Atomic Structure

Quantum NOS.

(1) Principal Q. No. (r) -> Shell No.

(2) Azimuthal O. NO. or secondary or subsidiary or angular 2. No. (1)

>>> Values of e can be 0,1,2 -- n-1

1 6

2 0,1

3 011,2

9 011,213

I -> type of subshell present in a shell

Subshell

Subshell

Sharip

P > sharip

P > trincipal spectral

d > diffused terms

f - fundamental

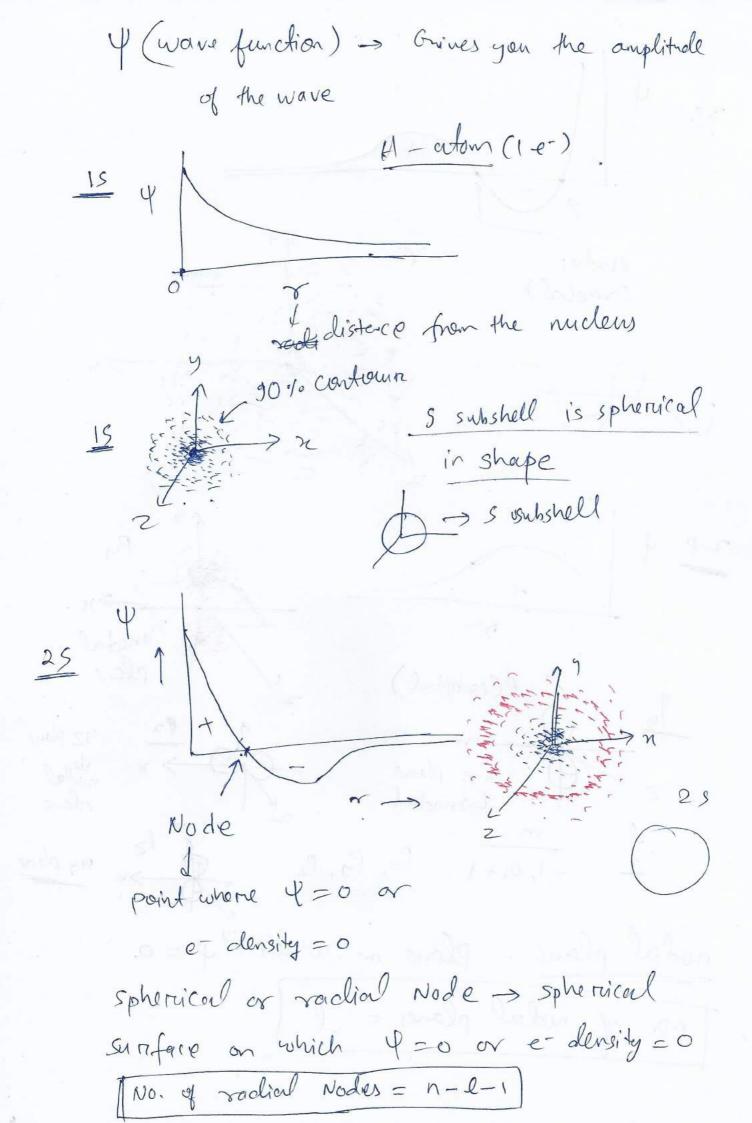
-> value of l gives the orbital angulare momentum [L = Je(let) h (3) magnetic Q. No. (m)

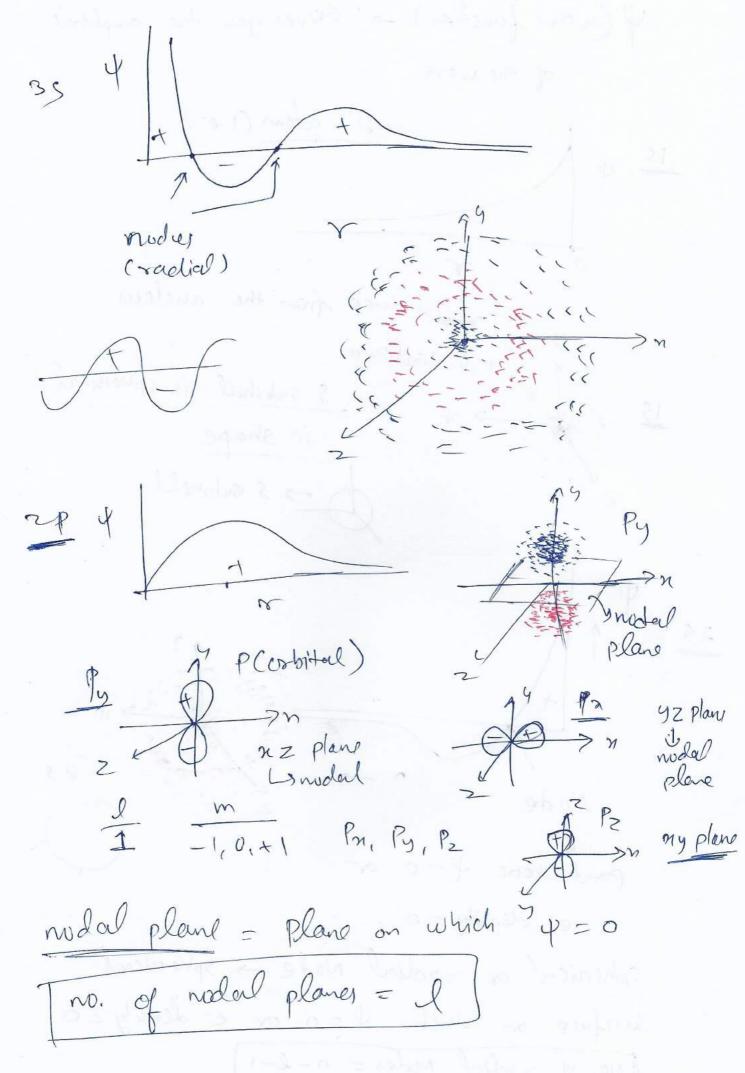
→ values can be -l to +l including zero l m one of m values 1 + 2x0+1 1 + 1 + 1

