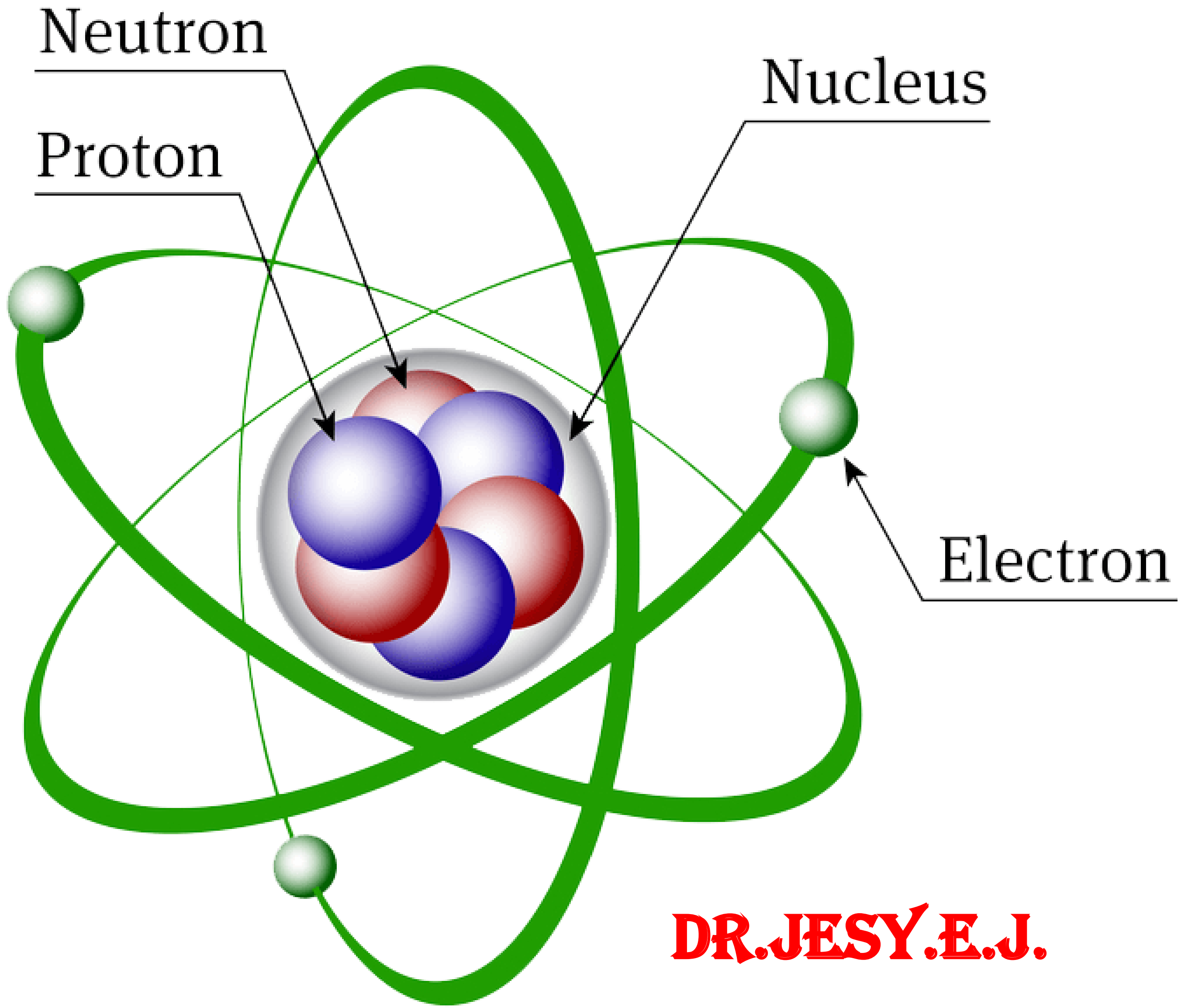

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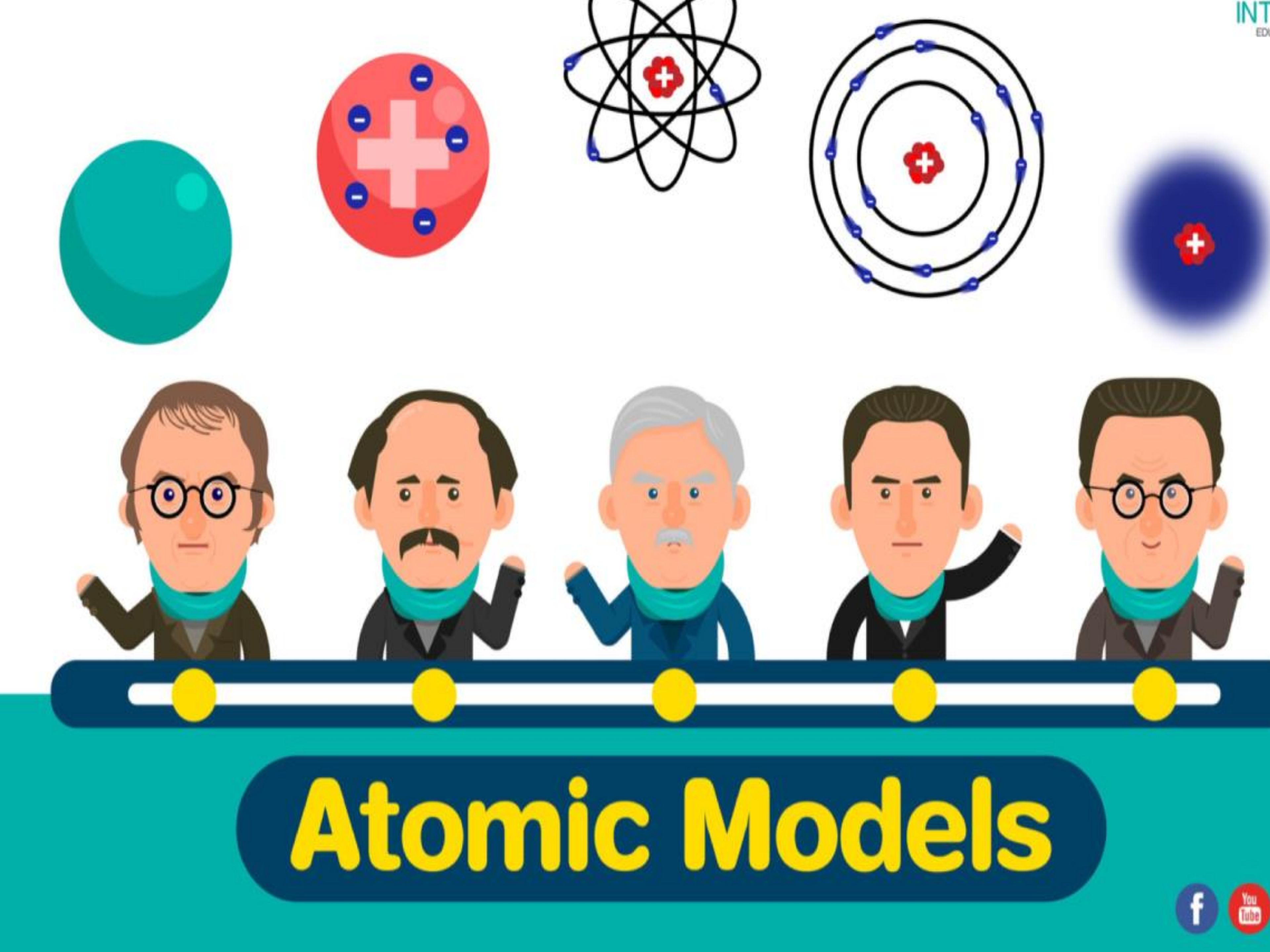
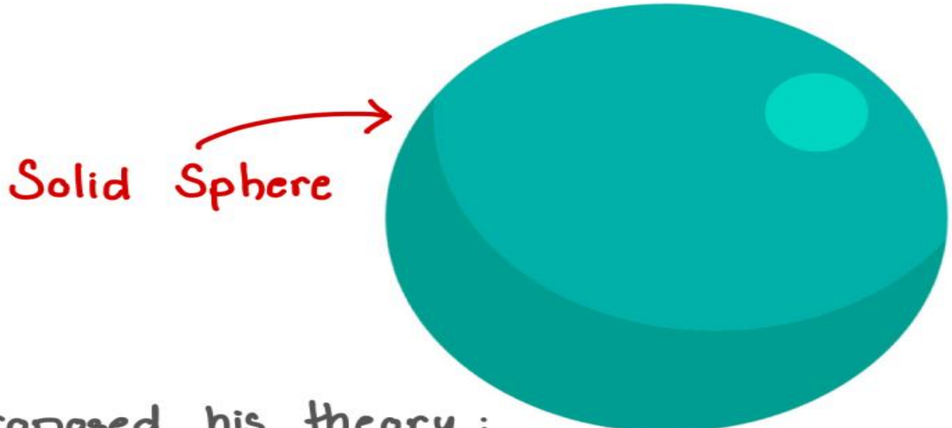

