Chem 2271 Sept 17/18

Orbitals Representations

- wave functions (after they are solved) can be written as the product of a radial function $R_{n,\ell}(r)$ r = radius
  - ↳ the radial component defines n and ℓ and is a function of the distance from the nucleus (r)

...

- and the angular components/coordinates of a point (e^-) within the spherical radius $Y_{\ell, m_\ell}(\theta, \phi)$
  - ↳ the angular component defines ℓ and m_ℓ and is a function of θ and ϕ

→ Table 1.2 and figure 1.4 from textbook

- Both the radial and angular components get more complex as the various quantum #'s increase (ie n, ℓ, m_ℓ)

$$\Psi_{n,\ell,m_\ell} = R_{n,\ell}(r) \times Y_{\ell,m_\ell}(\theta, \phi)$$

- from figure 1.4
  - ↳ black lines = cartesian coordinates
  - ↳ pink lines = spherical coordinates

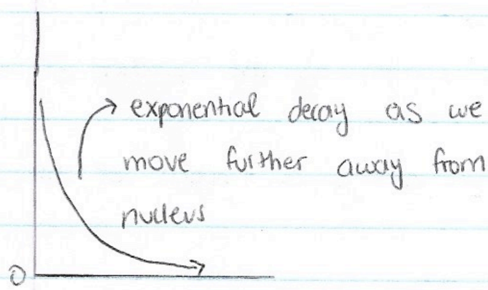
So why do we care about all this?

- ↳ by appreciating these details, we can begin to define the shapes of the orbitals
- ↳ this is our best tool to describe hydrogen-like orbitals (not a math class)

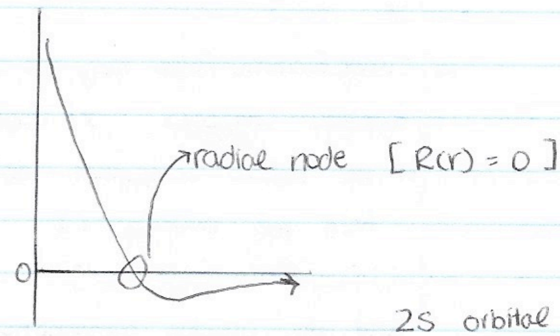
Radial Variation

- qualitatively, all orbitals decay exponentially from the nucleus
  - ↳ farther away from nucleus, less chance of finding e^-

Radial Nodes - occur where the radial components of the wavefunction passes through ~~zero~~ zero



1s orbital



2s orbital

* wavefunction can have +ve or -ve values

figure 1.6 contains: 3p, 3d, 4p, 2p

* wavefunction tends to be more complex as the quantum numbers increase. we can predict the #'s of radial nodes easily

*→ radial nodes = $n - \ell - 1$ (important, can be tested)

example:

1s e⁻ : $n = 1$, $\ell = 0$, $m_\ell = 0$, $m_s = \pm 1/2$, $s = 1/2$

↳ magnitude of spin

* radial nodes = 1 - 0 - 1 = 0

↳ ∴ no radial nodes (figure 1.5)

3p e⁻ : $n = 3$, $\ell = 1$, $m_\ell = \pm 1, 0$, $m_s = \pm 1/2$, $s = 1/2$

* radial nodes = 3 - 1 - 1 = 1

3d e⁻ : $n = 3$, $\ell = 2$, $m_\ell = \pm 2, \pm 1, 0$, $m_s = \pm 1/2$, $s = 1/2$

* radial nodes = 3 - 2 - 1 = 0

- the probability of finding an e^- in a spherical shell of radius r and thickness dr over all angles is:

$$P(r)dr = \int \Psi^2 \, d\tau$$

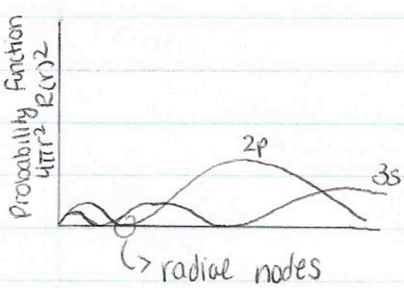
↑ overall all angles

- where $P(r)$ is the radial distribution function (probability)

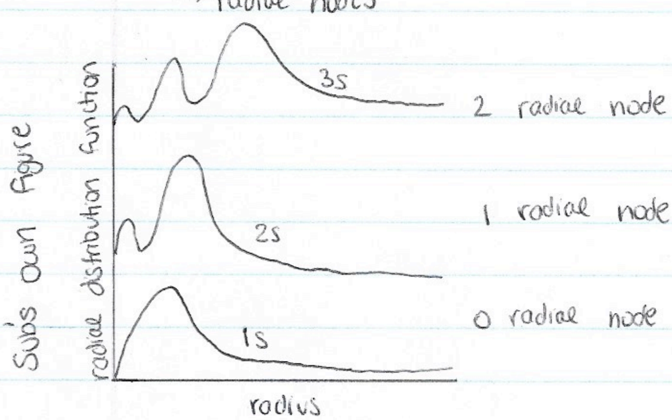
$$P(r) = 4\pi r^2 R(r)^2 \quad \text{or} \quad P(r) = 4\pi r^2 R^2$$

↑ depends on radius

→ Figure's 1.7 + alternative



* note all probability functions only have + or 0 values



↳ denotes radial nodes (shells of 0 probability) where $\Psi = 0$ and $\Psi^2 = 0$

↳ remember to consider these radial distributions like onions