for a particular I value there are total 21+1 m values

 $\frac{1}{0} \frac{\text{Subshell}}{\text{os}} \frac{\text{m}}{\text{onientations}(\text{onbitals})}$ $\frac{1}{2} \frac{P}{-1,0,1+1} \frac{3(P_{K}, P_{Y}, P_{Z})}{3(P_{K}, P_{Y}, P_{Z})}$ $\frac{1}{3} \frac{1}{4} \frac{1}{-3, +0+3} \frac{1}{4} \frac{1}{3} \frac{1}{4} \frac{1}{3} \frac{1}{4} \frac{1}{3} \frac{1}$

78.5...





spherical modes two modes so moder planes (spherical) radial moder = n-1-1 modal planes = I Total no. of nodes dumbell shapp -2,-1,0,+1,+2 I - shape of an orbital m > tells the orientation of orbitals

•

Size of Forbiorbitals 15 < 25 < 35 -2PZ 3P < 4P -orbitals Shell Subshell 15 0 or 1 -- 2 Pm, 2Py2Pz 2 5 d orbitals or 5 orientations in my plane at us to the n dy axes) 3d => nodal planes =?= 1=2 Nodal ple + 42 plane nz plan double dumbell shape dyz - in the yz place at us to y & z two model plans my 4 nz plenes

drz in the nz plene at us to nlz two model pleases Certs the or & yarres

has two model

planes Cuts the zaris -7 n l=2 ring => two mod no of spherical modes = ? = 3 - 7 - 1 = 0f -> 7 f orbitals -> complex shapes $d \rightarrow l = 2, m = -2, -1, 0, 1, 2$ IJJJ dry dyz dry dry dry dz?

forbitals (7 forbitals) $f_{n(n^2-y^2)}$, $f_{y(n^2-y^2)}$, $f_{z(n^2-y^2)}$, f_{nyz} , f_{z^3} , f_{yz} 4 nzz If wave function can be broken in to $\Psi(\gamma,\theta,\phi) = \underbrace{R(\gamma)}_{n \mid m} \underbrace{\Phi(\phi)}_{m} \underbrace{\Phi(\phi)}_{m}$ r > distance part angular part the nucleus represents the edensity w.r.t. + e density w.r.t. to l'et disterce for muclen 0 -> angle w.r.t. the zakis & I-> despuds on σ ∈ [0, π]

σ = cogle of projection of γ

ω. γ-1. the yan's

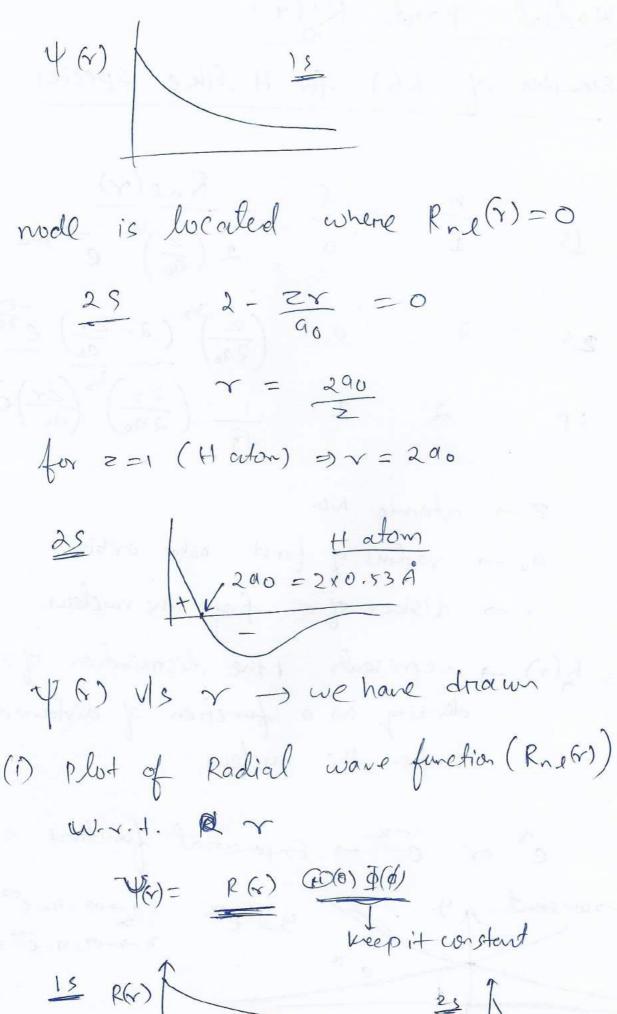
α- NOS.