Atomic Models

Atomic Model



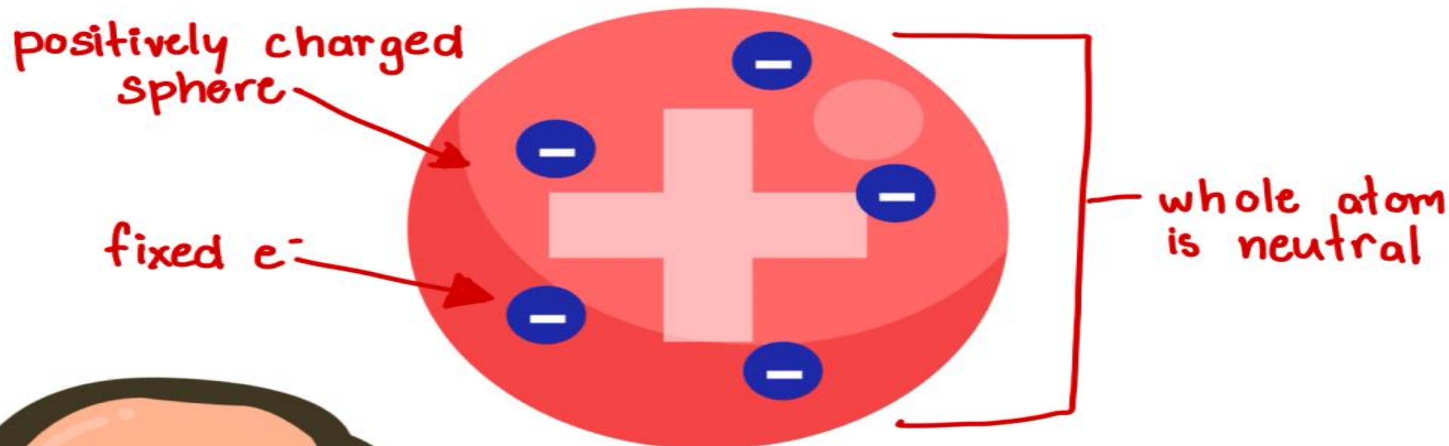
He proposed his theory :

- Atoms are small, indivisible
- Can't be divided, created, destroyed
- An element = identical
- Different elements = different properties
- Atoms of different elements combine to form compounds

John **Dalton**

Plum-Pudding Model

INTLINK EDUCATION

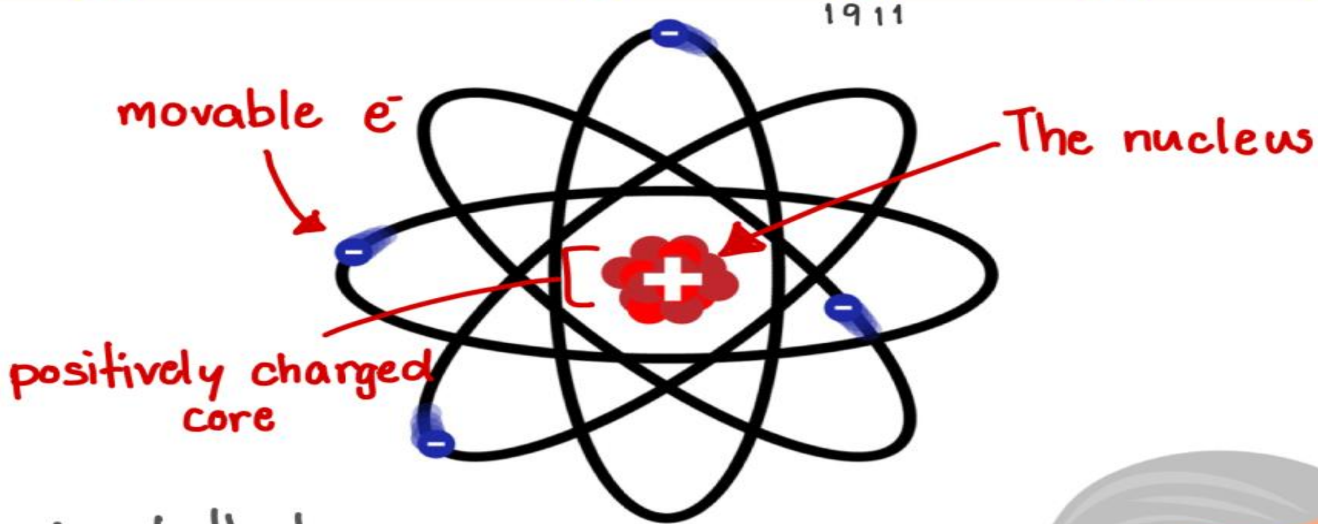


He found that :

- An atom consists of
  - positive charge
  - negative charge
- An atom is electrically neutral
  - ↳ positive = negative
- Negatively charged electrons are fixed in the positive sphere

Joseph John Thomson

Nuclear Model

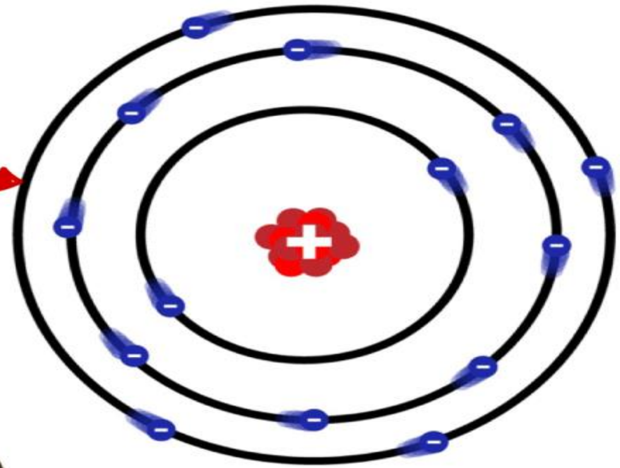


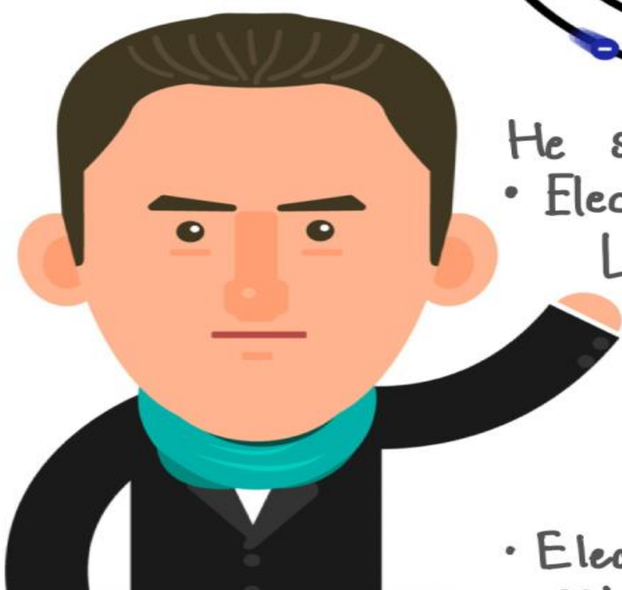
He theorized that :

