

$$H\psi = E\bar{\psi}$$

CLASSICAL
PARTICLE
NEWTON'S LAW

$$x, p_x$$

DETERMINISTIC

QUANTUM MECH.

WAVE

SCHRÖDINGER EQ.

$$\psi(x, y, z, t)$$

PROBABILISTIC

ALL THE PROPERTIES OF THE QUANTUM
"PARTICLE" IS IN $\psi(x, y, z, t)$.

Probability of finding the particle ΔT
in $\tau + dV$ IS GIVEN BY

$$P(\tau) dV = |\psi(\tau)|^2 dV$$

$$\tau = (x, y, z)$$

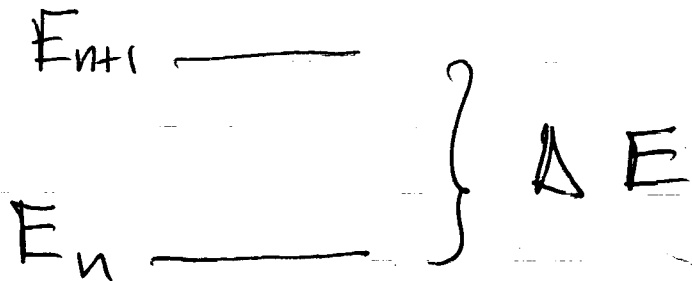
CARTESIAN COOR.

$$dV = dx dy dz$$

SPHERICAL COOR.

$$dV = r^2 \sin \theta dr d\theta d\phi$$

GIVEN THE ENERGY LEVELS

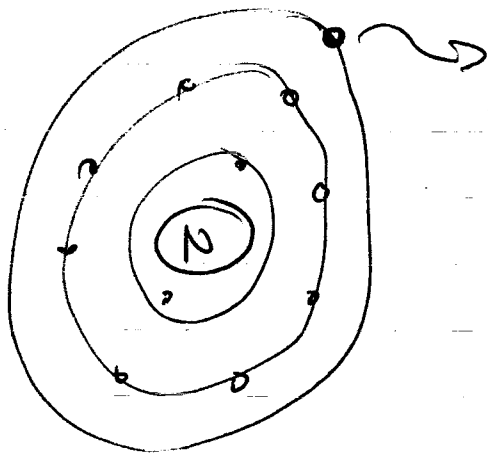


IF $\Delta E \gg kT \Rightarrow QM$

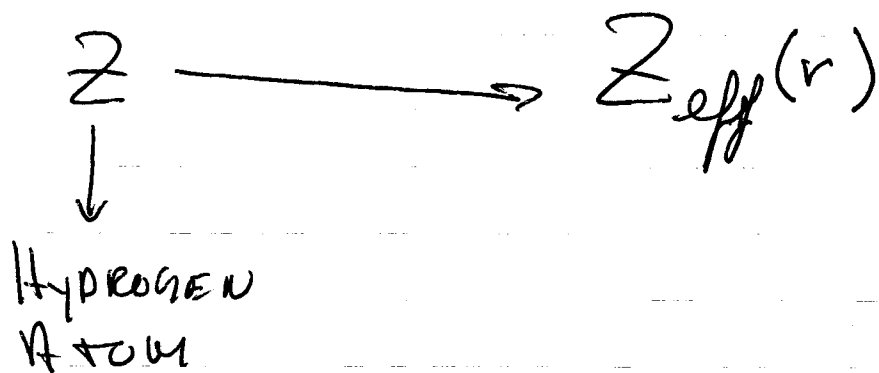
IF $\Delta E \ll kT \Rightarrow CM$

$kT \sim$ ENERGY EXCHANGE DUE
TO COLLISIONS

Multi Electron ATOMS



e^- DOES NOT SEE THE FULL NUCLEAR CHARGE DUE TO THE OTHER ELECTRONS



ATOMS - still preserve the SPHERICAL SYMMETRY!

$$\Phi_{n, l, m}(r, \theta, \varphi) = F_{n, l, m}(r) G_{l, m}(\theta, \varphi)$$

$$G_{l, m} \longrightarrow Y_l^m(\theta, \varphi)$$

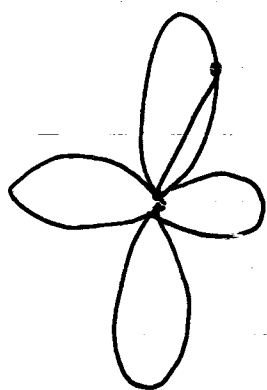
ORBITALS

POLAR REPRESENTATION

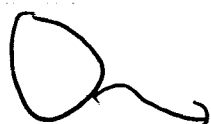
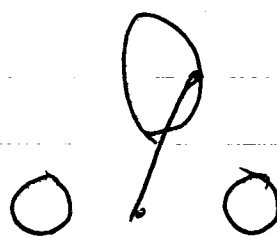
UNIQUE!