α = [0,2π]

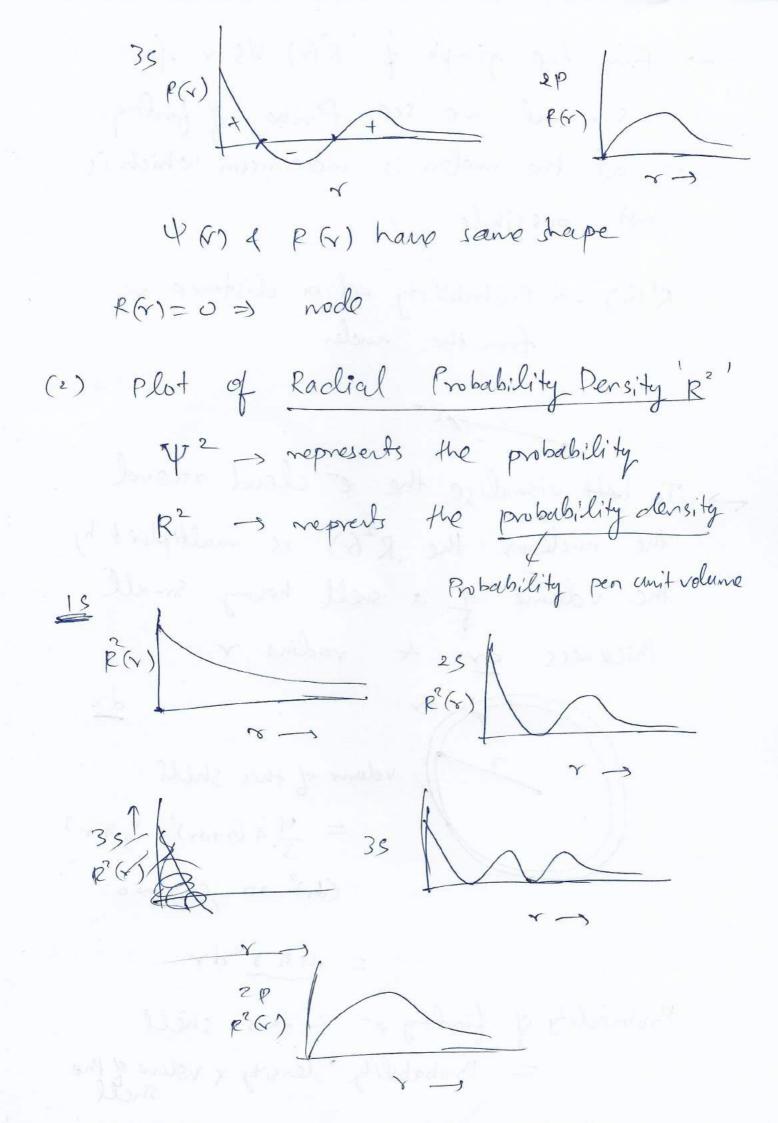
α congular part depends on

ex m. O E LOIT]

Radial part R (8) Examples of RG) for H like species Rne (r) $2\left(\frac{z}{a_0}\right)^{3/2} e^{-zr/a_0}$ $\left(\frac{z}{2a_6}\right)^{3/2}\left(\lambda - \frac{zr}{a_6}\right) e^{\frac{-zr}{2a_0}}$ $\frac{1}{\sqrt{3}} \left(\frac{z_{\gamma}}{2 a_0} \right)^{3/2} \left(\frac{z_{\gamma}}{a_0} \right)^{-2\gamma/2 a_0}$ Z -> atomic No. ao - rading of first bohr orbit r -> distace of e- from the nucleus. R(r) - represents the distribution of edensity as a function of distance r from the nucleus. er or en = Enponential functions e > constant qy y= ex $x \rightarrow co$, $y = e^{co} = \infty$ $\gamma \rightarrow -0$, $\gamma = \overline{\ell}^{cs} = \frac{1}{\rho_{os}}$