- Atoms are **mainly empty pace**
- **Positive charge** is concentrated at the center of atom, the **nucleus**
- The center of atom = the nucleus
- Electrons move around the nucleus

Ernest **Rutherford**

Planetary Model





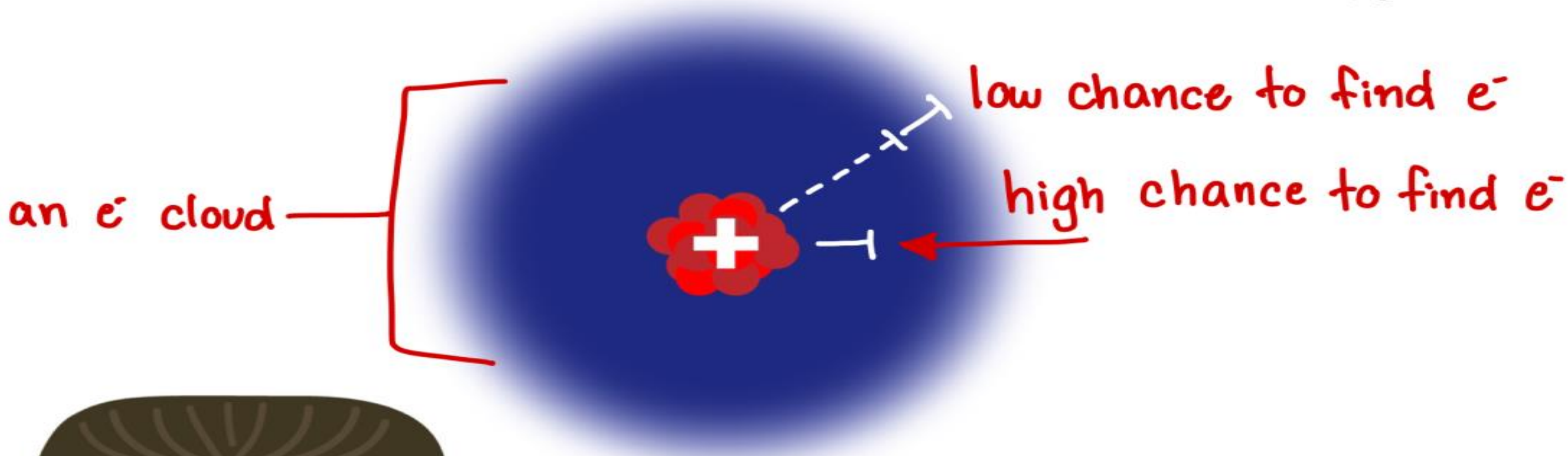
He said that:

- Electrons orbit the nucleus
  - ↳ The orbits have specific size and energy
    - ↳ The energy is related to it size
      - ↳ The lowest energy is found in the smallest orbit
- Electrons can move between each shell when gaining or losing energy

Niels Bohr

Quantum Mechanical Model

1926

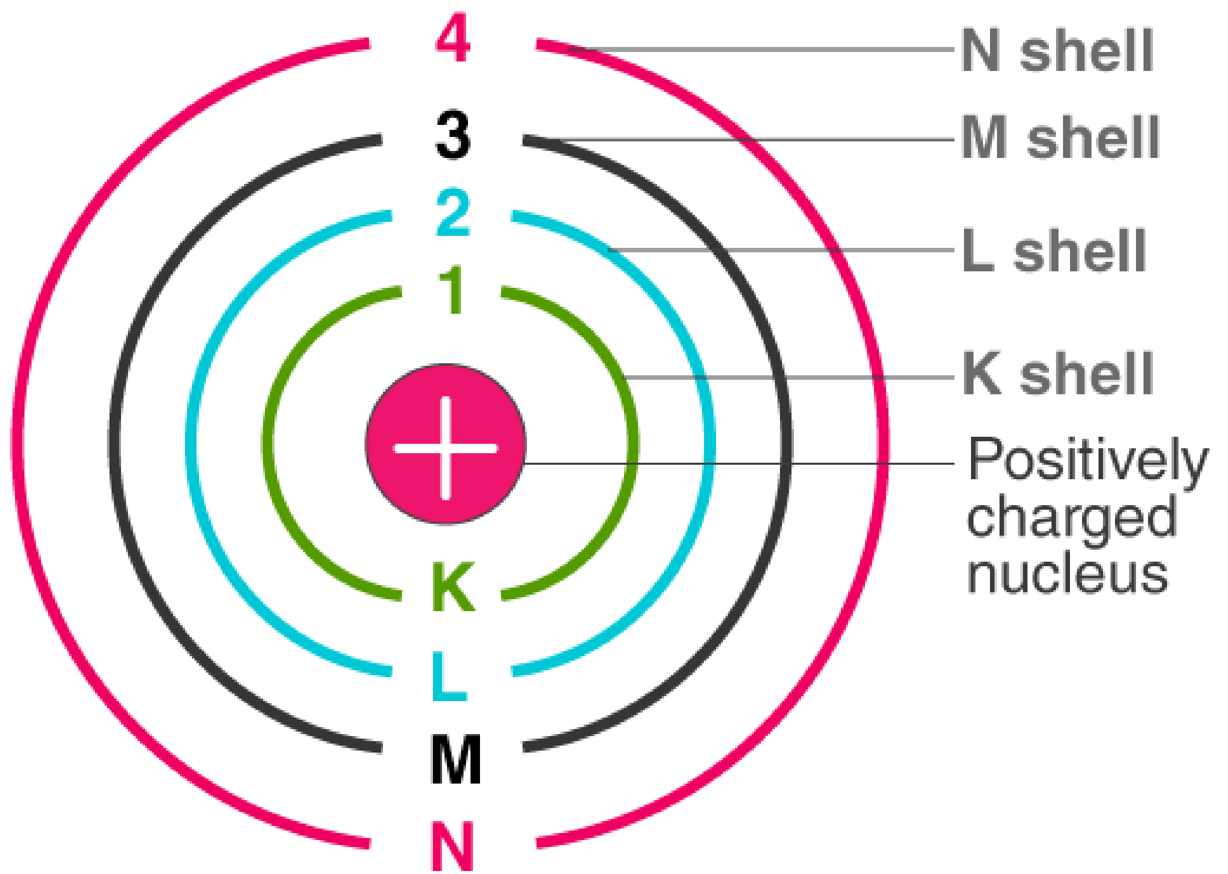


He discovered that:

- Electrons move around the nucleus in 'a cloud' not 'orbits'
- Orbital helps us predict the area where we can find electrons
- The closer position to the nucleus, the higher chance to find electrons

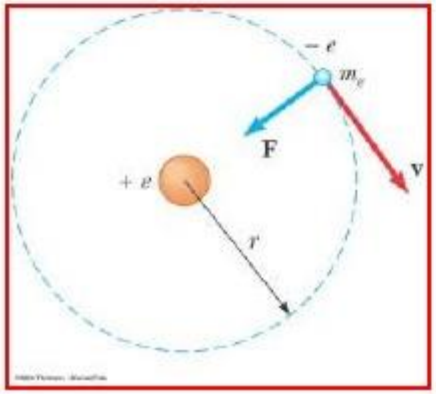
Erwin Schrodinger

BOHR'S MODEL OF AN ATOM



Bohr’s Postulates

- Bohr started from the assumption that the electron moves in circular orbits around the proton under the influence of the attractive electric field.



