Atoms Lecture 3: Hydrogen Atom

Learning Objective	Openstax 2e Chapter
Quantum theory for Hydrogen Atom	6.3
Orbital Quantum Numbers	6.3
3-Dimensional Representations of the Hydrogen Orbitals	6.3

Suggested Practice Problems

Chapter 6 Exercises – Questions: 41

Answers can be found in the Chapter 6 Answer Key

Hydrogen Atom

Based on Schrödinger's equation, how is the electron distributed around the nucleus?

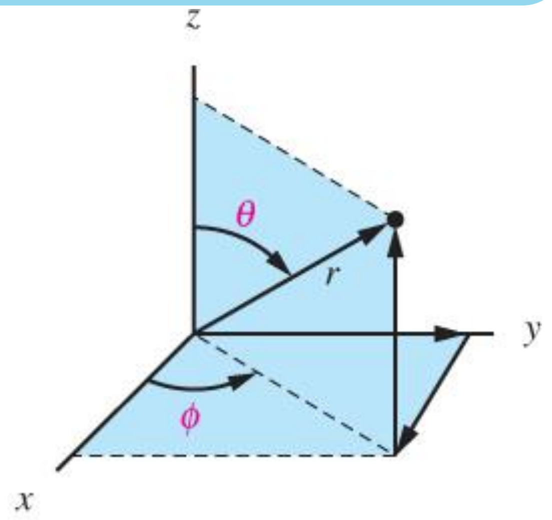
$$\hat{H}\psi = E\psi$$

E: Energy
ψ: wave function
$\hat{H}$: Hamiltonian Operator

$$\begin{cases} \psi_{n,\ell,m_\ell}(r,\theta,\phi) = R_n(r)Y_{\ell,m_\ell}(\theta,\phi) \\ E_n = -\dfrac{R_\mathrm{H}}{n^2} \qquad n = 1,2,3,\cdots \end{cases}$$

- **R(r)** describes how ψ changes as we move away from the nucleus
  - Called the radial function
- **Y($\boldsymbol{\theta}$, $\boldsymbol{\phi}$)** describes how ψ changes as we move around the nucleus
  - Called the angular function
- $\boldsymbol{n}, \boldsymbol{\ell}, \boldsymbol{m_\ell}$ are quantum numbers
  (integers with rules about relative values)

Each unique set of $\boldsymbol{n}, \boldsymbol{\ell}, \boldsymbol{m_\ell}$ will give a different wavefunction.



Spherical polar coordinates
$x^2 + y^2 + z^2 = r^2$
$x = r \sin\theta \cos\phi$
$y = r \sin\theta \sin\phi$
$z = r \cos\theta$

Quantum Numbers

n, ℓ, m_ℓ are related to each other so you have to choose them in a specific order

n → Principal Quantum Number → Principal Shell

- Can take on positive integer values
  (n = 1, 2, 3, 4, …)
- Determines the energy of the orbital
- Determines the **most probable distance** of finding an electron from the nucleus

ℓ → Orbital Angular Momentum Quantum Number → Sub Shell

- Restricted integer numbers < n
- Can take on positive integer values from 0 to n-1
  - e.g. if n = 5, ℓ = 0, 1, 2, 3, and 4
- Determines the **shape** of the orbital

m_ℓ → Magnetic Quantum Number → Orbital

- Determined by the value of ℓ
- Can take on integer values from $-\ell$ to $+\ell$
  - e.g. if ℓ = 3, m_ℓ = -3, -2, -1, 0, 1, 2 and 3
- Determines the **orientation** of the orbital

Quantum Numbers: Notation

- Different sub-shells are given different labels
- Labels depend on the value of ℓ
- Labels are related to the shapes of the orbitals (later slides)

Notation:

- $\ell = 0 \rightarrow$ label = s
- $\ell = 1 \rightarrow$ label = p
- $\ell = 2 \rightarrow$ label = d
- $\ell = 3 \rightarrow$ label = f

- To completely specify the sub-shell we also have to include the principal quantum number, *n*
- We do this by putting *n* in front of the label

Examples:

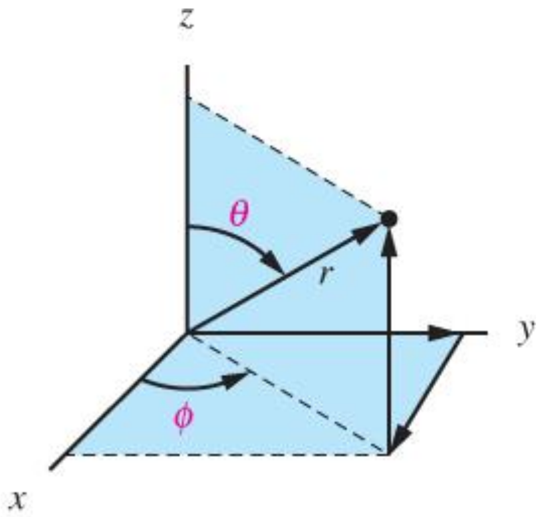
- n = 3, $\ell = 1 \rightarrow$ 3p
- n = 2, $\ell = 1 \rightarrow$ 2p
- n = 2, $\ell = 0 \rightarrow$ 2s
- n = 2, $\ell = 3 \rightarrow$ not allowed

Hydrogen Atom

Based on Schrödinger's equation, how is the electron distributed around the nucleus?

$$\psi_{n,\ell,m_\ell}(r,\theta,\phi) = R_n(r)Y_{\ell,m_\ell}(\theta,\phi)$$

$$E_n = -\frac{R_H}{n^2} \qquad n = 1, 2, 3, \cdots$$



Spherical polar coordinates
$x^2 + y^2 + z^2 = r^2$
$x = r \sin\theta \cos\phi$
$y = r \sin\theta \sin\phi$
$z = r \cos\theta$

E	Subshells			Shell
	$3s$ —	$3p$ — — —	$3d$ — — — — —	$n = 3$
	$2s$ —	$2p$ — — —		$n = 2$
	$1s$ —			$n = 1$
	$\ell = 0$	$\ell = 1$	$\ell = 2$	
	$m_\ell = 0$	$m_\ell = -1, 0, +1$	$m_\ell = -2, -1, 0, +1, +2$	

Angular momentum quantum number → ℓ

Magnetic quantum number → m_ℓ

Principal quantum number → n

Each subshell is made up of $(2\ell + 1)$ orbitals.

How do the Hydrogen orbitals look?

We should look at the 3D probability density distributions of various Hydrogen orbitals.

$$\psi_{n,\ell,m_\ell}(r,\theta,\phi) = R_{n,\ell}(r)Y_{\ell,m_\ell}(\theta,\phi) \quad \rightarrow \quad \left(\psi_{n,\ell,m_\ell}(r,\theta,\phi)\right)^2 = ?$$

$$E_n = -\frac{R_\mathrm{H}}{n^2}$$

The quantum numbers are:

$$n = 1, 2, 3, \cdots$$

$$\ell = 0, 1, \cdots, n-1$$

$$m_\ell = -\ell, \cdots, 0, \cdots, +\ell$$

n	***ℓ***	***m_l***	***type***	***# orbitals***
1	0	0	1s	1
2	0	0	2s	1
	1	-1,0,+1	2p	3
3	0	0	3s	1
	1	-1,0,+1	3p	3
	2	-2,-1,0,+1,+2	3d	5

Degenerate Orbitals

Radial Function of Hydrogen Orbitals

$$\psi(x,y,z) = \psi_{n,\ell,m_\ell}(r,\theta,\phi) = \boxed{R_{n,\ell}(r)}\, Y_{\ell,m_\ell}(\theta,\phi)$$