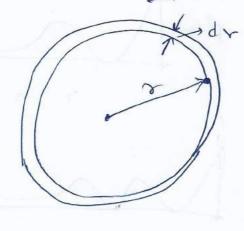
 $rac{2}{8}$



-> from the gruph of Re(r) VIS ~ for s arbitul we see Proba. of finding e- at the molen is maximum which is nut possible

R°(r) -> Probability at a distence ~ from the nucles

To bett visualize the e- cloud attord the nucleurs the R260) is multiplied by the volume of a shell having small thickness dr & radius ~

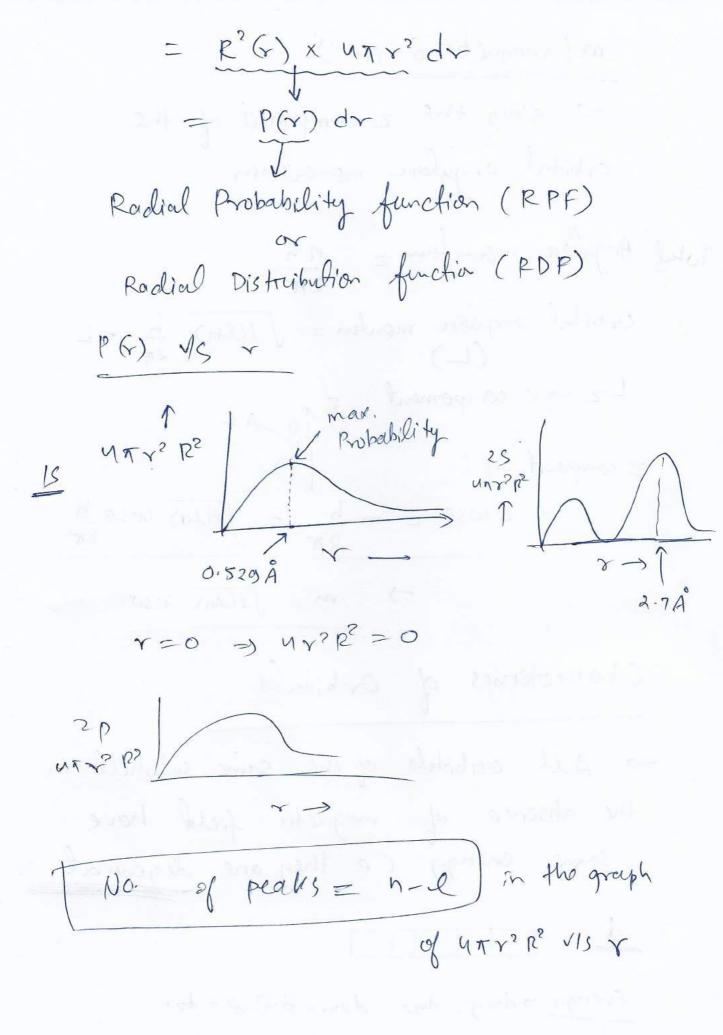


volume of this Shell

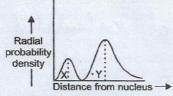
= $\frac{4}{3}\pi (r+dr)^3 - \frac{4}{3}\pi r^3$ (dr) 2 -> 0 (dr) 3 -> 0

= UTY2dr

Probability of finding or in this shell = Probability density x volume of the



Objective Questions



If the above radial probability curve indicates '2s' orbital, the distance between the peak points X, Y is:

(a) 2.07Å

(b) 1.59Å

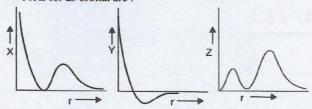
(c) 0.53Å

(d) 2.12Å

[Ans. (a)] [Hint:

X = 0.53Å, Y = 2.6Å Y - X = 2.6 - 0.53 = 2.07Å1

Plots for 2s orbital are:



X, Y and Z are respectively:

(a) R, R^2 and $4\pi r^2 R^2$

(b) R^2 , R and $4\pi r^2 R^2$

(c) $4\pi r^2 R^2$, R^2 and R

(d) R^2 , $4\pi r^2 R^2$ and R

[Ans. (b)]

[Hint: Y will be definitely 'R' because value of R cannot be negative, thus X will be R^2 and Z will be $4\pi r^2 R$. Z represents radial probability function; its value will be zero at origin]

3. The wave function (Ψ) of 2s is given by:

$$\Psi_{2s} = \frac{1}{2\sqrt{2\pi}} \left(\frac{1}{a_0}\right)^{1/2} \left\{ 2 - \frac{r}{a_0} \right\} e^{-r/2a_0}$$

At $r = r_0$, radial node is formed. Thus for 2s, r_0 in terms of a_0

(a) $r_0 = a_0$ [Ans. (b)]

(b) $r_0 = 2a_0$ (c) $r_0 = a_0 / 2$ (d) $r_0 = 4a_0$

[Hint: When $r = r_0$, $\psi_{2s} = 0$, then from the given equation:

$$2 - \frac{r}{a_0} = 0$$

 $r=2a_0$]

The wave function for 1s orbital of hydrogen atom is given by:

$$\Psi_{1s} = \frac{\pi}{\sqrt{2}} e^{-r/a_s}$$

where, a_0 = Radius of first Bohr orbit

r = Distance from the nucleus (Probability of finding the electron varies with respect to it)

What will be the ratio of probabilities of finding the electrons at the nucleus to first Bohr's orbit a_0 ?