- **Postulate 1:** Only certain orbits are stable. These are ***stationary*** or more precisely ***quasi-stationary states***. An electron ***does not*** emit EM radiation when in one of these states (orbits)

•Bohr’s Postulates

•**Postulate 2.** The electron can only have an orbit for which the angular momentum of the electron, *L,* takes on discrete values (the orbits are quantized):

$$L = m_e v r = n\hbar$$

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

•Orbits characterized by angular momentum since this depends on both the distance of the electron from nucleus and its velocity

•Bohr's Postulates

• **Postulate 3.** If the electron is initially in an allowed orbit (stationary state), *i*, having the energy, *Ei*, goes into another allowed orbit, *f*, having energy, *Ef* (< *Ei*), EM radiation is emitted, with ***energy*** and ***frequency,***

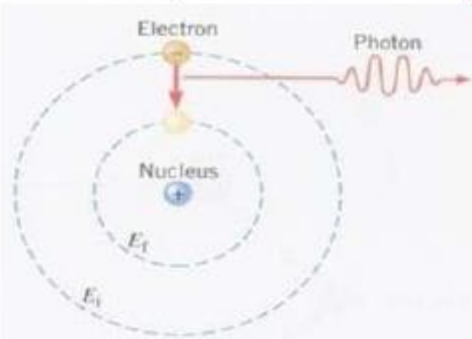
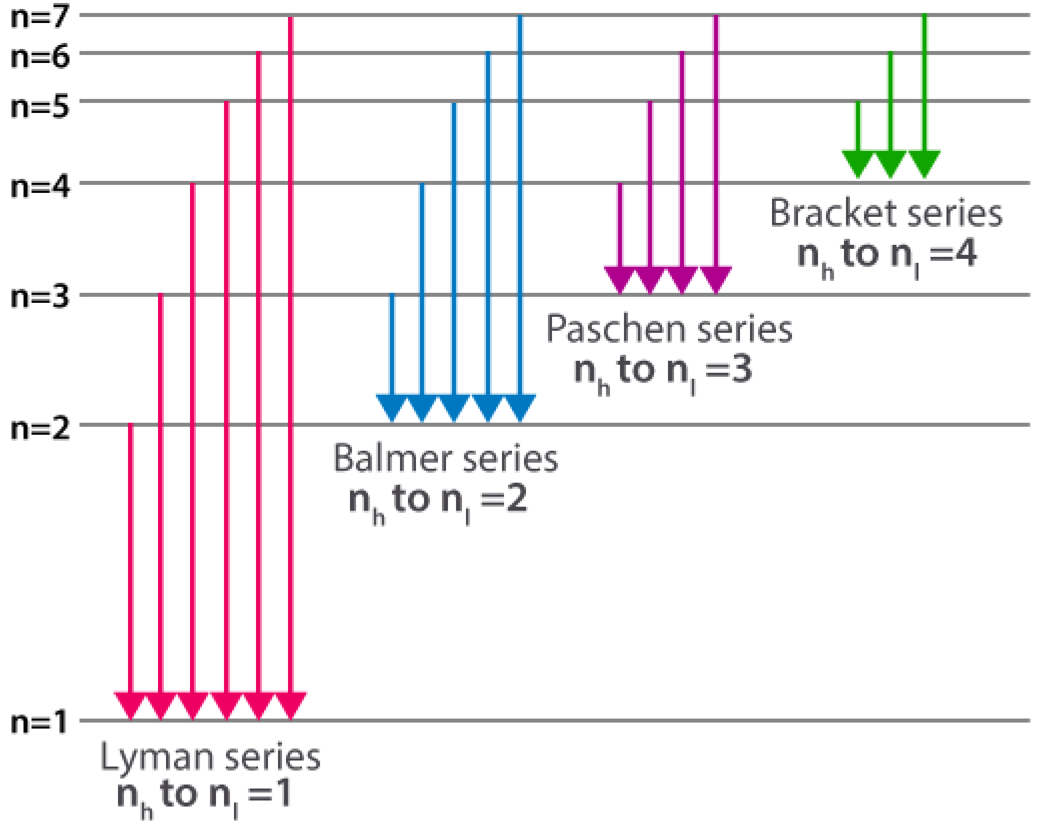


Figure 30.5 In the Bohr model, a photon is emitted when the electron drops from a larger, higher-energy orbit (energy = E_i) to a smaller, lower-energy orbit (energy = E_f).

$$h\nu = E_i - E_f$$

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

ELECTRON TRANSITIONS FOR THE HYDROGEN ATOM



spectral lines for hydrogen

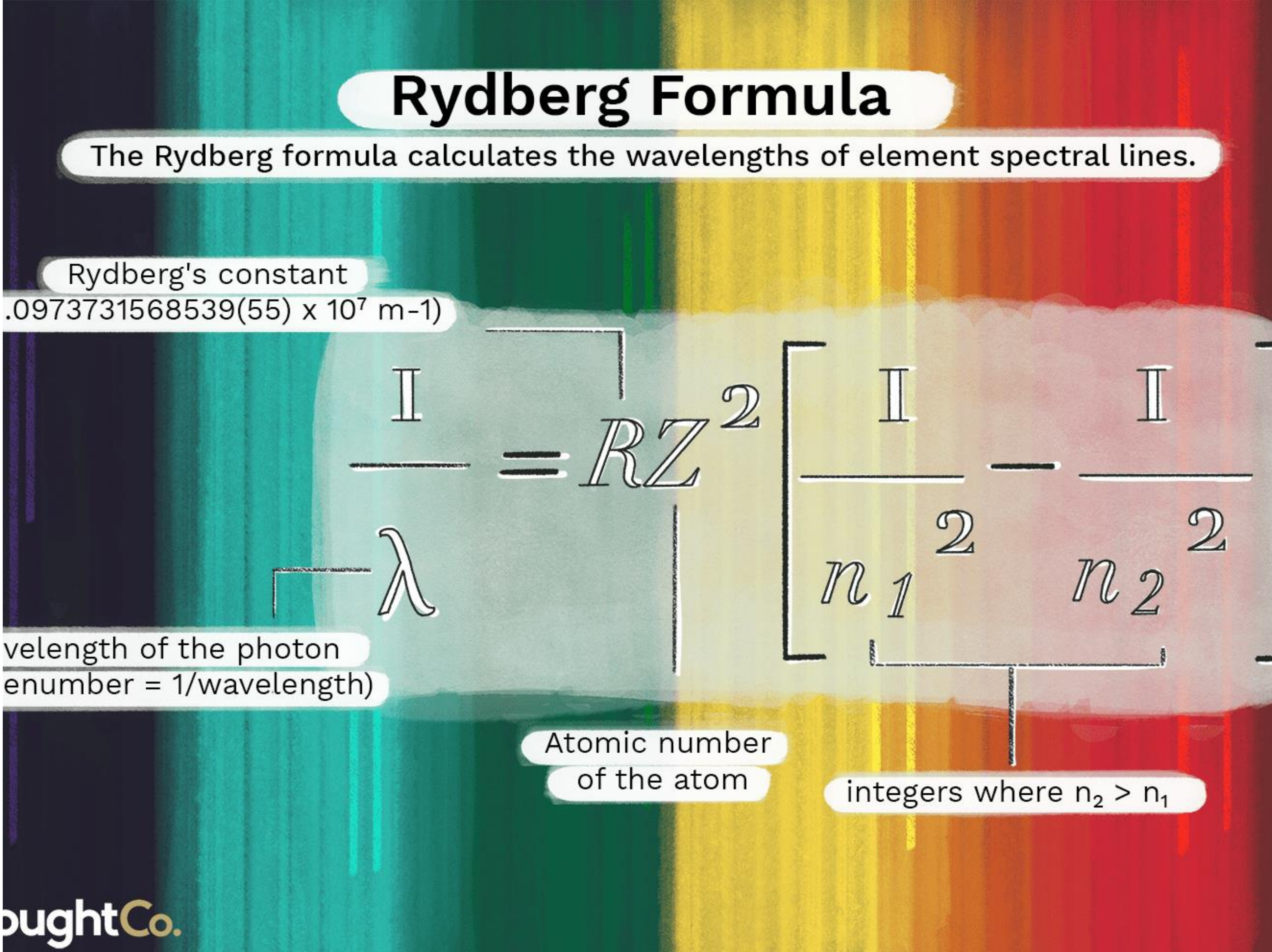
series	n_1	n_2	*spectral region*
Lyman	1	2, 3..	*UV*
Balmer	2	3, 4..	*Visible*
Paschen	3	4, 5..	*IR*
Brackett	4	5, 6..	*IR*
Pfund	5	6, 7..	*IR*

Hydrogen Spectral Lines

Bohr calculated the energy, frequency and wave number of the spectral emission lines for hydrogen atom.

$$\bar{\upsilon} = R\left[\frac{1}{n_1^2} - \frac{1}{n_2^2}\right]$$

The wave number of different spectral lines can be calculated corresponding the values of n_1 and n_2.