 # radial nodes = $\boldsymbol{n - \ell - 1}$

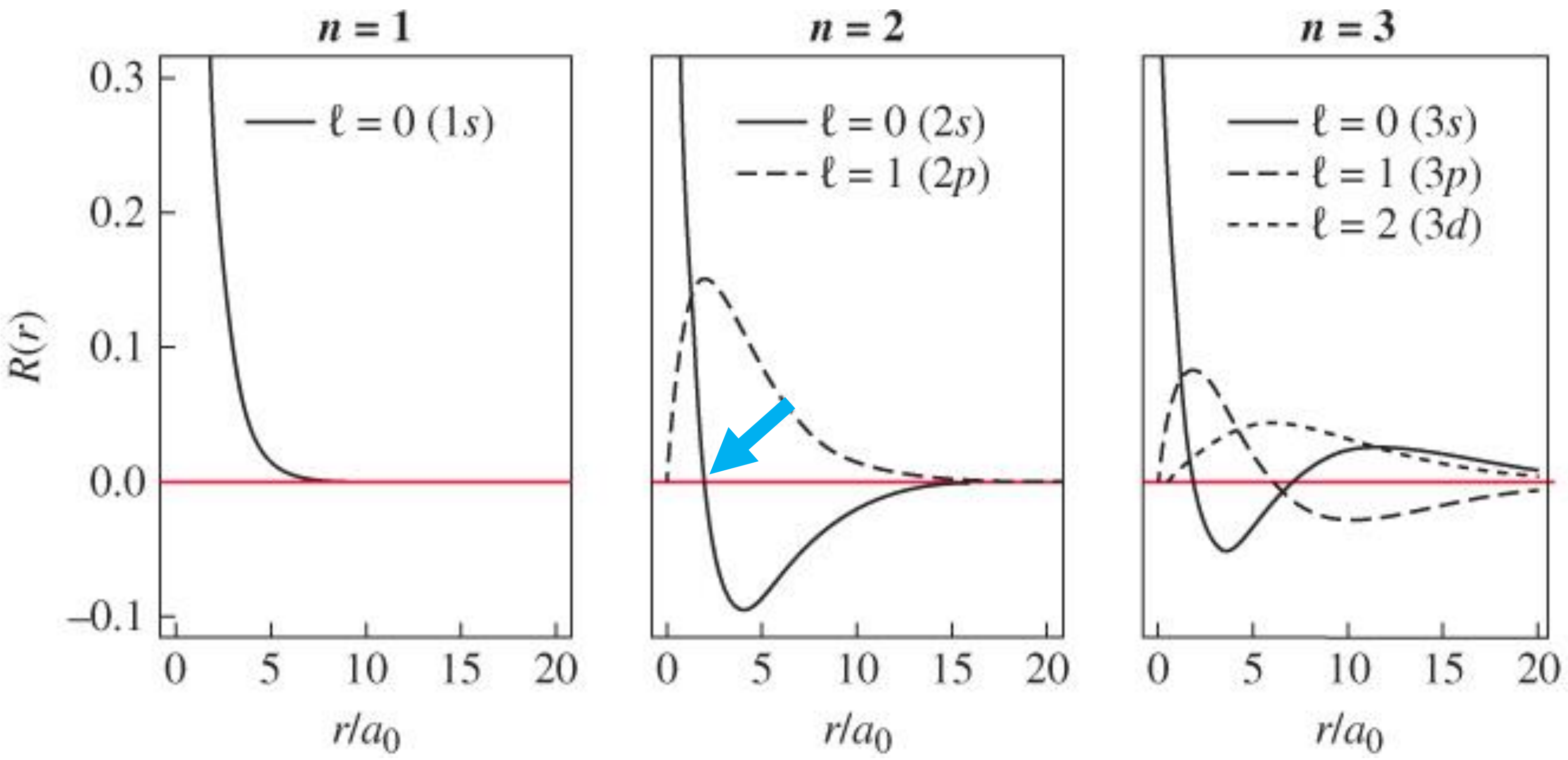


Figure 1: Radial functions of Hydrogen Orbitals

Bohr radius: a_0 = 5.29177x10^{-11} m = 0.529177 angstrom

- $R_{n\ell}(r)$ has its maximum at $r = 0$ for *s* orbitals, whereas for other orbitals it has a zero value at $r = 0$.

Angular Function of Hydrogen Orbitals

$$\psi(x,y,z) = \psi_{n,\ell,m_\ell}(r,\theta,\phi) = R_{n,\ell}(r)\boxed{Y_{\ell,m_\ell}(\theta,\phi)}$$

