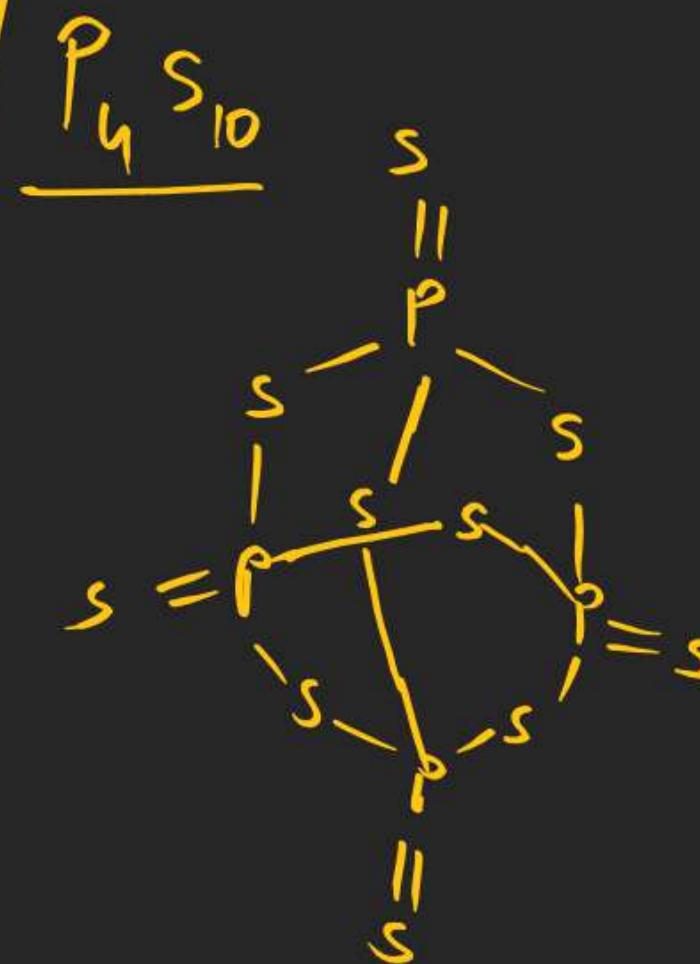
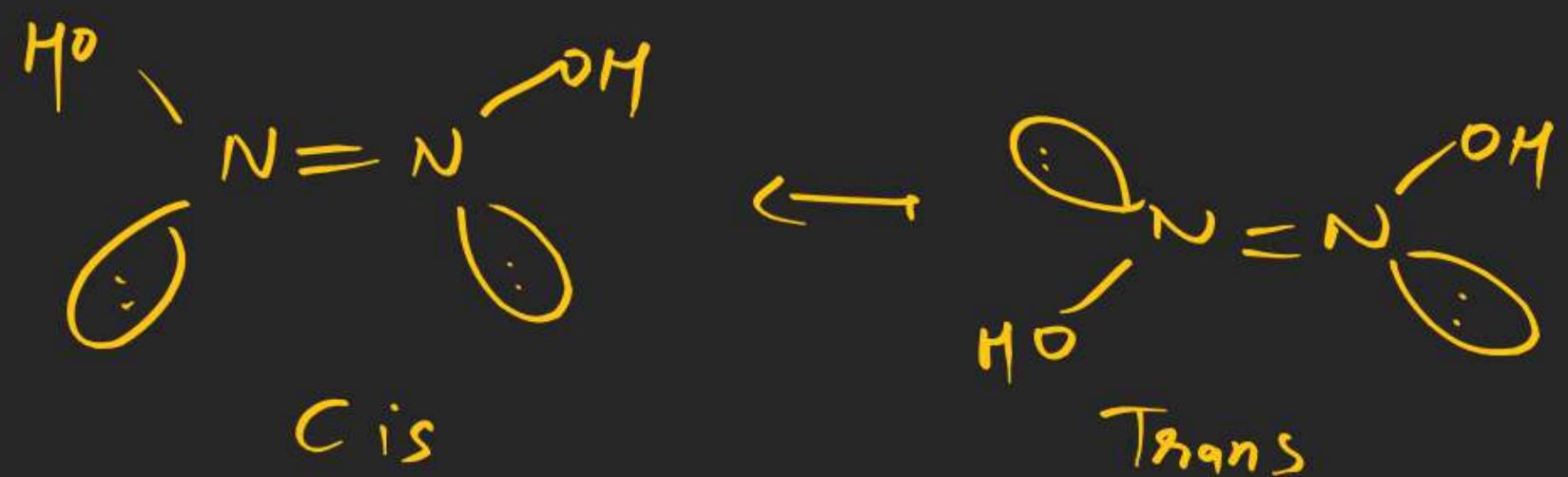