(a) e

(b) e2

(c) $1/e^2$

(d) zero

[Ans. (d)] [Hint: For 1s orbital, probability of finding the electron at the nucleus is zero.]

The radial wave equation for hydrogen atom is:

$$\Psi = \frac{1}{16\sqrt{\pi}} \left(\frac{1}{a_0}\right)^{3/2} \left[(x-1)(x^2 - 8x + 12) \right] e^{-x/2}$$

where, $x = 2r/a_0$; $a_0 = \text{radius of first Bohr orbit.}$

The minimum and maximum position of radial nodes from nucleus are:

(a)
$$a_0$$
, $3a_0$

(b) $\frac{a_0}{2}$, $3a_0$ (c) $\frac{a_0}{2}$, a_0 (d) $\frac{a_0}{2}$, $4a_0$

[Ans. (b)]

i.e.,

[Hint: At radial node, $\Psi = 0$

.. From given equation,

$$x-1 = 0$$
 and $x^2 - 8x + 12 = 0$
 $x-1 = 0 \implies x = 1$
 $\frac{2r}{a_0} = 1; r = \frac{a_0}{2}$ (Minimum)

$$x^{2}-8x+12=0$$

$$(x-6)(x-2)=0$$
when
$$x-2=0$$

$$x=2$$

$$\frac{2r}{a_{0}}=2, i.e., r=a_{0} \text{ (Middle value)}$$
when
$$x-6=0$$

$$x=6$$

$$\frac{2r}{a_{0}}=6$$

$$r=3a_{0} \text{ (Maximum)}$$

m (magnetic Q. NO-)
orbital orgular momentum
Total Angular monutum = nh
c) hild and
LZ > 2 component 2 for L Zor L Zor L
z compont of L
$= L \cos \theta = m \frac{h}{2\pi} = \sqrt{l(1+1)} \cos \theta \frac{h}{2\pi}$
=) m = Section wso
Characterics of orbitals
-> All orbitals of the same subshell in
the absence of magnetic field have some energy i.e they are degenerate
same energy i.e they are degenerate
d The Indian
Energy > dny = dn2 = d2n = dn2y2 2 d22

effect -> splitting of Z elman spectral lines in the presence of field (B) magnetic d orbitaly In the absence of B In the presence of B m >can emplain Grives diff. orientations of dorbital 2P (4) Spin a. No. (5) Ispin of e- around its own axis (1) For clockwise spin s=+1/2 (1) () For anticlockwise spin s=-1/2 (1) Pauli's Enclusion principle -> No two es in an atom can have the same value of all the four

Quantum Nos.

1

10 mars. capacity of a subshell: 2(21+1) each can have max re--l ---0, --+l = 21+1 > whitaly > No. of subshells in a main energy shell = n. n I No. of subshells 1 0 15 = 1 2 - 0,1 - 25, 2P = 23 0,1,2 35,3P,3d => 3 n subshells no. of orbitals in a main energy shell = n2 n ogerhitaly 2 0,1 25,2Pm,2Ps,2Pz 4

3 0,1,2 35, 3Pm, 3Py 3P, 5dny -- = 9

Exuple 2 Pm 2 Py 2 Pz 2 p | 1 | 1 | 1 | 1 | 1 | $/ n = 2, l = 1, m = -1, s = + \frac{1}{2}$ $> n = 2, l = 1, m = -1, s = -\frac{1}{2}$ MY Not possible in an orbital Than arbital there can be maximum of 2 emax. capacity of subshells P -> Pm, Py, P2 -> 64d -> 5d orbital -> 10 e-2 f -> 7 ferbitu -> INP-No of orbitals in a given subshell = (2/+1) 1=0 => 5 = 2x0+1=1 (15) 1=1 => P => 2X1+1=3 (Pm, Pu P,) 1 = 2 = 1 d = 1 2x 2+1 = 5 (drydyz, dron, dw?-y, dr?)

11

max. Capouity of a main energy-shell

- 2 x n²

max. capouity no of orbitals

of each orbital

5 -> spin angulerre mes Q. No.

Spin angular montum $L_S = \sqrt{s(S+1)} \frac{h}{2\pi}$ where $S \rightarrow Spin$ of the Q. NO. of the $e - (1_2)$ for H order e^- , $L_S = \sqrt{\frac{s(S+1)}{2\pi}} \frac{h}{2\pi}$ $S = \frac{1}{2} \times \frac{h}{2\pi} + \frac{1}{2\pi} = \frac{1}{3} \times \frac{h}{2\pi}$ $= \frac{\sqrt{3}}{3} \times \frac{h}{3}$

Excuples

(8)
$$n=4$$
 4 subshells 4s, 4p, 4d, 4f

 $N=0$
 $N=0$

1.