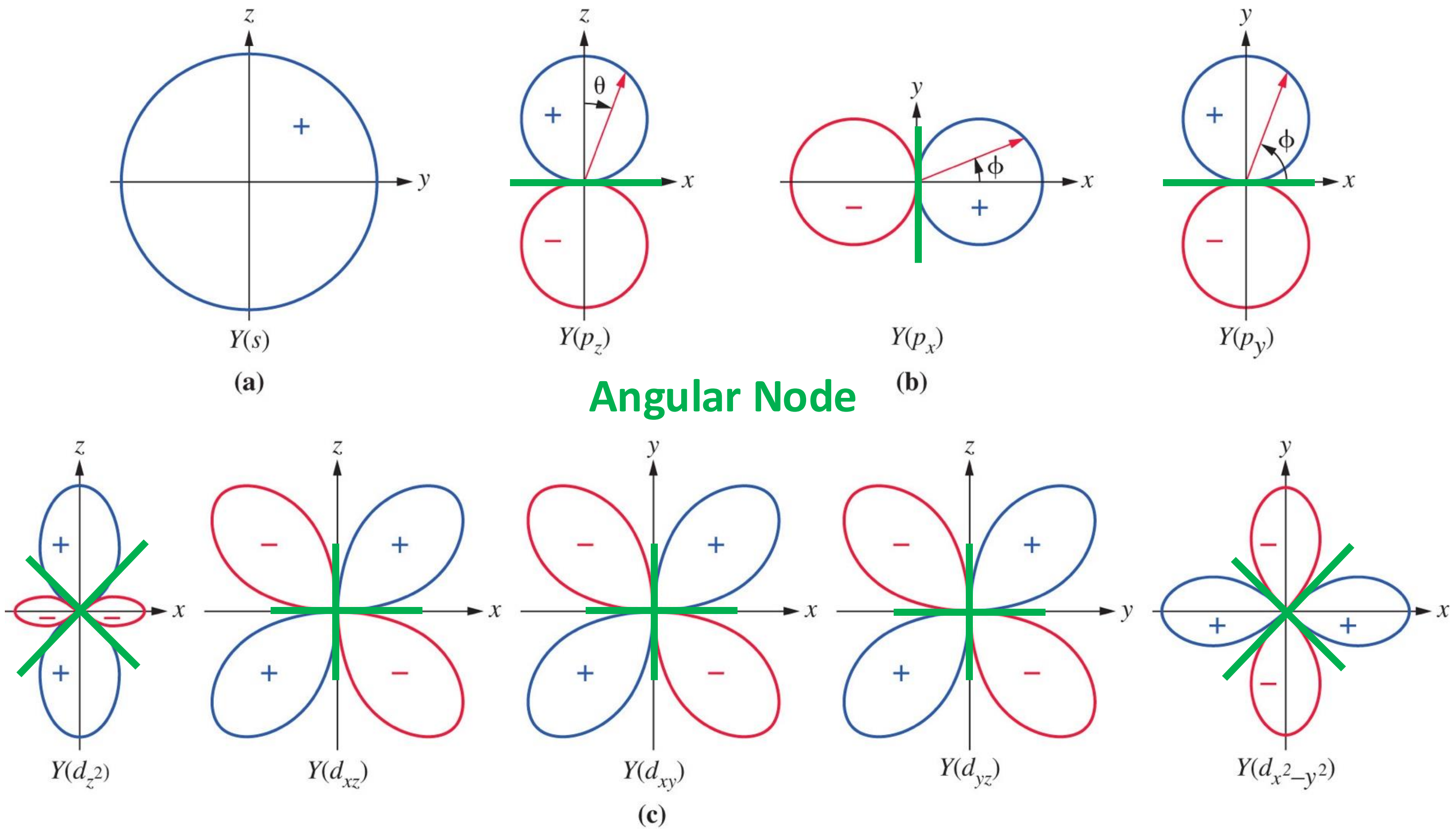


Figure 2: Cross-sections of the angular functions of the s, p, and d orbitals.

 # angular nodes = ℓ

***s*-orbitals**

- have no angular dependence
- posses 0 angular nodes

***p*-orbitals**

- have identical shape but orient differently in space
- posses 1 angular node

***d*-orbitals**

- are more complicated
- posses 2 angular nodes

s-orbitals of Hydrogen Atom

We do __not__ expect you to know (memorize) these wavefunction equations, but we show them so you can see where the shapes come from

$$\psi(1s) = \overbrace{R(r)}^{\text{radial function}} \times \underbrace{Y(\theta,\phi)}_{\text{angular function}} = \frac{2e^{-r/a_0}}{a_0^{3/2}} \times \frac{1}{\sqrt{4\pi}} = \boxed{\frac{e^{-r/a_0}}{\sqrt{(\pi a_0^3)}}}$$