CaCN_2 [Calcium cyanide]



$\underline{\text{P}_4\text{S}_3}$ (Match box)
 fine Cr.
 (explosive)





M.O.T [Molecular orbital theory]

$$\text{H}-\text{H} = 1^{\text{B.O}}$$

$$\text{O}=\text{O} = 2$$

$$\text{N}\equiv\text{N} \quad 3$$

$$\text{N}\overset{*}{\equiv}\text{O} \quad 2.5$$

Drawback of V.B.T

① acc. to V.B.T O_2 is diamagnetic but actually it is paramagnetic

$$\text{B.O} = [\text{Bond order}] \quad : \text{O} = \ddot{\text{O}}:$$

② V.B.T can't explain formation of odd e- bond.

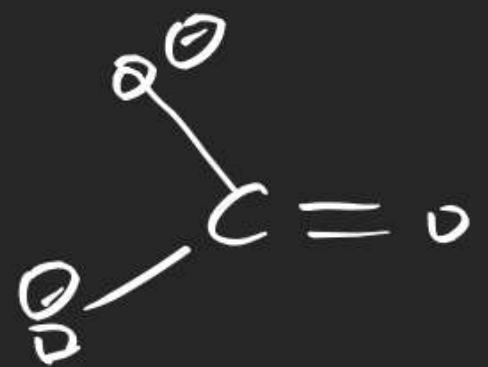
$\text{B.O} = 2.5$

$$\text{N}\overset{*}{\equiv}\text{O}$$

③ V.B.T can't explain fractional bond order in diatomic molecules but in polyatomic molecule