Examples

1) The orbital angular momentum of an electron in a d-orbital is?

Ans.
$$L = \sqrt{2(2+1)} \frac{h}{2\pi} = \sqrt{6} \frac{h}{2\pi}$$

- 2) which of the following sets of quantum numbers is contract for an electron in 4 f-orbital?
 - (a) n = 4, l = 3, m = +4, $s = +\frac{1}{2}$
 - (6) n = 4, l = 4, m = -4, S = -1/2
 - (c) n=4, l=3, m=+1, $s=+\frac{1}{2}$
 - (d) n=3, l=2, m=-2, $S=+\frac{1}{2}$

Ans.(c)

ι

3 Match the following:

(A) The number of sub-energy levels (P) n2 in an energy level

(B) The number of oribitals in (9) 3d a sub-energy level

(c) the number of orbitals in (x)21+1
an energy level

(p) n=3, l=2, m=0 (3) n

 \underline{Ans} $(A) \rightarrow (S)$, $(B) \rightarrow (Y)$, $(C) \rightarrow (P)$, $(D) \rightarrow (2)$

(4) Which of the following is not possible?

(a) n=2, l=1, m=0 (b) n=2, l=0, m=-1

(c) n=3, l=0, m=0 (d) n=3, l=1, m=-1

Ans. (b)

(3) What is the maximum numbers of electrons in on atom that can have quantum numbers n=4, $m_0=+1$?

(a) 4 (b) 15 (c) 3 (d) 1 (e) 6

Ans. (e)

Aufbau Principle
-> Gives the energy order of various
orbitals
s German word means building up
the state of the said with the
h = 1 (15)
N=2 (25) (2P)
n=3 (3d)
n=4 4 9 40 (4d) (4f)
n=5 (53) (51) (F) - (53)
n=6 (63) (67) (67) (67) -
n=7 (15) (1P)
n=8 85 $$
Energy orden
1s < 2s < 2p < 3s < 3p < 4s < 3d < 4p < 5s
-> rule which determines the energy order is called (n+1) rule

(n+1) rule

-) highers the value of n+l higher is the energy of the orbital

if n+l is same for two different orbitals then his the orbital with higher n has higher energy.

 $\frac{3d}{3+2} > \frac{4s}{4+0}$ = 5 = 4

Electric a

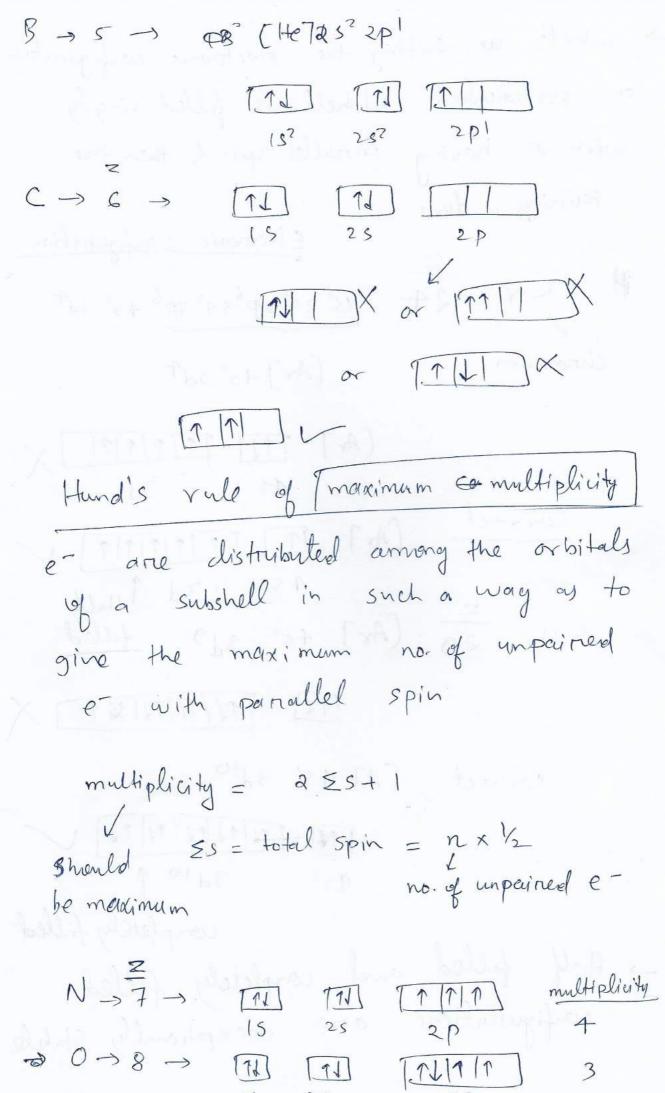
Electronic configuration & Hund's rule
of maximum multiplicity