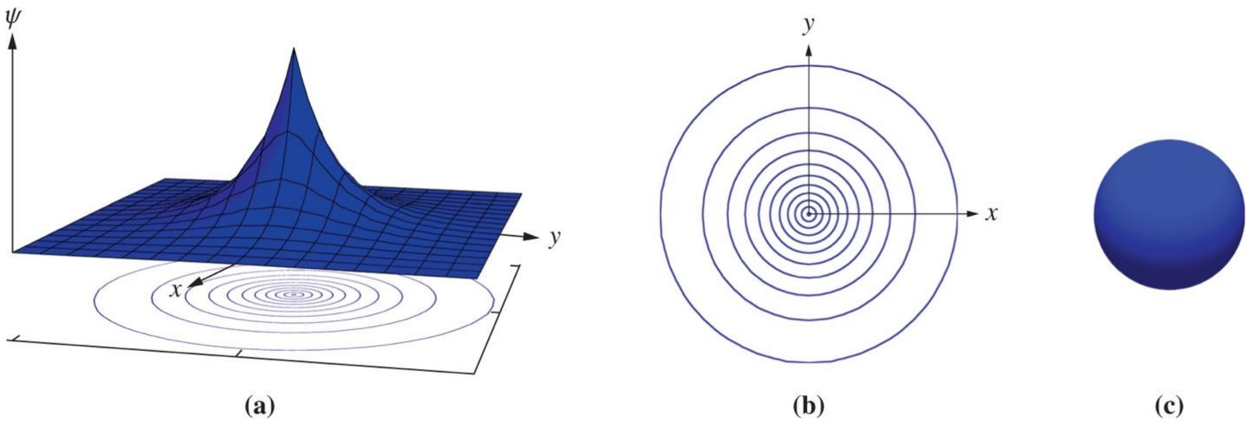


Figure 3: Wave function of the 1*s* orbital.

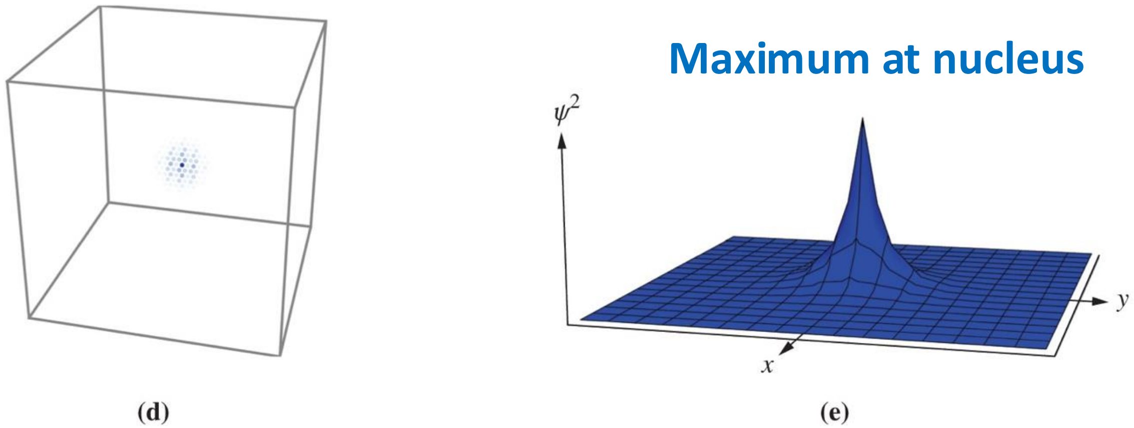
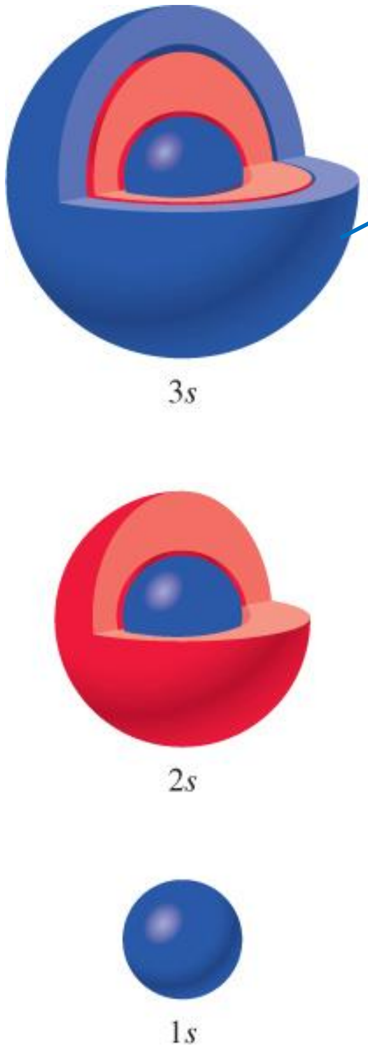


Figure 4: Electron probability density of the 1*s* orbital.

s-orbitals of Hydrogen Atom

For s-orbitals ($\ell = 0$), the ψ^2 only depends on r. What makes s orbitals different when n=1, 2, 3…?