Rydberg Formula
The Rydberg formula calculates the wavelengths of element spectral lines.
Rydberg's constant
.0973731568539(55) x 10^7 m-1)
$\frac{1}{\lambda} = RZ^2 \left[\frac{1}{n_1^2} - \frac{1}{n_2^2} \right]$
velength of the photon
enumber = 1/wavelength)
Atomic number
of the atom
integers where $n_2 > n_1$
oughtCo.

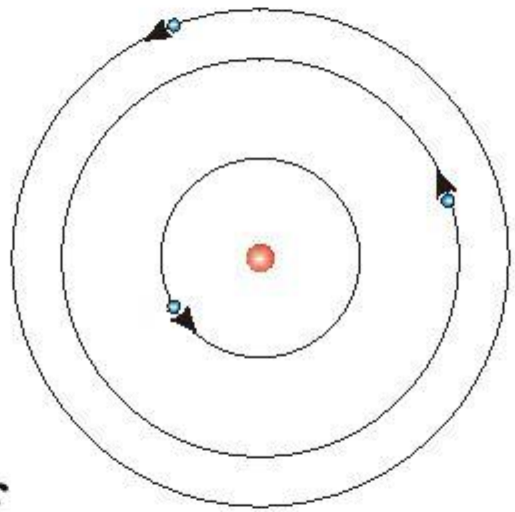
Limitations of the Bohr Model

a. Model could not calculate the wavelengths of observed spectra of multi-electron atoms.

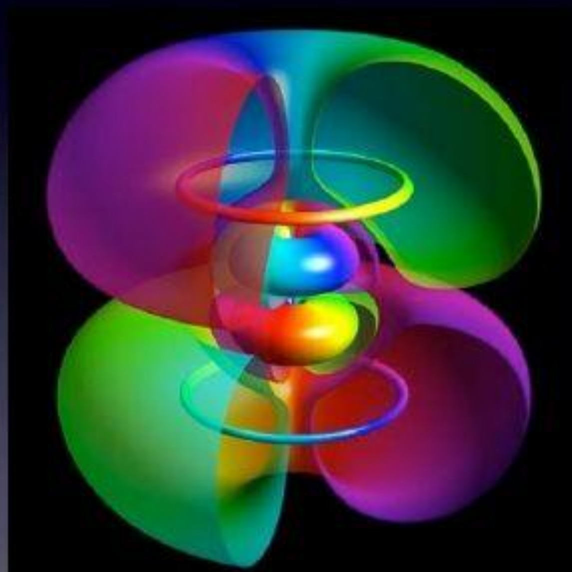
b. Model could not explain the chemical behavior of atoms.

c. Bohr used classical mechanics to understand the behaviors of small particles.

d. The Bohr model is also known as the planetary, solar system, or satellite model.



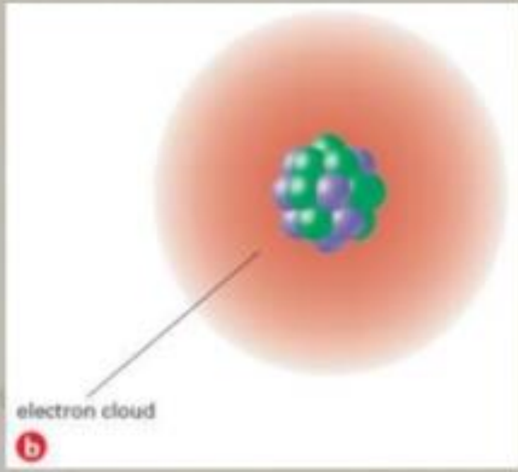
Quantum Mechanical Model



- The quantum mechanical model is the most advanced and accurate model of the atom, used today by chemists and physicists
- In this model, electrons do not exist as tiny points inside the atom, but instead surround the nucleus in a form resembling a cloud

The Quantum Mechanical Model

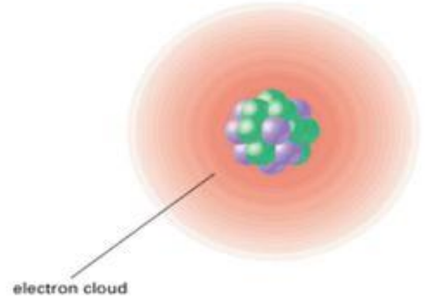
- The probability of finding an electron within a certain volume of space surrounding the nucleus can be represented as a fuzzy cloud.
  - The cloud is more dense where the probability of finding the electron is high.



Quantum Mechanical Model

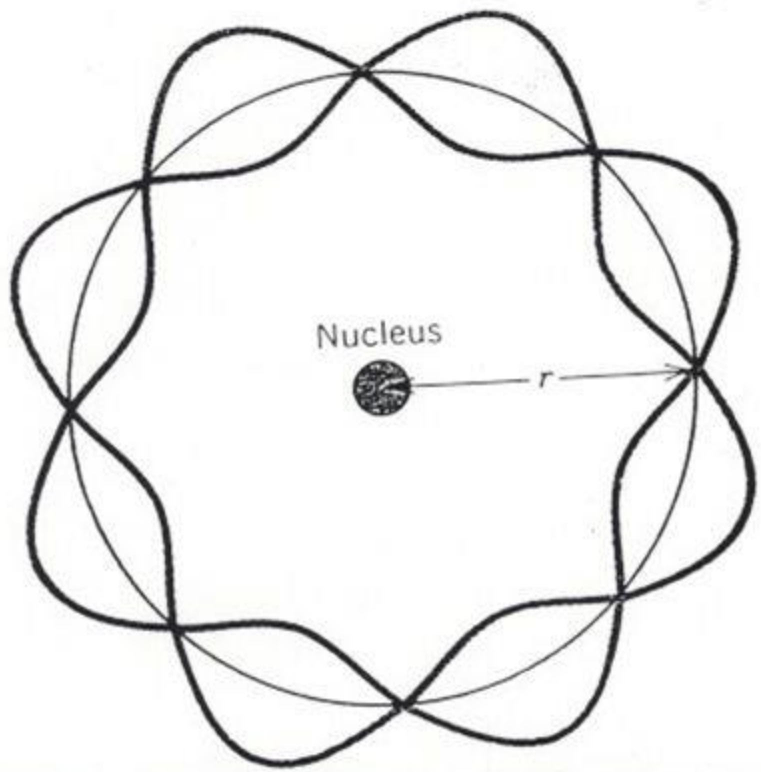
- In 1926, **Erwin Schrodinger** derived an equation that described the energy and position of the electrons in an atom.
  - e^- are not found in specific orbitals. Electrons are in a 'cloud'.

$$-\frac{h^2}{8\pi^2 m}\frac{d^2\psi}{dx^2} + V\psi = E\psi$$



Equation for the probability of a single electron being found along a single axis (x-axis)

de Broglie and Wave Model



- An electron in its path is associated with a wavelength.
- The wavelength depends on the mass:

De Broglie's Equation

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

Where

λ = wavelength in meters

v = the velocity in meters/sec

m = the mass in kilograms

h = Plancks's constant in J/Hz

de Broglie wavelength in terms of KE

Consider a particle of mass *m* moving with a velocity *v*

Kinetic Energy of the particle

$$E = \frac{1}{2}mv^2 = \frac{1}{2m}m^2v^2 = \frac{p^2}{2m}$$

$$E = \frac{p^2}{2m} \Rightarrow p^2 = 2mE \Rightarrow p = \sqrt{2mE}$$

de Broglie wavelength

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

de Broglie wavelength in terms of KE

$$\lambda = \frac{h}{\sqrt{2mE}}$$

What is the de Broglie wavelength of a proton whose kinetic energy is 2.0 MeV? $\lambda = ?$

de Broglie Wavelength

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

KE = 2.0 MeV

$$\lambda = \frac{\left(6.626\times10^{-34}\ \frac{m^2kg}{s}\right)}{\sqrt{2(1.67\times10^{-27}\ kg)(2.0\ MeV)}} = \boxed{20\ fm}$$