fractional bond order is explain by

Resonance

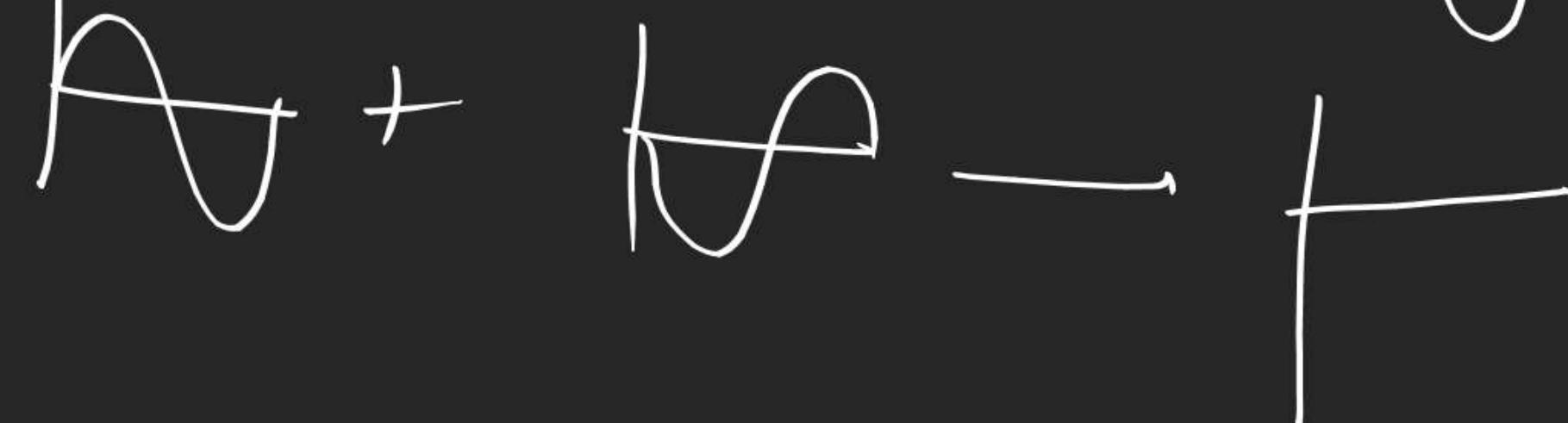
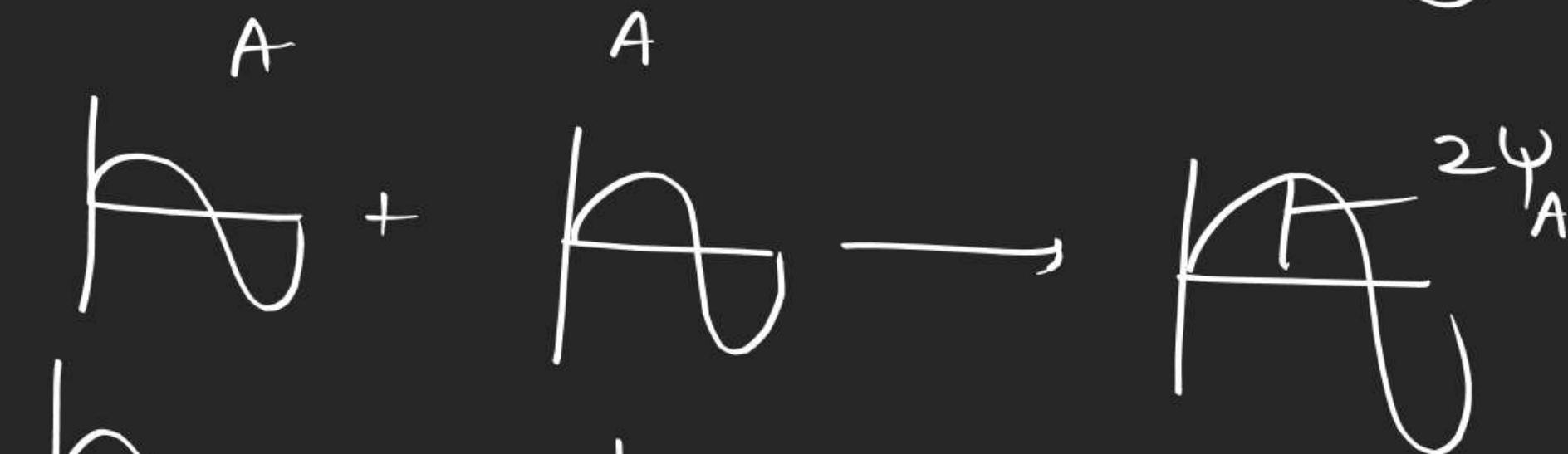
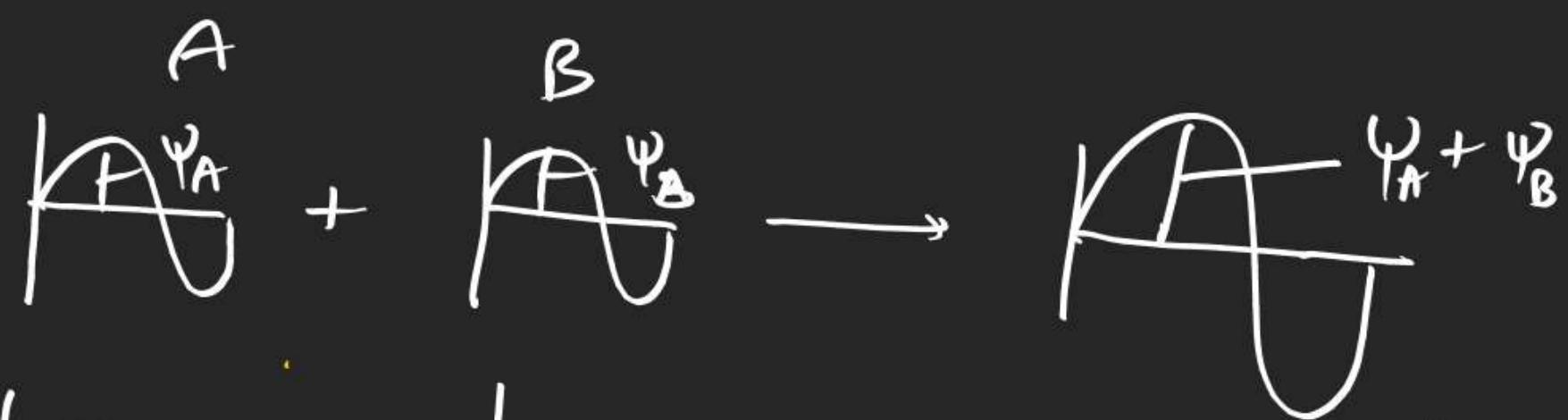


