$1e^-$ vs multi-electron

- How to write $\hat{H}$?
- Explicit solution not done.
- Nature of solutions.
- Nature of ψ_n

$\hat{H}_n \psi_n = E_n \psi_n$

$dr.r^2.\sin\theta.d\theta.d\phi$

$\psi(r, \theta, \phi) = R(r).Y(\theta, \phi)$

Start: $\hat{H} = \hat{KE} + \hat{PE}$

For $l = 0 \longrightarrow E_n \longrightarrow$ Exact as Bohr soln.

$V = -\frac{e^2}{4\pi\varepsilon_0 r}$

For $l > 0$,

$V_{eff} = -\frac{e^2}{4\pi\varepsilon_0 r} + \frac{l(l+1)\hbar^2}{2\mu r^2}$

For $1e^-$ problem:

KE of nucleus

" " e^-

PE of interaction (Coulomb interaction)

$\mu = \frac{m_e m_{nn}}{m_{nn} + m_e} \simeq m_e$

H-problem

He^+

Li^{2+}

⋮

Radial Distribution function RDF $= r^2 R(r)$

$\frac{d}{dr}(RDF)^2$ & finding minima & maxima

↔ probability

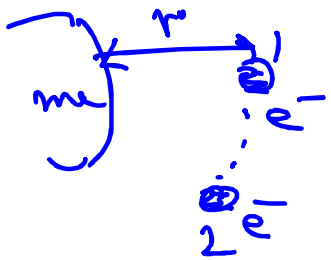
Orbital → $1e^-$ wave f^n. Schrödinger Eqn. → $n \to 1, 2, \ldots$

→ $l \to 0, 1, \ldots (n-1)$

→ $m_l \to (2l+1)$

$\Rightarrow 0, \pm 1, \pm 2, \ldots \pm l.$

$$\hat{H}_{relative} = -\frac{\hbar^2}{2\mu}\nabla^2 - \frac{e^2}{4\pi\varepsilon_0 r}$$



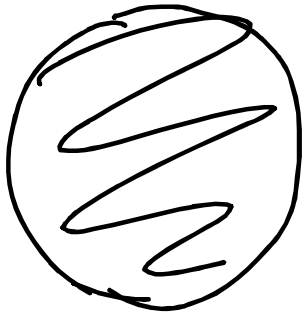
$-$ e^--e^- repulsion

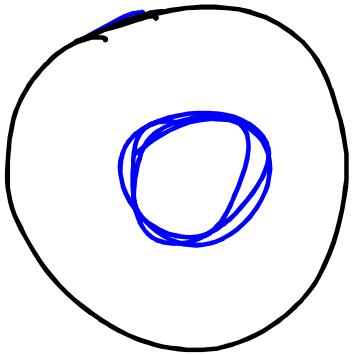
$n = 1$, $n = 2$ $\quad \ell = 0 \quad \alpha \exp\left(-\frac{r}{a_0}\right)$

1s → $r^2 R(r)$

2s → $r^2 R(r)$ → $\left(2 - \frac{r}{a_0}\right) \exp\left(-\frac{r}{2a_0}\right)$ Bohr radius

$(n-1)$ radial nodes.





$\boxed{\ell > 0}$

$\hat{H}\Psi_1 = E\Psi_1$ & $\hat{H}\Psi_2 = E\Psi_2$

$\hat{H}(a\Psi_1 + b\Psi_2) = E(a\Psi_1 + b\Psi_2)$

$\psi_{2,1,0}$ $\psi_{2,1,-1}$ $\psi_{2,1,+1}$

p_0 p_{-1} p_{+1}

$\propto R_{2,\pm1}^{(r)} \cdot \sin\theta \exp(i\phi)$

Real $\begin{cases} R_{2,0}^{(r)} \hookrightarrow \theta \text{ dependent} \\ \phi \text{ independent} \end{cases}$

$\propto R_{2,\pm1}(r) \sin\theta \cdot \exp(-i\phi)$

p_z

$(\psi_{2,1,+1} + \psi_{2,1,-1}) \propto R_{2\pm1} \sin\theta \cdot \cos\phi \rightarrow p_x$

$(\quad " \quad - \quad " \quad) \propto R_{2\pm1} \sin\theta \cdot \sin\phi \rightarrow p_y$

Hybridization $\Rightarrow$ $E \simeq E'$ $\longrightarrow$

$l = 0$: S - orbital
$= 1$: p - ..
$= 2$: d - ..

Total # of Nodes $\rightarrow n-1$
Radial # of Nodes $\rightarrow n-l-1$

k^- $\longrightarrow$ H-like Rydberg Atoms

Multi-e^- $\longrightarrow$ Molecules

$e^- - e^-$ repulsion ignored

Frozen fixed distance between the nuclei