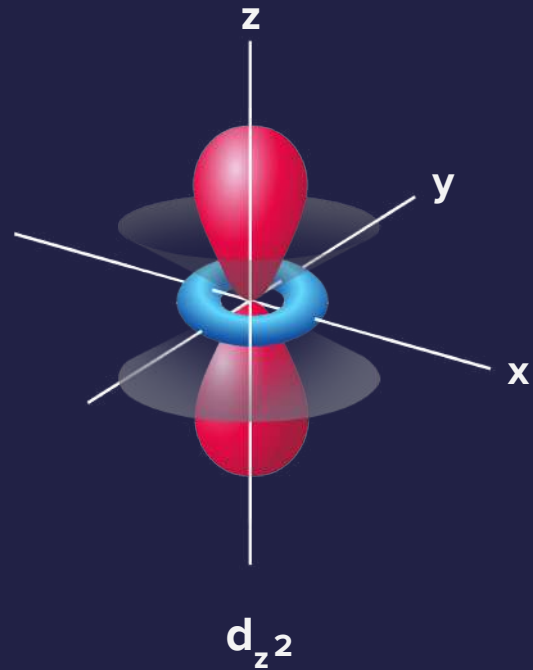
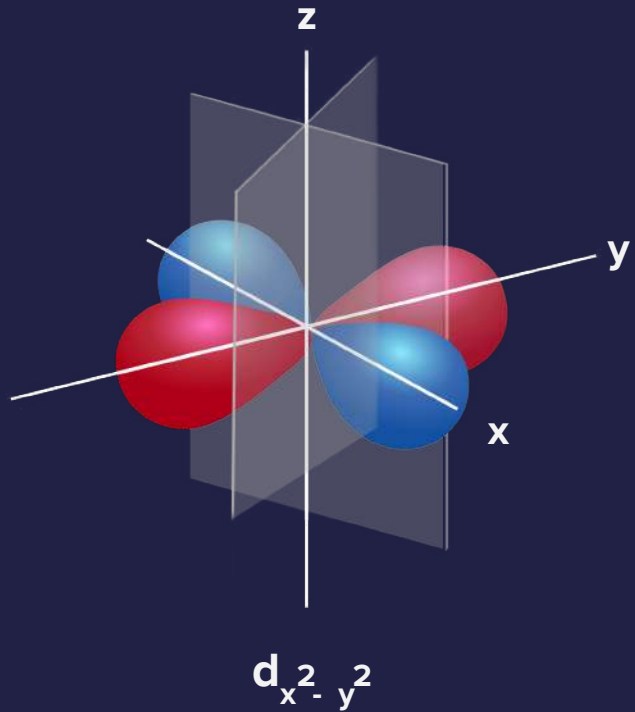
Angular Nodes of 'p' orbitals



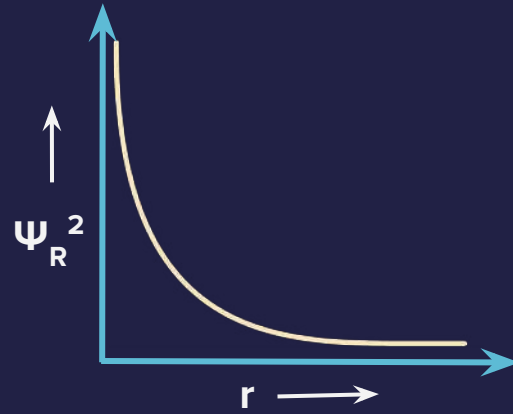
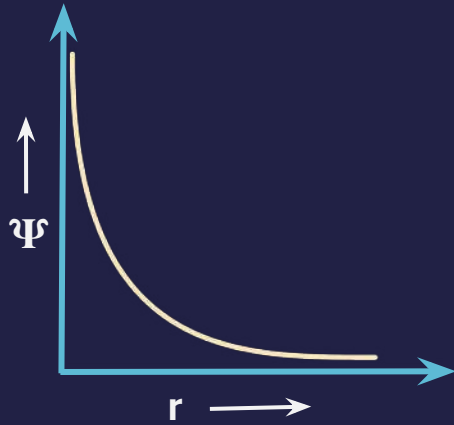
Angular Nodes of 'd' orbitals



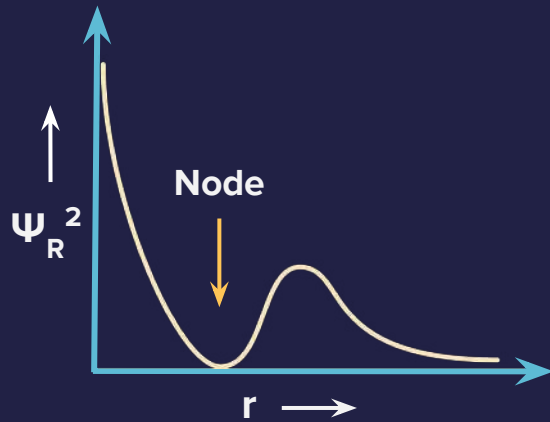
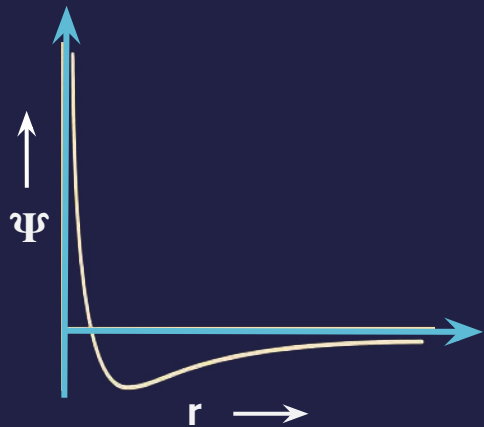
Angular Nodes of 'd' orbitals