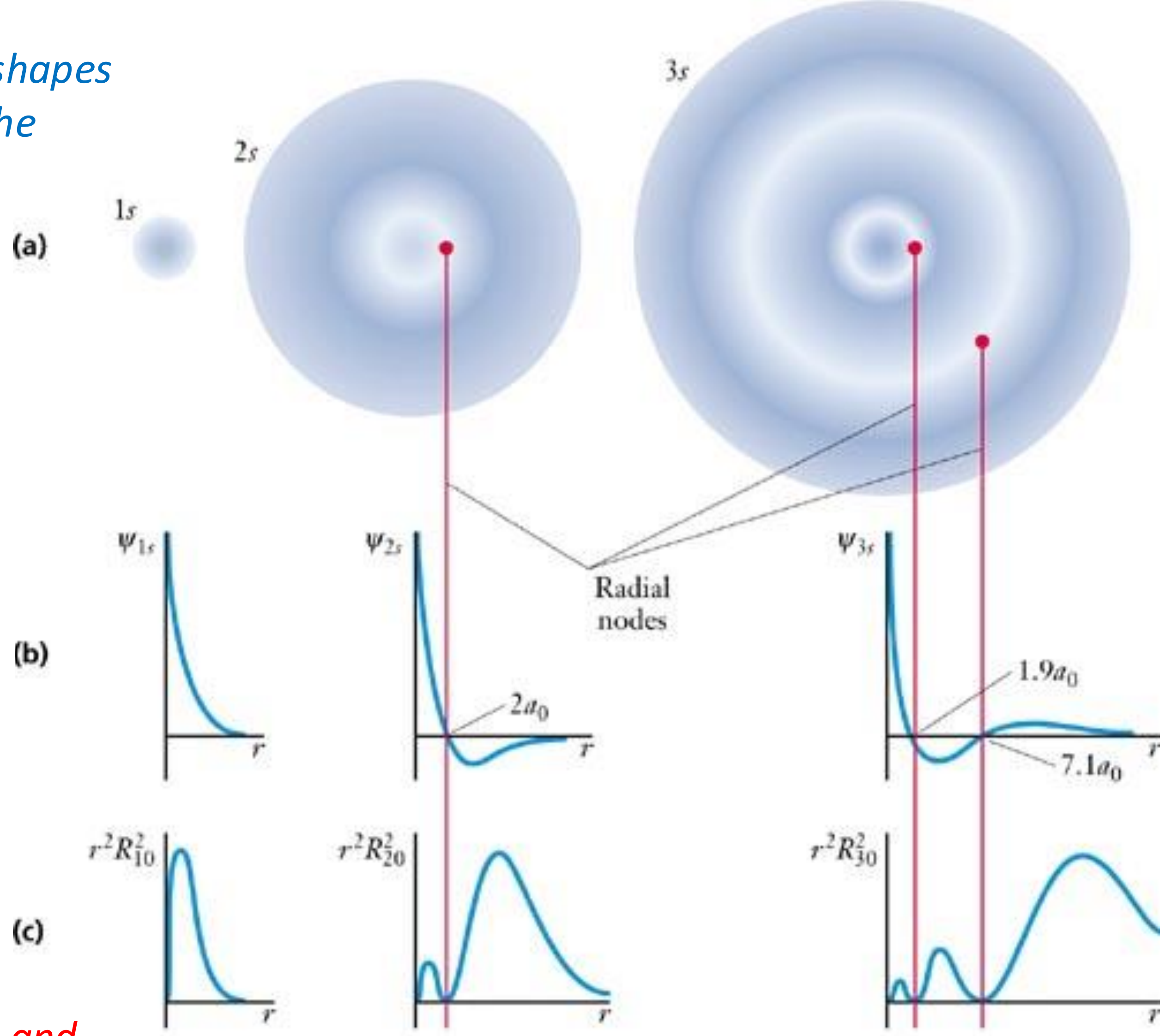


The surfaces of these 3D shapes represent where 95% of the electron density is found

Size & # nodes increases

Wave function

Radial Probability



We expect you to know (memorize) the 3D shape of s orbitals and the number of nodes in the radial distribution, but not the equations

p-orbitals of Hydrogen Atom

*We do **not** expect you to know (memorize) these wavefunction equations, but we show them so you can see where the shapes come from*

$$\psi(2p_x) = R(r) \times Y(\theta,\phi) = \frac{1}{2\sqrt{6}}\frac{1}{a_0^{3/2}}e^{-r/2a_0} \times \left(\frac{3}{4\pi}\right)^{1/2}\sin(\theta)\cos(\phi) = \boxed{\frac{1}{4}\left(\frac{1}{2\pi a_0^3}\right)^{1/2} e^{-r/2a_0}\sin(\theta)\cos(\phi)}$$