1.33

for removal of these difficulties Hund's and
Mulliken introduce a theory which is
Known as Molecular theory

$$\downarrow -t = \frac{h}{mv}$$

e^- mass $\downarrow -t$ (wave nature)



e^- wave meet in same phase then there would be constructive interference then e^- probability \uparrow between nucleons of both bonded atoms due to attraction and formed molecular orbital named as bonding molecular orbital $[B \cdot M \cdot O]$ which has lower energy than the atomic orbital.

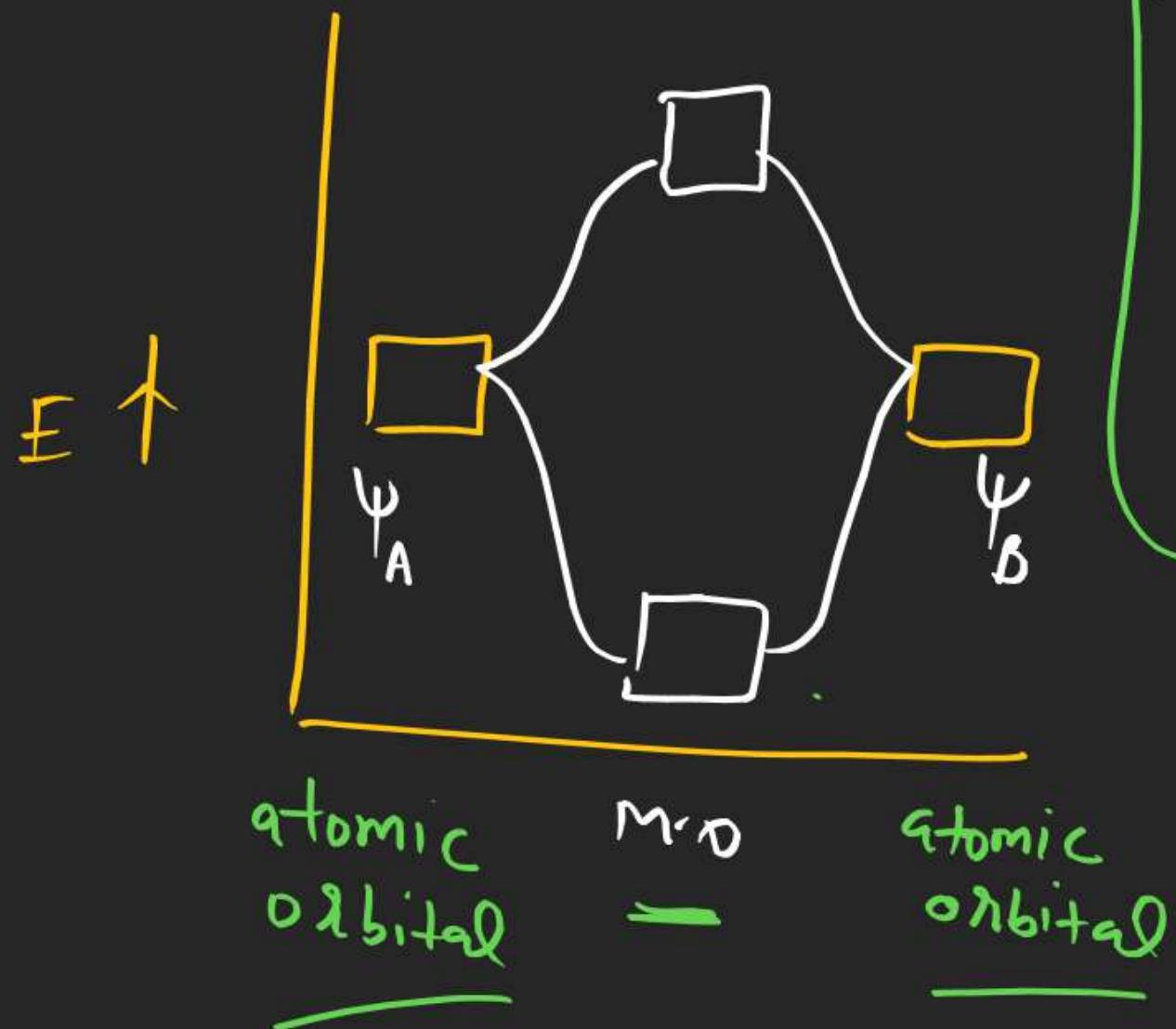
If e^- wave meet in opposite phase then there would be destructive interference then e^- probability \downarrow between nucleons of atomic orbitals due to repulsion formed molecular orbital named as anti bonding molecular orbital $[A \cdot B \cdot M \cdot O]$ which has higher energy than the atomic orbital.