INFINITE
CONTOUR (OF EQUAL PROBABILITY)

REPRESENTATION.



d_{22}



Points of equal
probability

d_{22}

Polar

$(|d_{22}|, \theta, \varphi)$

(r, θ, φ)

ORBITAL

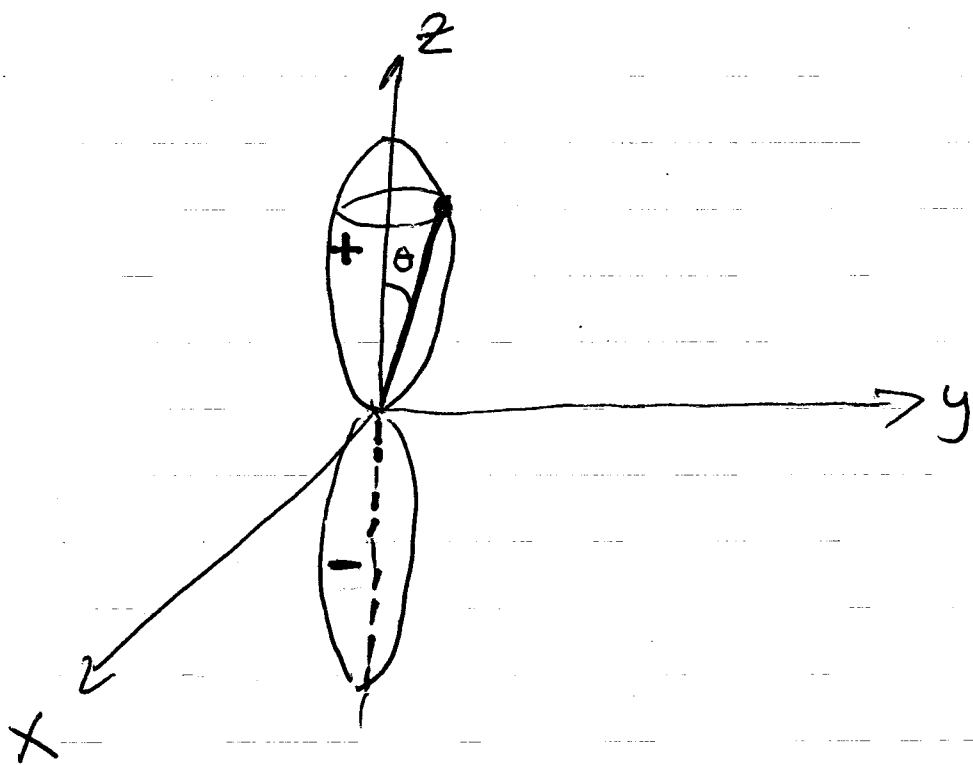
$$Y_l^m \in \mathbb{C}$$

$$\left. \begin{array}{l} s \\ p \\ d \end{array} \right\} \text{ ORBITALS } \in \mathbb{R}$$

$$P_z = \sqrt{\frac{3}{4\pi}} \cos \theta$$

P_z (part) WAVE FUNCTION

$|P_z|^2 \sim$ Probability OF FINDING
THE ELECTRON



$$\varphi = \frac{\pi}{2}$$

DISTANCE FROM THE ORIGIN = $\sqrt{|P_z|^2}$

~ PROBABILITY

Plotting $(|P_z|, \theta, \varphi)$

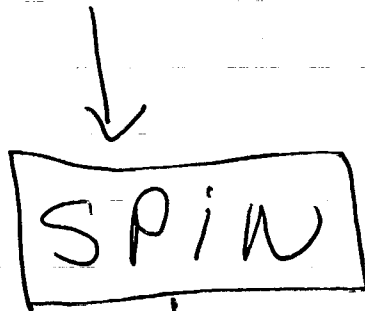
Probability in direction (θ, φ)

NO RADIAL PART!

Solve the multi-electron

$$SE \Rightarrow E_{nem}$$

$$\Phi_{nem}$$



HUND'S RULE