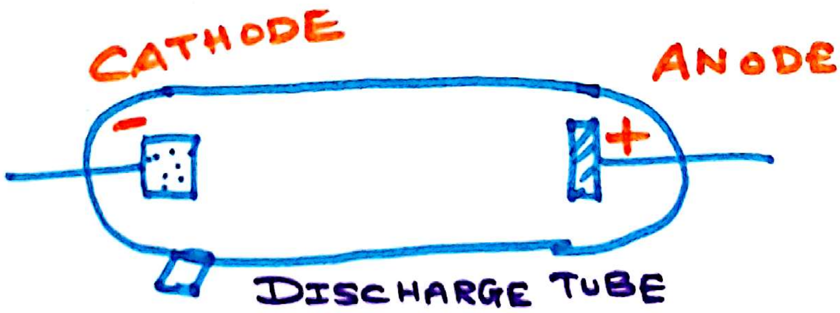
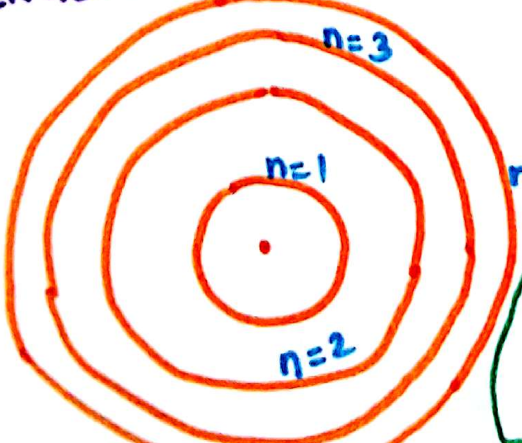
ATOMIC SPECTRA

- SIMPLEST ATOM: HYDROGEN ATOM
- HOW DO WE OBTAIN THE LINE SPECTRA OF HYDROGEN ATOMS?
  - → H_2 MOLECULE
  - → H_2O
  - → CH_4, C_2H_6, ...
- DISSOCIATION OF H_2 MOLECULE

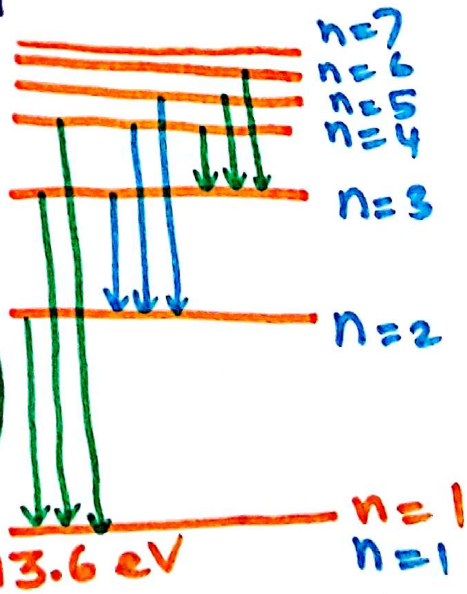


- BOHR'S MODEL OF THE HYDROGEN ATOM

FINGER PRINT OF HYDROGEN



$$\boxed{E_n = \frac{-R}{n^2}}$$



R → RYDBERG CONSTANT
R = 13.6 eV

n=1 ⇒ LYMAN (ULTRAVIOLET)
n=2 ⇒ BALMER (VISIBLE)
n=3 ⇒ PASCHEN (NEAR INFRARED)
n=4 ⇒ BRACKETT (FAR IR)
n=5 ⇒ PFUND (FAR IR)