V.T sir book

11th Class Chemical bonding

Part B → H-W

12th Class Chemical bonding
Part - A



Wave function of molecular orbital is explained by
L.C.A.O [Linear Combination of atomic orbital]
that may be of two type.
① axial ② sideways

Axial

here +, - sign show phase
of orbital



+

 $\Psi_{(A)}$

$$\frac{B \cdot M \cdot O}{N \cdot P = 0}$$



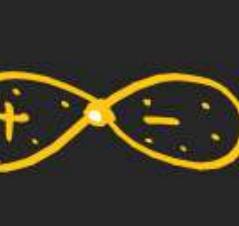
+



$$\frac{N \cdot P = 1}{A \cdot B \cdot M \cdot O} \Psi_{(u)}$$



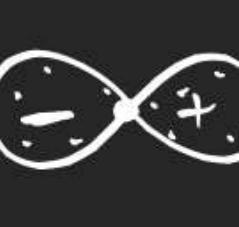
+

 $\Psi_{(S)}$

$$\frac{B \cdot M \cdot O, N \cdot P = 0}{ABMO}$$



+



$$\frac{ABMO}{N \cdot P = 1} \Psi_{(u)}$$



+



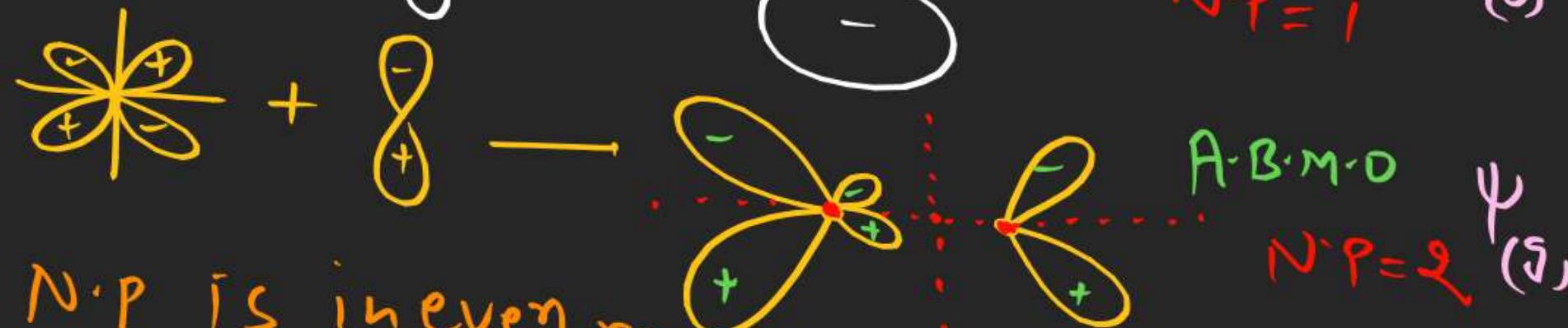
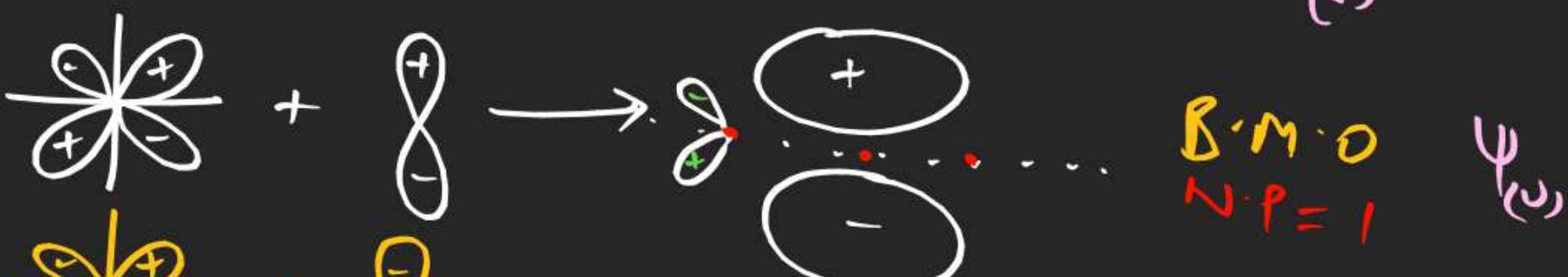
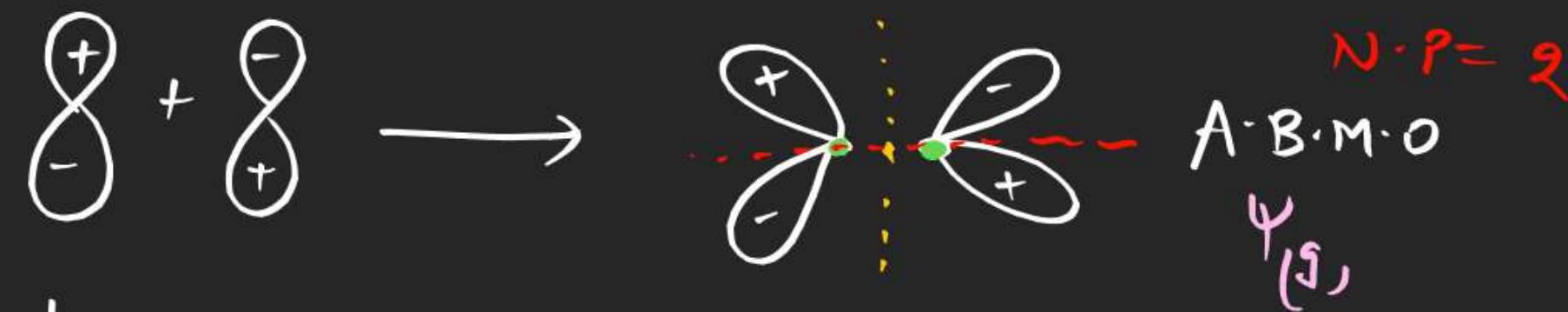
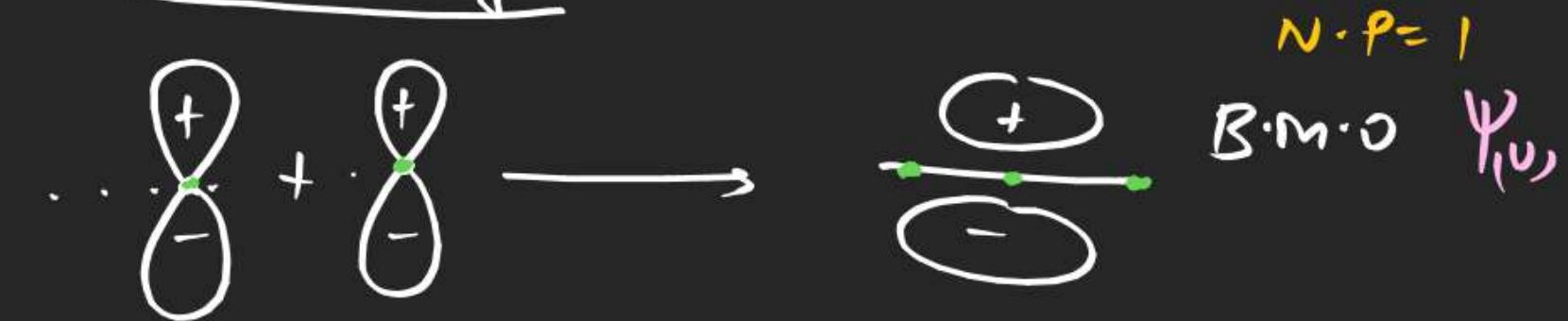
$$\frac{B \cdot M \cdot O}{N \cdot P = 0} \Psi_{(S)}$$