H 1 1 or 1 or 15'

1te 2 [1] 08 132 = (He]

Li 3 [1] [1] 0 152 251 = [He] 251

Be 4 [1] [1] or 152 252 = (He) 252



-> while so writing the electronic configuration a particular subshell is filled singly with e- having parallel spir & then the Perirring is done Electronic configuration 24 15° 25° 29635° 396 45° 3d⁴ Chromium (Ar] 45° 3dt (A) [1] [1/1/1] X
45 3d Correct (A) IN [1/1/1] Cu = 3d 1 Half Cu = 3d (Ar) 45° 3d9 filled TTD TTL/12/12/12/1 correct [A] 45' 3d'0 95/ 3410 1 completely filled - Half filled and completely filled configurations are exceptionally stable

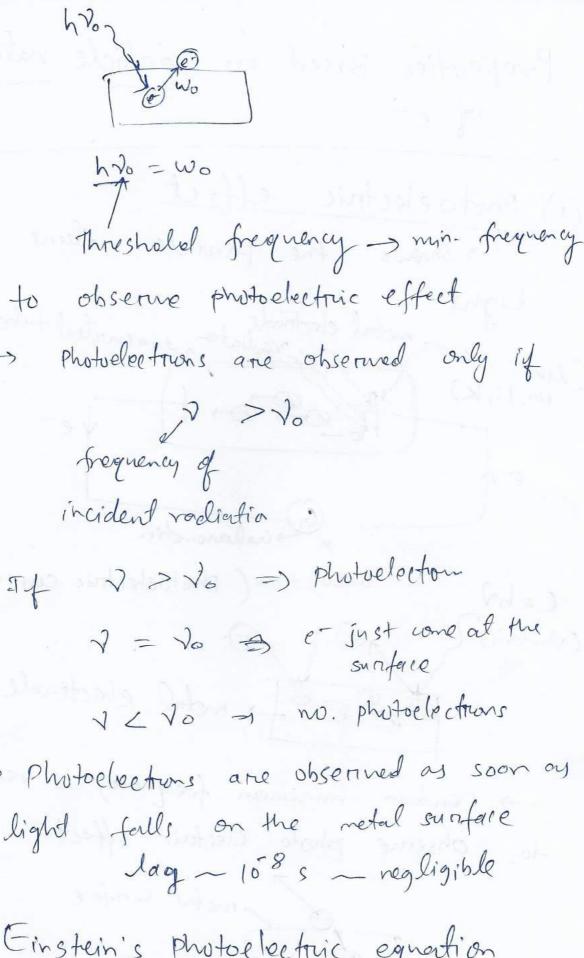
Enplanation (i) Symmetry -> half filled & completely filled configurations and more symmetric, Symmetry always leads to stability. (") Encharge energy -> where there is enclouge between ethere is energy released. energy released => stability V/S 4+3+2+1=10 total enchage, morp enchanges =) more stubility more energy is released Li l'esser energy => more stability. Para magnetic material - material having attens with atteast one unpaired e-- weakly attracted by magnetic field

01

(Ar) 452 3d6 Ar7 [1] [11/1/1/1]
45? 3d6 Fe metal is parramagnetic in nature how 4 unpaired e-Diamagnetic material (No attraction for magnetic field) - has no unperined eexemples
Be = 2 152 252 Zn 32 (Ar) 45°3210 Magnetic moment (Determines the - strength of magnetic nature of an atom) M = In(n+2) B. M. init of M n -> no. of unpowered Buhr magneton. 1 B.M. = eh 4 Tmc

Properties Based on particle nature 4 e-(i) Photoelectric effect Is shows the particle nature metal electrode vadration evacuated tube (G) Gralianometer deflection (photoelectric current) 666) noted electricale -> certain minimum frequency is required photo electric effect observo 5 metal sunface wo - work function - min. energy nequired to bring e- from inside the metal or to the sunface.