$(2.0\times10^{6} \times 1.602\times10^{-19})\ J$

Planck's Constant

$$h = 6.626\times10^{-34}\ \frac{m^2kg}{s} \qquad 1eV = 1.602\times10^{-19}\ J$$

$$p = mv \qquad KE = \frac{1}{2}mv^2 \Rightarrow v = \sqrt{\frac{2KE}{m}} \qquad m_p = 1.67\times10^{-27}\ kg$$

Einstein's equation: $\mathrm{E} = mc^2$

Planck's equation: $\mathrm{E} = hf$

Equating both, we get

$$mc^2 = hf$$

We know that $f = \dfrac{c}{\lambda}$

$$mc^2 = \frac{hc}{\lambda}$$

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

or, $$\lambda = \frac{h}{mc}$$

For macroscopic objects, velocity "v" can replace speed of light "c"

Thus our equation becomes:

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

Now, $mv = p$ (momentum of particle) and therefore,

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

Problem 2.14

Calculate the mass of a photon with wavelength 3.6 Å.

Solution

$\lambda = 3.6 \text{ Å} = 3.6 \times 10^{-10}$ m

Velocity of photon = velocity of light

$$m = \frac{h}{\lambda \nu} = \frac{6.626 \times 10^{-34} \text{ Js}}{(3.6 \times 10^{-10} \text{ m})(3 \times 10^{8} \text{ m s}^{-1})}$$

$= 6.135 \times 10^{-29}$ kg

Heisenberg's Uncertainty Principle

uncertainty in momentum

$$\Delta x \Delta p \geq \frac{h}{4\pi} = \frac{\hbar}{2}$$

uncertainty in position

The more accurately you know the position (i.e., the smaller Δx is), the less accurately you know the momentum (i.e., the larger Δp is); and vice versa

Uncertainty Principle $\Delta x \times \Delta v \geq \frac{h}{4\pi}\left(\frac{1}{m}\right)$

- Heisenberg stated that the product of the uncertainties in both the position and speed of a particle was inversely proportional to its mass
  - ✓ x = position, Δx = uncertainty in position
  - ✓ v = velocity, Δv = uncertainty in velocity
  - ✓ m = mass
- the means that the more accurately you know the position of a small particle, like an electron, the less you know about its speed
  - ✓ and visa-versa

$$\Delta x \times \Delta P_x \geq \frac{h}{4\pi}$$

or $$\Delta x \times \Delta (mv_x) \geq \frac{h}{4\pi}$$

or $$\Delta x \times \Delta v_x \geq \frac{h}{4\pi m}$$

Example: Uncertainty Principle

An electron is confined to a region of width 5.00×10^{-11} m, which is its uncertainty in position Δx. Estimate the minimum uncertainty in its momentum.

$$\Delta x \, \Delta p_x \geq h$$

so

$$\Delta p_x \geq \frac{h}{\Delta x} = \frac{6.626 \times 10^{-34}\ \mathrm{J\ s}}{5.00 \times 10^{-11}\ \mathrm{m}} = 1.33 \times 10^{-23}\ \mathrm{kg\ m\ s^{-1}}$$

Schrödinger Equation

$$\frac{d^2\Psi}{dx^2}+\frac{8\pi^2 m}{h^2}(E-V)\Psi=0$$

- Schrödinger Equation 1926
- $\psi(x,t)$ is a solution of this equation
- the wave equation for matter waves

Second derivative with respect to X

Shrodinger Wave Function

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{8\pi^2 m}{h^2}(E - V)\psi = 0$$

Position

Energy

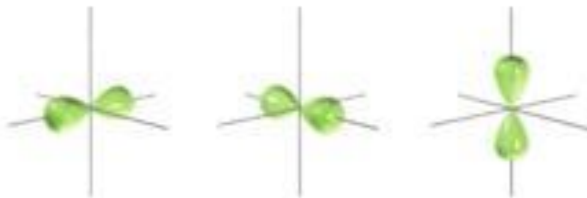
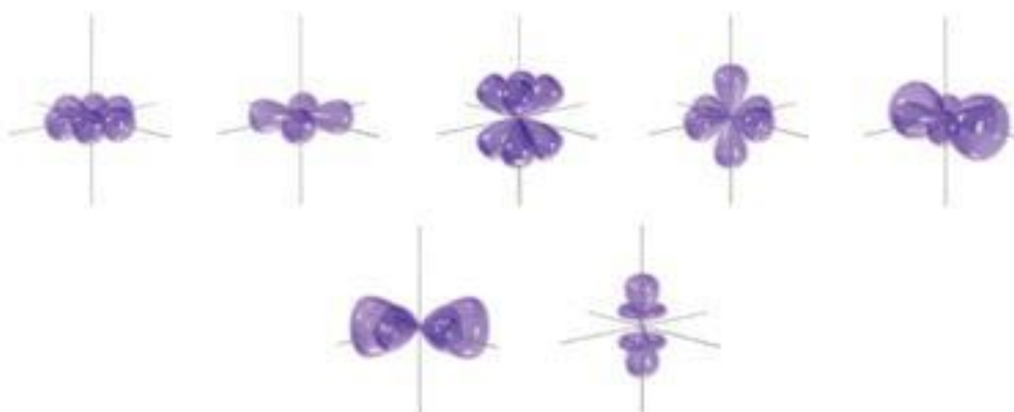
Potential Energy