+

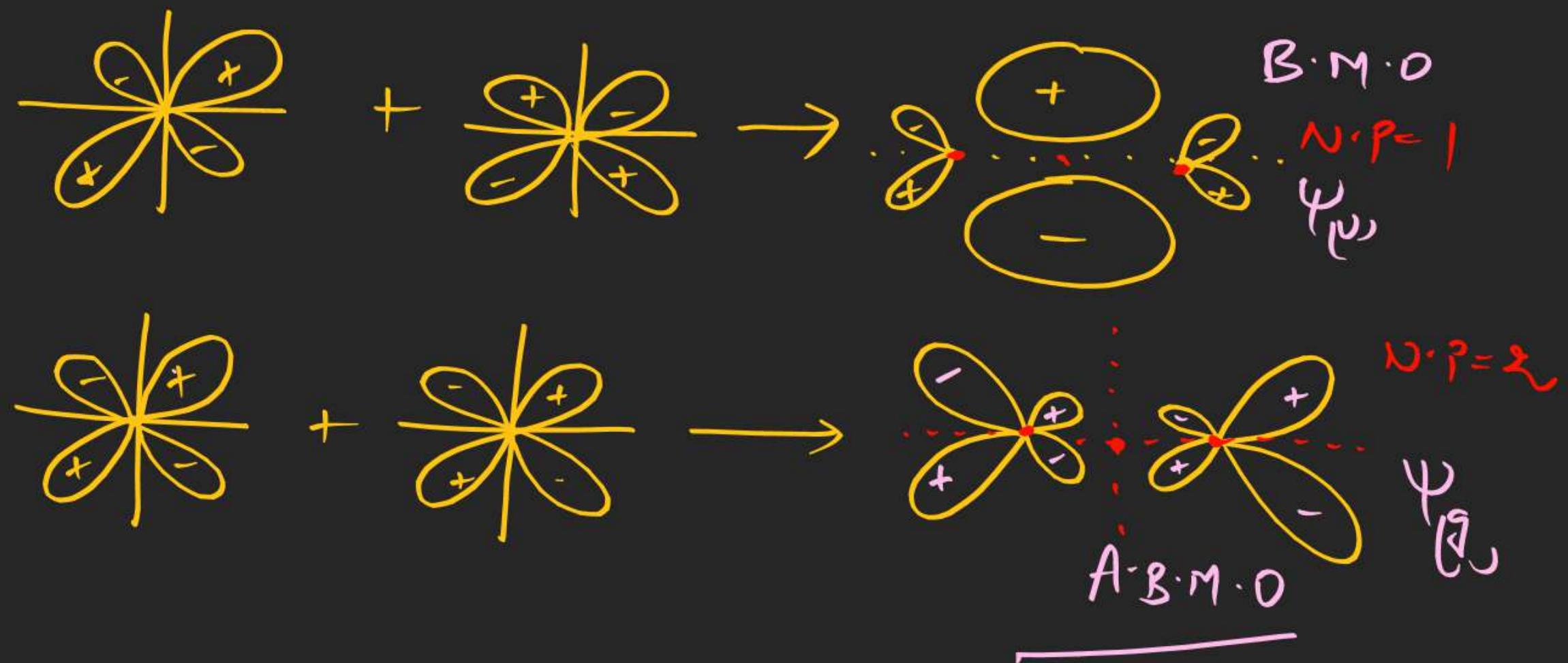


$$\frac{N \cdot P = 1}{ABMO} \Psi_{(u)}$$

Sideways

if $N \cdot P$ is even number = gerade orbital

if $N \cdot P$ is odd number = ungerade orbital



$N \cdot P$ = any imaginary plane which has zero e^- probability and must be passed through nucleus of atomic orbital in case of molecular orbital must be passed through mid point.