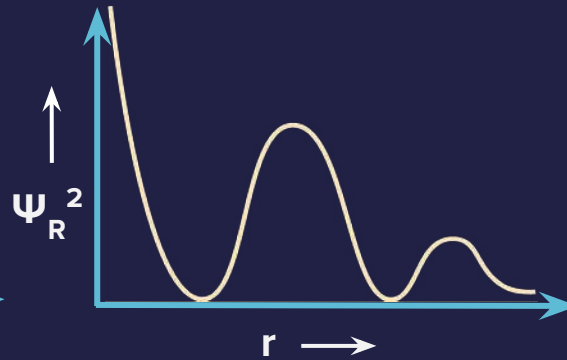
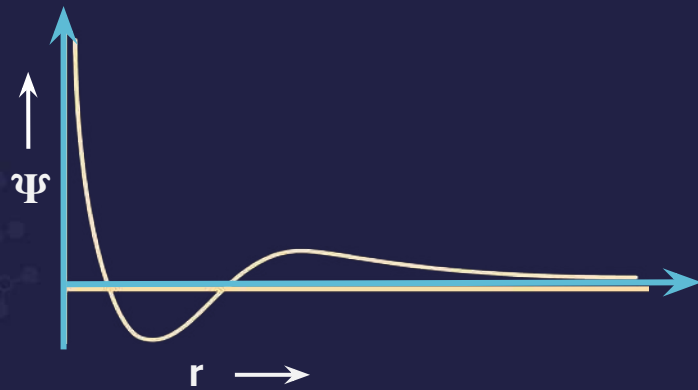
Radial Probability of 1s



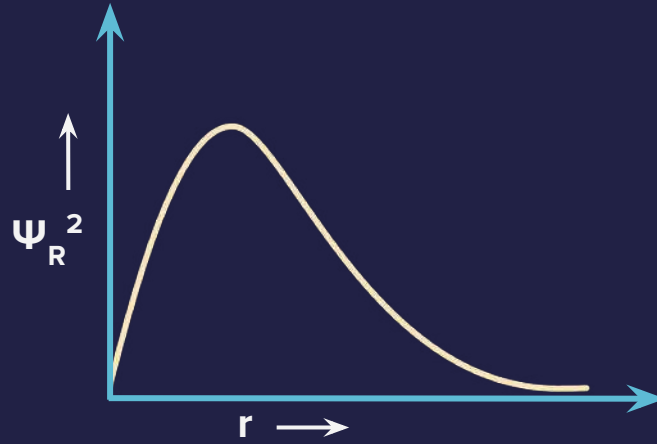
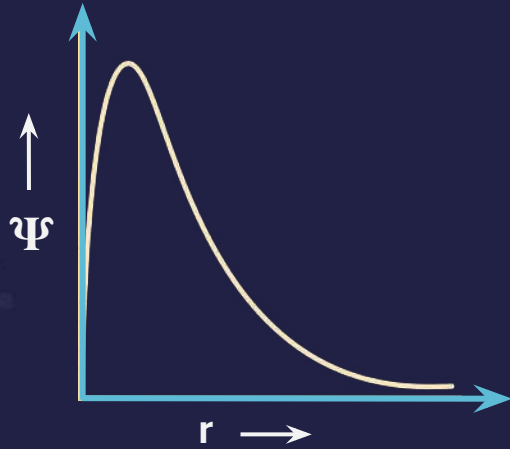
Radial Probability of 2s



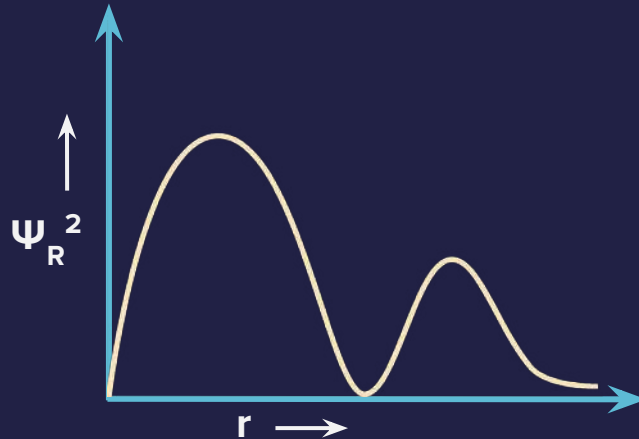
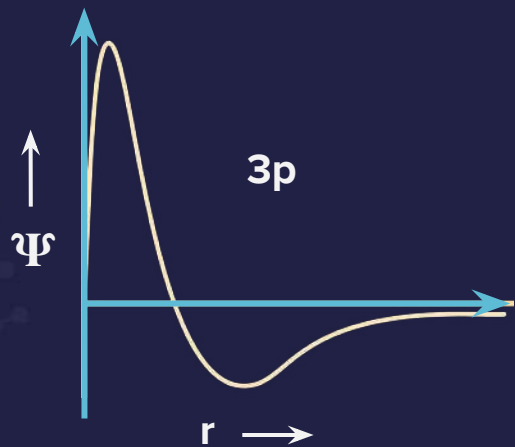
Radial Probability of 3s



Radial Probability of 2p



Radial Probability of 3p



Nodes in p-orbital