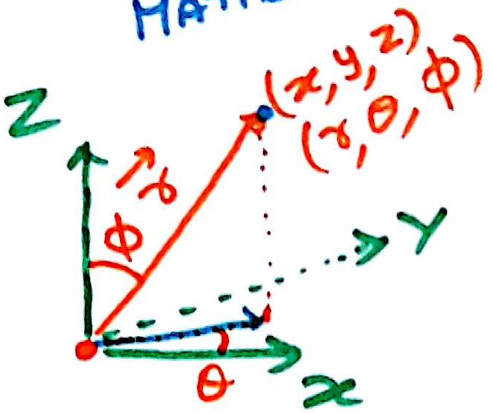
Quantum Mechanics of Hydrogen Atom

MATHS

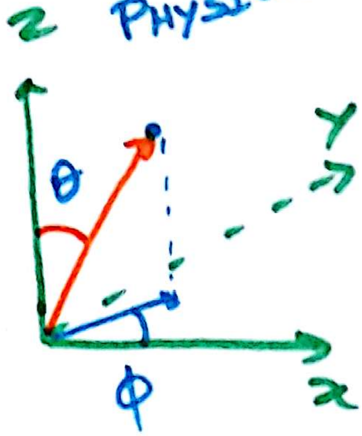
$0 \le \theta \le 2\pi$

$0 \le \phi \le \pi$

$0 \le r \le \infty$



PHYSICS



$$x = r \sin\phi \cos\theta$$
$$y = r \sin\phi \sin\theta$$
$$z = r \cos\phi$$

$x = r \sin\theta \cos\phi$
$y = r \sin\theta \sin\phi$
$z = r \cos\theta$
$0 \le \phi \le 2\pi$
$0 \le \theta \le \pi$

→ WAVE FUNCTION $\psi(x, y, z)$

OR $\psi(r, \theta, \phi)$

→ PROBABILITY DENSITY AT $\vec{r}$

$$\psi^*(x, y, z)\, \psi(x, y, z)$$

(OR)

$$\psi^*(r, \theta, \phi)\, \psi(r, \theta, \phi)$$

→ PROBABILITY OF FINDING THE ELECTRON IN AN INFINITESIMAL VOLUME

$$\psi^*(x, y, z)\, \psi(x, y, z)\, dx\, dy\, dz$$

(OR)

$$\psi^*(r, \theta, \phi)\, \psi(r, \theta, \phi)\, r^2 \sin\theta\, dr\, d\theta\, d\phi$$

- CONSTRUCT THE HAMILTONIAN
  - → KINETIC ENERGY OPERATOR

$$-\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right]$$

(OR)

PHYSICS CONVENTION

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]$$

  - → POTENTIAL ENERGY $\dfrac{-e^2}{4\pi\epsilon_0 r}$

- SOLVE THE SCHRODINGER EQUATION

$$H_0\psi(x,y,z)=E\psi(x,y,z)$$

(OR)

$$H_0\psi(r,\theta,\phi)=E\psi(r,\theta,\phi)$$

- SOLUTION:

$$\psi_{nlm}(r,\theta,\phi)=R_{nl}(r)\,Y_{lm}(\theta,\phi)$$

$R_{nl}(r)$ → RADIAL PART

$Y_{lm}(\theta,\phi)$ → ANGULAR PART → SPHERICAL HARMONICS

• QUANTUM NUMBERS

$n \rightarrow$ PRINCIPAL QUANTUM NUMBER

$l \rightarrow$ ORBITAL OR AZIMUTHAL QUANTUM NUMBER

$m \rightarrow$ MAGNETIC QUANTUM NUMBER

$S \rightarrow$ SPIN

$\Rightarrow$ ALLOWED VALUES:

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

$$l = 0, 1, 2, \dots, n-1$$

$$m = -l, -l+1, -l+2, \dots, 0, \dots, l-1, l$$

$$S = \pm \frac{1}{2}$$

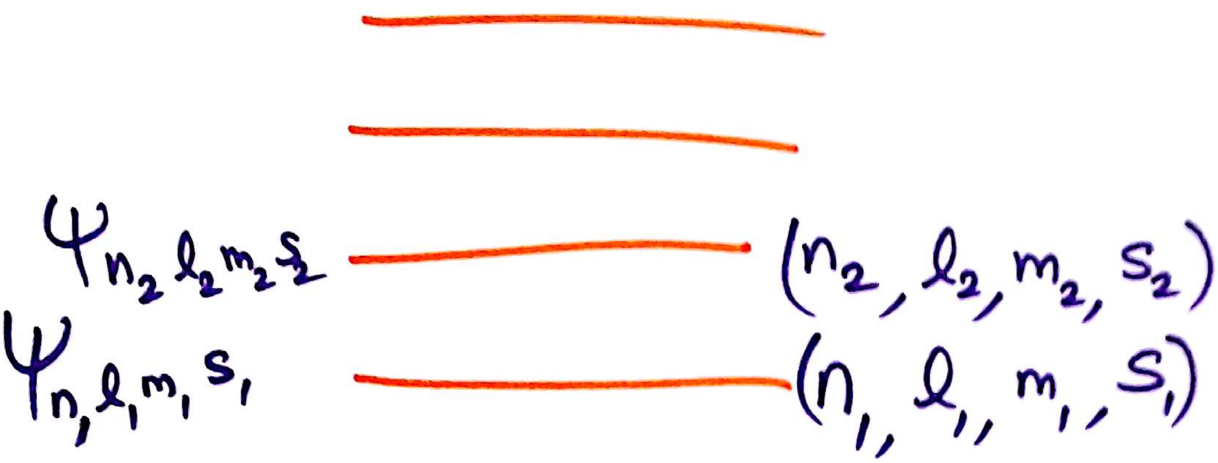
$\Rightarrow$ n GOVERNS THE ENERGY AND SIZE OF THE ORBITAL

l GOVERNS THE SHAPE OF THE ORBITAL AND THE ELECTRONIC ANGULAR MOMENTUM

m GOVERNS THE DIRECTION OF THE ORBITALS AND THE BEHAVIOUR OF ELECTRON IN A MAGNETIC FIELD

S GOVERNS THE AXIAL ANGULAR MOMENTUM OF THE ELECTRON.

- STATES ARE DEFINED BY THESE QUANTUM NUMBERS



- ENERGIES OF ATOMIC ORBITALS

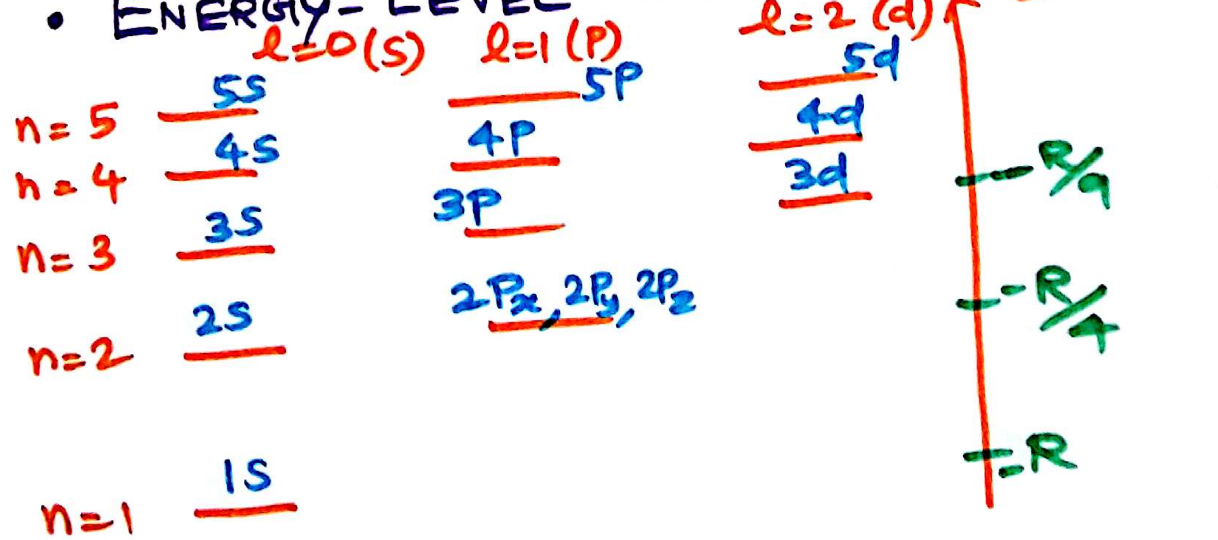
$\Rightarrow$ CALCULATE THE ENERGIES of 1S, 2S, $2P_x$, $2P_y$, $2P_z$, 3S, $3P_x$, $3P_y$, $3P_z$ and 3d

