

$$\psi(r, \theta, \phi) = R(r) \cdot \Theta(\theta) \cdot \Phi(\phi)$$

quantum # $\begin{matrix} \downarrow & \downarrow & \downarrow \\ n & l & m \end{matrix}$

each is a known analytical function.

relationship to chemical notation

$n \rightarrow K, L, M$ "shells" $n = 1, 2, 3, \dots \rightarrow$ energy.

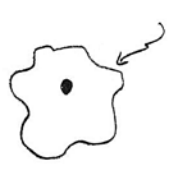
$l \rightarrow s, p, d$ "orbitals" $l = 0, 1, 2, \dots, n-1$

$m \approx p_x, p_y, p_z$ "orientation" $m = -l, -l+1, \dots, 0, \dots, l-1, l$ } angular momentum.

$s = \frac{1}{2}$ or $-\frac{1}{2}$ additional spin quantum number (up or down).

Physical interpretation of quantum # n , Bohr atom

assumption: electron orbits nucleus \rightarrow restricts r



such that

recall

$$n\lambda = 2\pi r_n \quad \left. \begin{matrix} \uparrow \\ \lambda = \frac{h}{p} \end{matrix} \right\} = \frac{nh}{p} = 2\pi r_n$$

$$\Rightarrow r_n = \frac{nh}{p} = \frac{nh}{mv}$$

Balance forces. ($F = \frac{dV}{dr}$)

electrostatic

centrifugal

$$\frac{Ze^2}{4\pi\epsilon_0 r^2} = \frac{mv^2}{r} \Rightarrow r = \frac{Ze^2}{4\pi\epsilon_0 mv^2} = \frac{nh}{mv}$$

velocity $\Rightarrow v_n = \frac{Ze^2}{4\pi\epsilon_0 nh}$

$$r_n = \frac{nh}{mv} = \boxed{4\pi\epsilon_0 \frac{(nh)^2}{mZe^2}}$$

Bohr radius

for hydrogen:

$$r_{n=1} = 0.529 \text{ \AA} = a_0$$

$Z=1$

What can we say about the energy?

$$E_{\text{tot}} = E_k + E_p$$

$$= \frac{1}{2}mv^2 + \frac{-Ze^2}{4\pi\epsilon_0 r}$$

want $E_{\text{tot}} = f(r)$. eliminate v .

$$\Rightarrow E_{\text{tot}} = f(n)$$

from balance of forces:

$$mv^2 = \frac{Ze^2}{4\pi\epsilon_0 r}$$

$$\Rightarrow E_{\text{tot}} = \frac{1}{2} \left(\frac{Ze^2}{4\pi\epsilon_0 r} \right) - \frac{Ze^2}{4\pi\epsilon_0 r}$$

$$= -\frac{1}{2} \frac{Ze^2}{4\pi\epsilon_0 r}$$

know $r_n = \frac{4\pi\epsilon_0 (n\hbar)^2}{mZe^2}$

$$\Rightarrow E_{\text{tot}} = -\frac{1}{2} \frac{mZ^2e^4}{(4\pi\epsilon_0)^2 (n\hbar)^2} = \frac{-13.6 Z^2}{n^2} \text{ eV}$$

$z=1 \quad n=1$
 $-13.6 \text{ eV} = 1 \text{ Ry}$

- Same result obtained from proper Q.M.
- Energy to change state (or to remove an electron)
- Degenerate w.r.t l, m_l, s

Electron state characterized by 4 QNs: n, l, m_l, s .

simplest: $\psi(r, \theta, \varphi) = A e^{-Zr/a_0}$

$\begin{matrix} \nearrow & \uparrow & \nwarrow \\ n & l & m_l \end{matrix}$
↑ known constant.

1s orbital