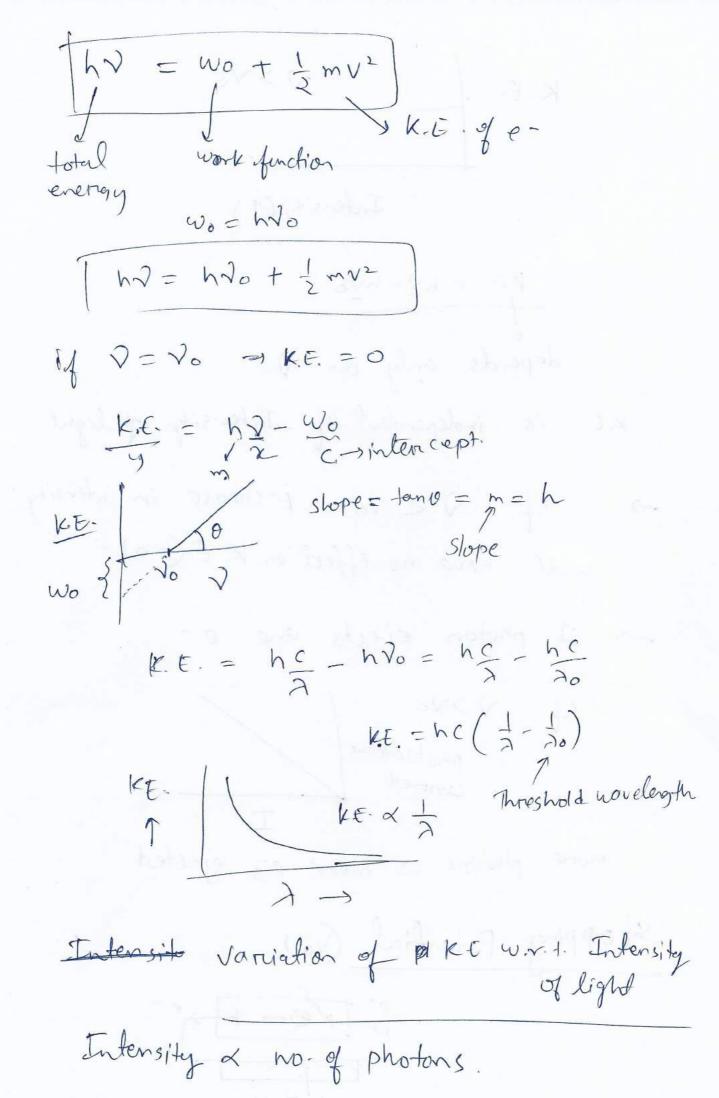
2



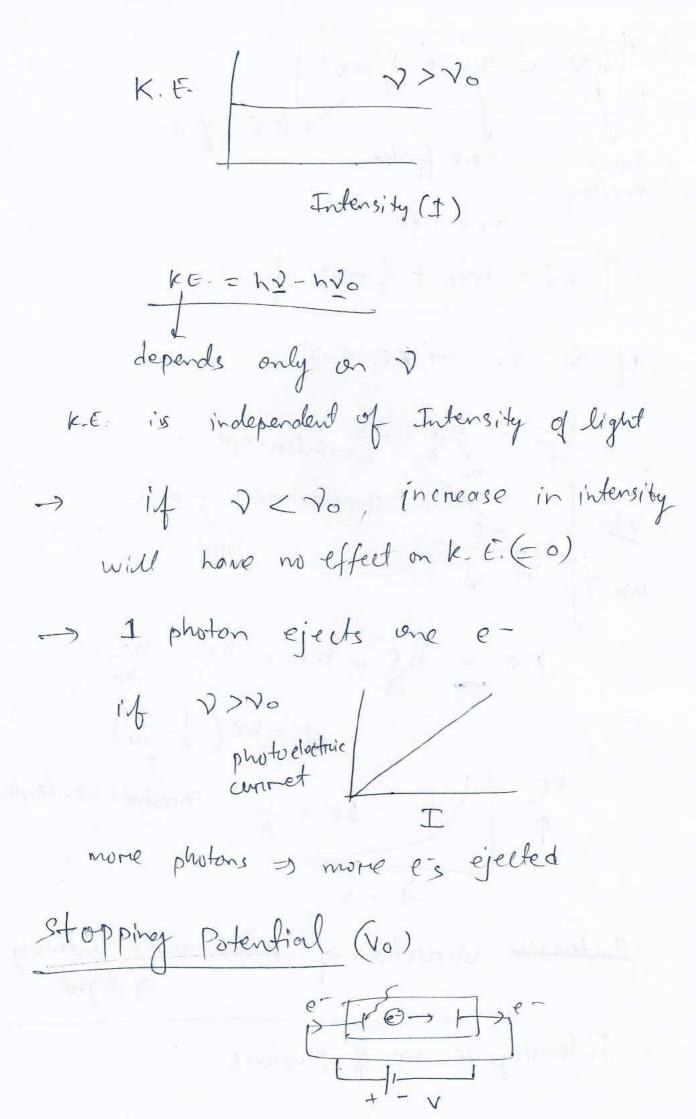
Einstein's photoelectric equation

h ? 3 (K.E.)

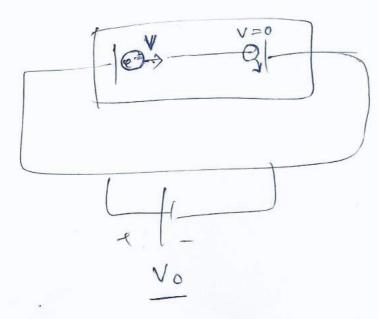
0,



(



Vo > minimum potential required to stop photo electric emission or for zero photo electric current



Vo

m=shope=tano= he
intencept = hive
wo

* Vo depends only on I not on intensity
of light used.