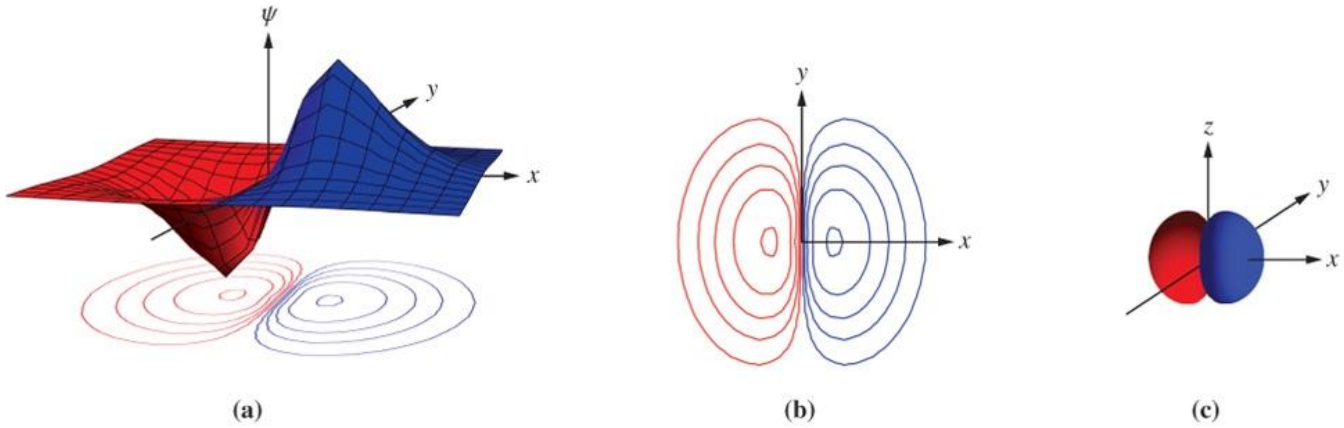
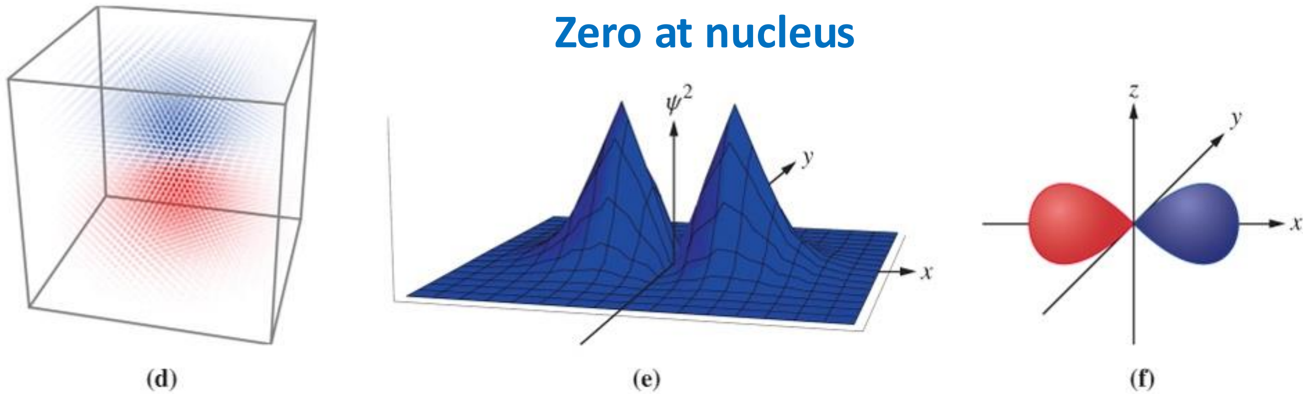


Figure 5: Wave function of the $2p_x$ orbital.

Figure 6: Electron probability density of the $2p_x$ orbital.