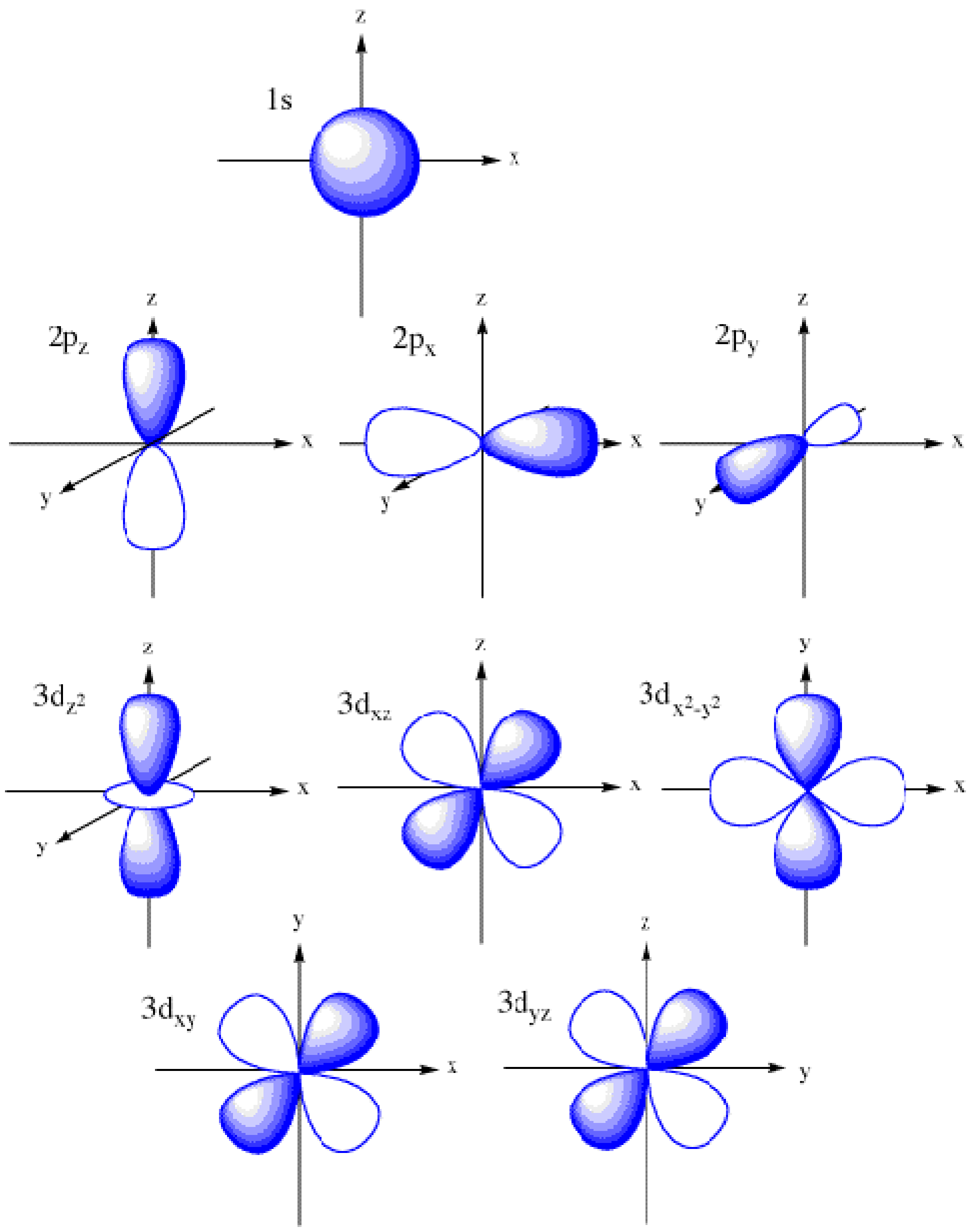
Concept of Orbit & Orbital

- An **orbit** is a circular path followed by an electron around the nucleus.
- An **atomic orbital** is a mathematical function that describes the wave-like behavior of either one electron or a pair of electrons in an atom. This function can be used to calculate the probability of finding any electron of an atom in any specific region around the atom's nucleus. The term may also refer to the physical region or space where the electron can be calculated to be present.

Table 5.1

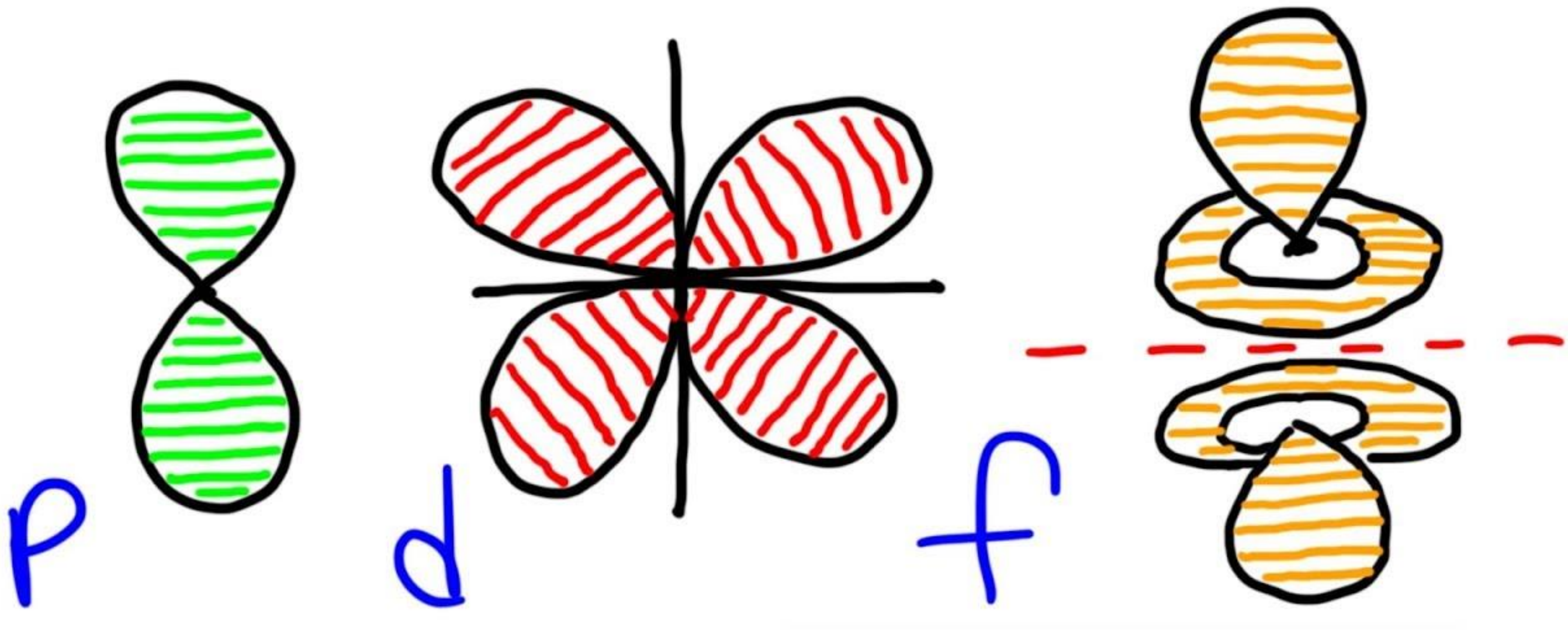
The First Four Atomic Orbitals: *s, p, d, f*

Orbital Type	Spatial Orientations
s The *s* orbital has only one shape, which is spherical.	
p There are three *p* orbitals. They differ by orientation.	
d There are five *d* orbitals.	
f There are seven *f* orbitals.	


1s
2p z
2p x
2p y
3d z2
3d xz
3d x2-y2
3d xy
3d yz
x
y
z

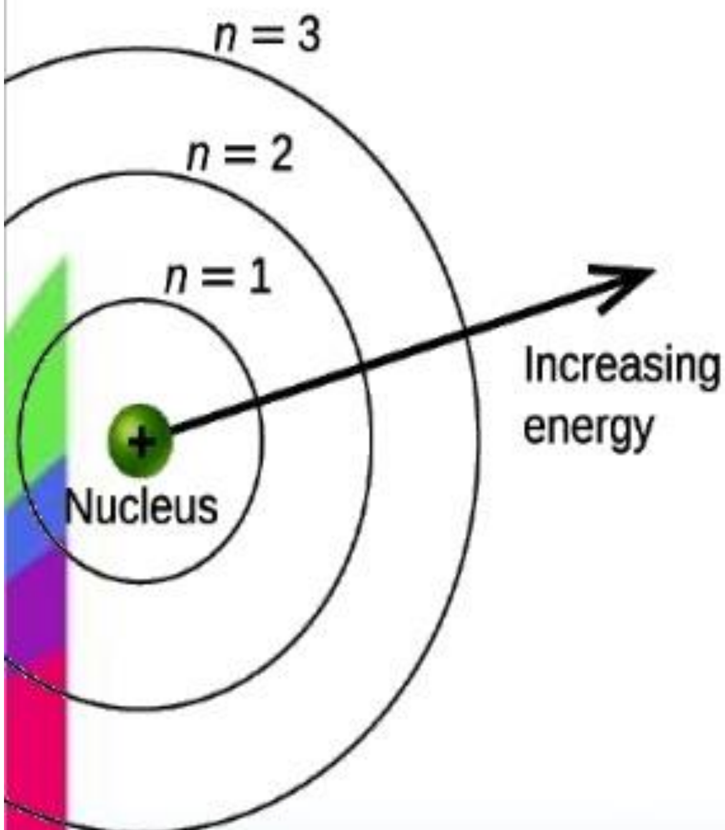
ORBIT	ORBITAL
It is well-defined circular path followed by electron around nucleus.	It is a region of space around the nucleus where the probability of finding an electron is maximum.
It represents two dimensional motion of electron around nucleus.	It represents three dimensional motion of electron around nucleus.
The maximum no. of electrons in an orbit is $2n^2$.	The maximum no. of electrons in an orbital is 2.
Orbit is circular in shape.	Orbitals have different shapes.