DEGENERATE

DEGENERATE

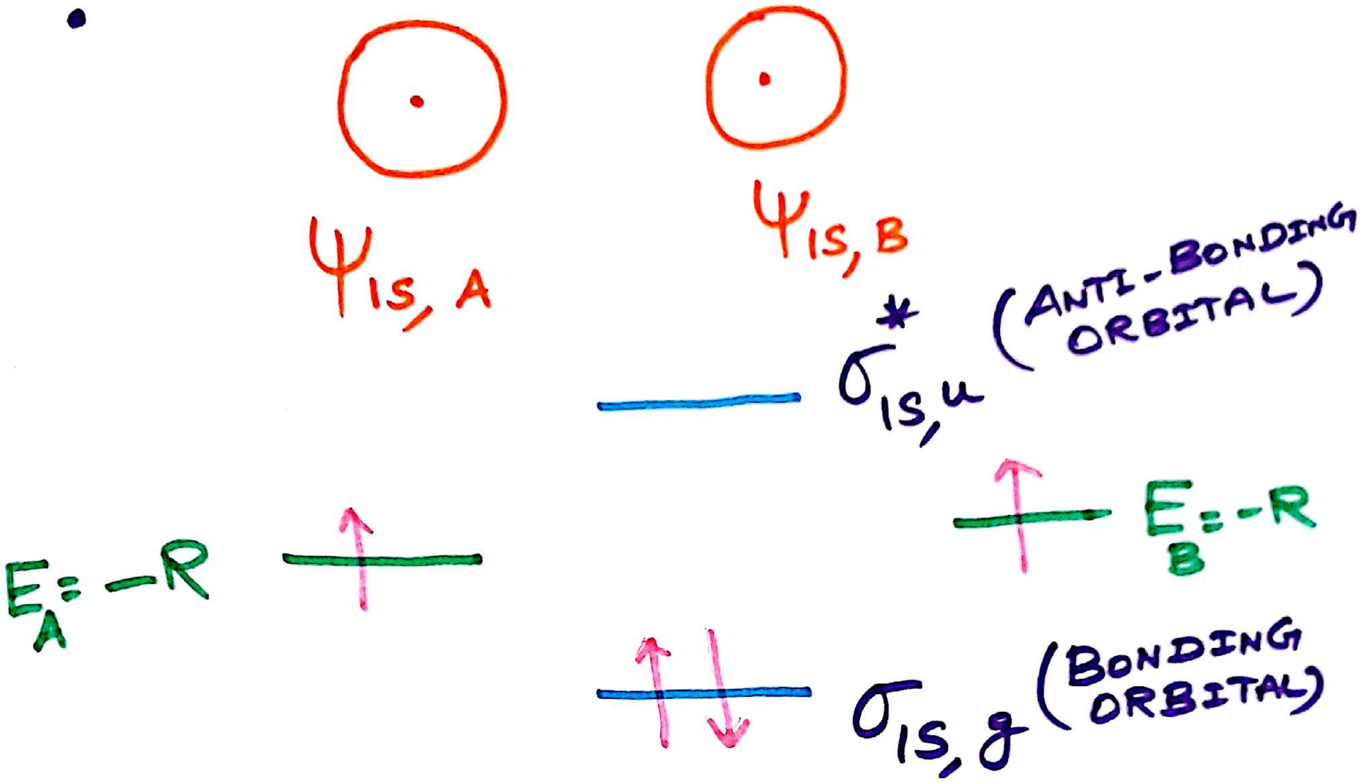
$$\Rightarrow \quad E_n = -\frac{R}{n^2}$$

- ENERGY-LEVEL DIAGRAM



HYDROGEN MOLECULE

- CONSIDER TWO HYDROGEN ATOMS IN THEIR RESPECTIVE GROUND STATES (1S ORBITALS)

- 

LINEAR COMBINATION OF ATOMIC ~~ORBITA~~ ORBITALS

$\Downarrow$

MOLECULAR ORBITALS

$$\psi_{1s,A} + \psi_{1s,B} \Rightarrow \sigma_{1s,g} \quad \text{(BONDING ORBITAL)}$$

$$\psi_{1s,A} - \psi_{1s,B} \Rightarrow \sigma^*_{1s,u} \quad \text{(ANTI-BONDING ORBITAL)}$$

CLASS WORK