Quantum Numbers



Name	Symbol	Allowed Values	Property
Principal	n	positive integers 1,2,3…	Orbital size and energy level
Secondary (Angular momentum)	*l*	Integers from 0 to (n-1)	Orbital shape (sublevels/subshells)
Magnetic	m_l	Integers –*l* to +*l*	Orbital orientation
Spin	m_s	+½ or –½	Electron spin Direction

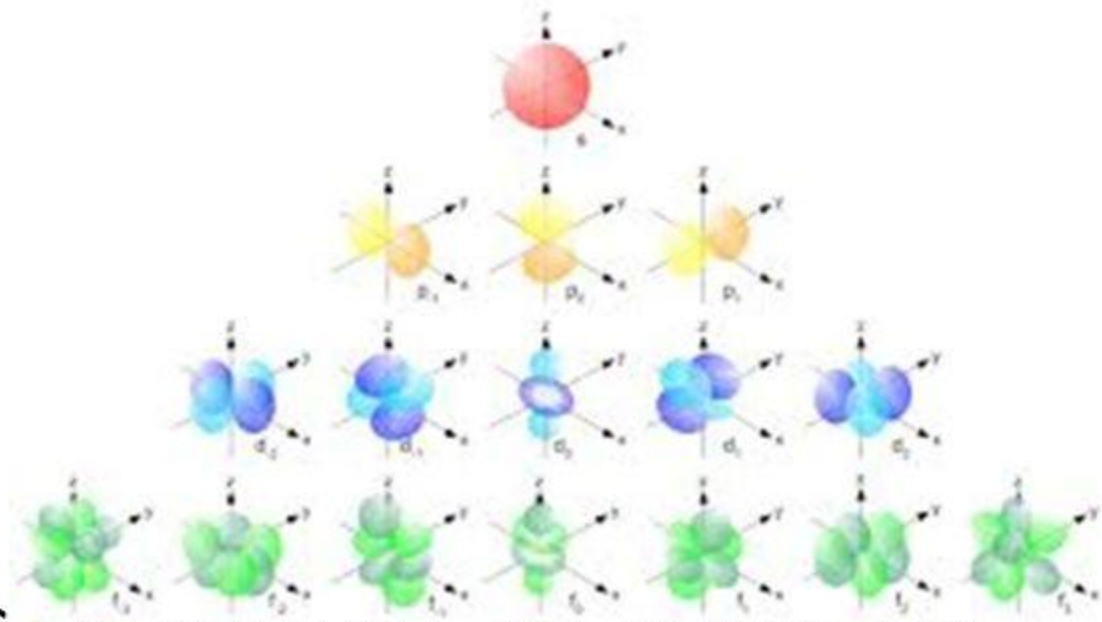
Principal Quantum Number (n)



- Size & Energy of an orbit/shell
- n=1, 2, 3, 4,....
- Greater value of n represents Bigger orbits with high energies
- Distance from the nucleus also increases.

Angular Momentum Quantum Numbers

- Definition: indicates the shape of the orbital
- Symbol: l
- Values:
  - 0 = s
  - 1 = p
  - 2 = d
  - 3 = f

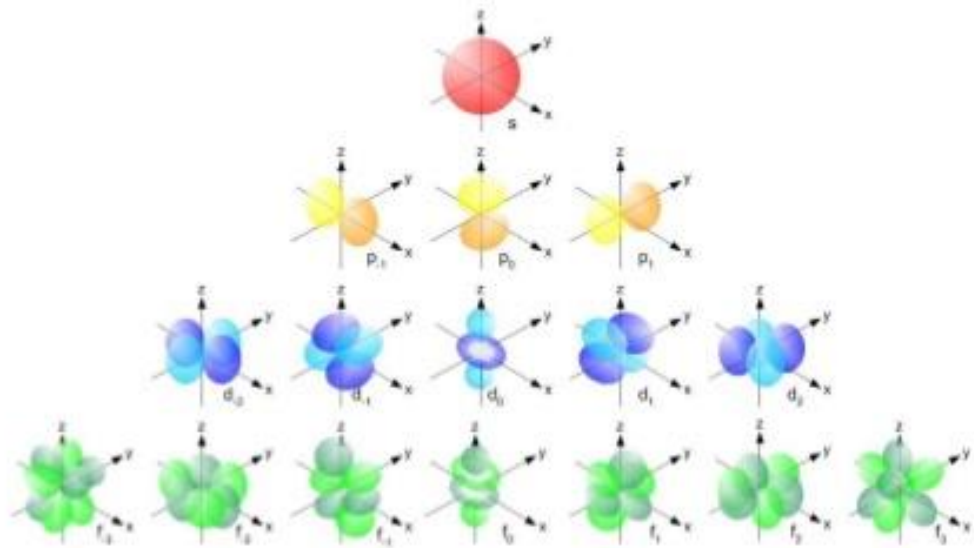


- For a specific energy level, the number of orbital shapes available is equal to n -1

The Magnetic Quantum Number (m_l)

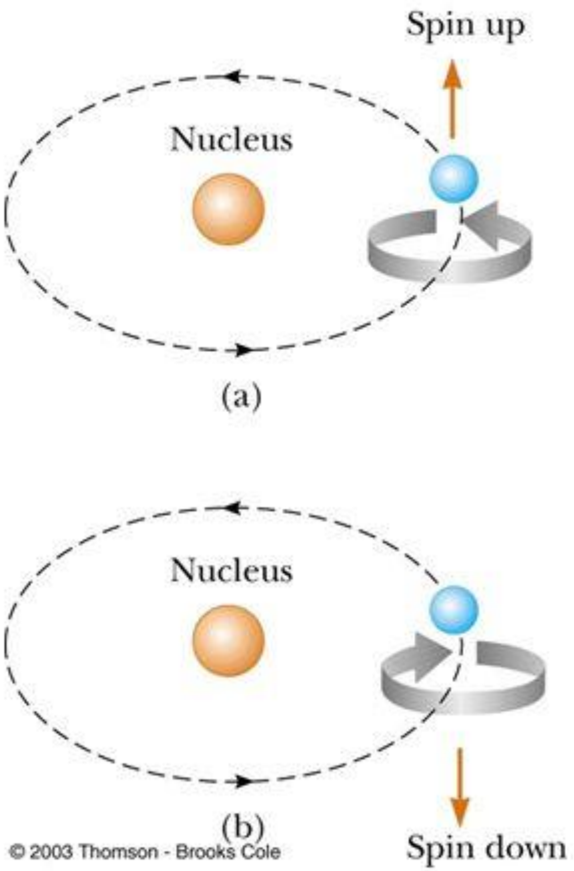
- Gives the exact *orbital*
- Describes the **orientation** of an atomic orbital in space (how it lines up on the xyz plane)
- m_l can have integer values from $-l$ to $+l$ including 0
- The Zeemen effect showed that if a gas discharge tube was placed near a strong magnet some single lines in the spectrum split into new lines that were not initially present

l	m_l
0	0
1	-1, 0, +1
2	-2, -1, 0, +1, +2
3	-3, -2, -1, 0, +1, +2, +3



Spin Magnetic Quantum Number

- It is convenient to think of the electron as spinning on its axis
  - The electron is *not* physically spinning
- There are two directions for the spin
  - Spin up, $m_s = ½$
  - Spin down, $m_s = -½$
- There is a slight energy difference between the two spins and this accounts for the doublet in some lines



Summary: Quantum Numbers

The three quantum numbers:

- n Principal quantum number
- ℓ Orbital angular momentum quantum number
- m_ℓ Magnetic quantum number

The boundary conditions wavefunctions go to zero at x goes to infinity result in :

- $n = 1, 2, 3, 4, \ldots$ Integer
- $\ell = 0, 1, 2, 3, \ldots, n - 1$ Integer
- $m_\ell = -\ell, -\ell + 1, \ldots, 0, 1, \ldots, \ell - 1, \ell$ Integer

The restrictions for quantum numbers:

- $n > 0$
- $\ell < n$, $\ell_{max} = n-1$
- $|m_\ell| \leq \ell$