p-orbitals and *d*-orbitals of Hydrogen Atom

Figure 7: Simplified representation of the three *2p* orbitals

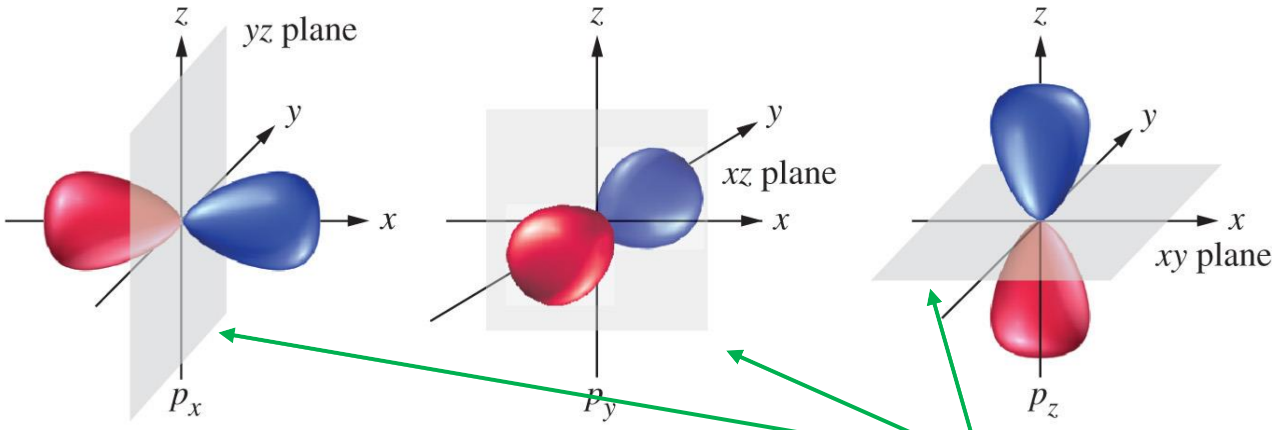
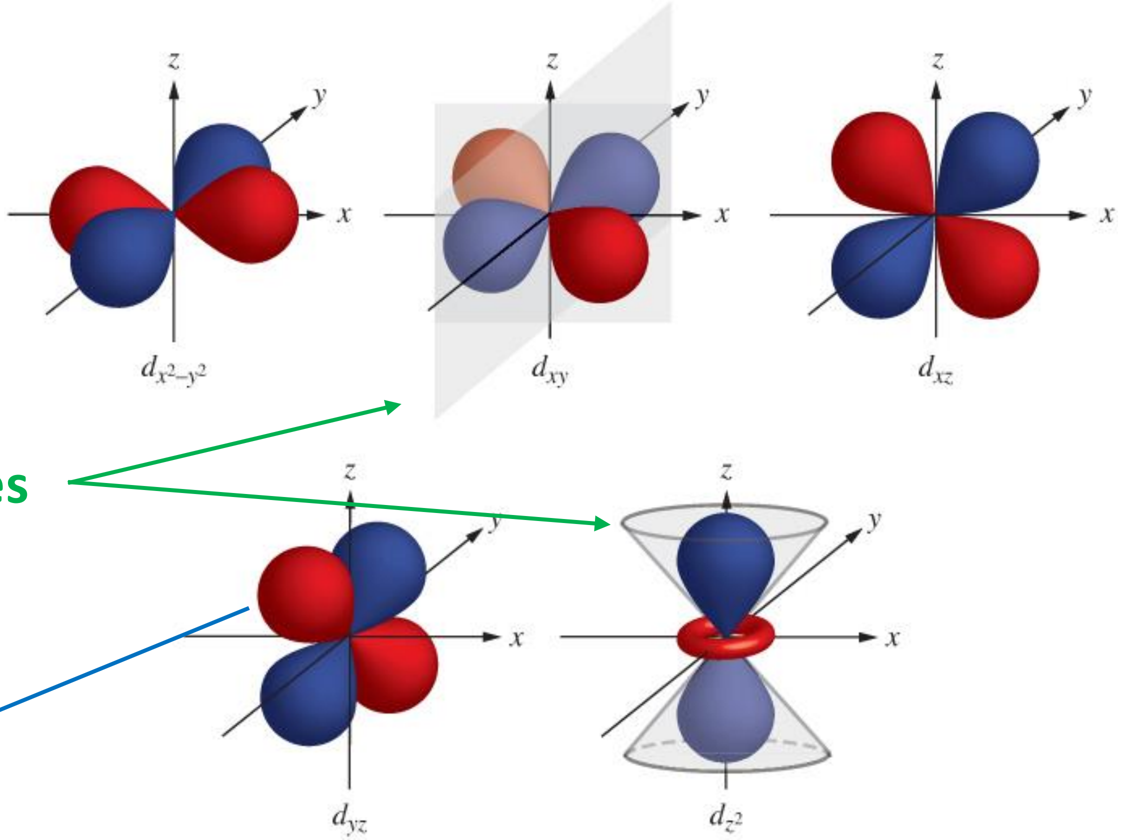


Figure 8: Simplified representation of the five 3*d* orbitals



Nodal Surfaces

The surfaces of these 3D shapes represents where 95% of the electron density is found

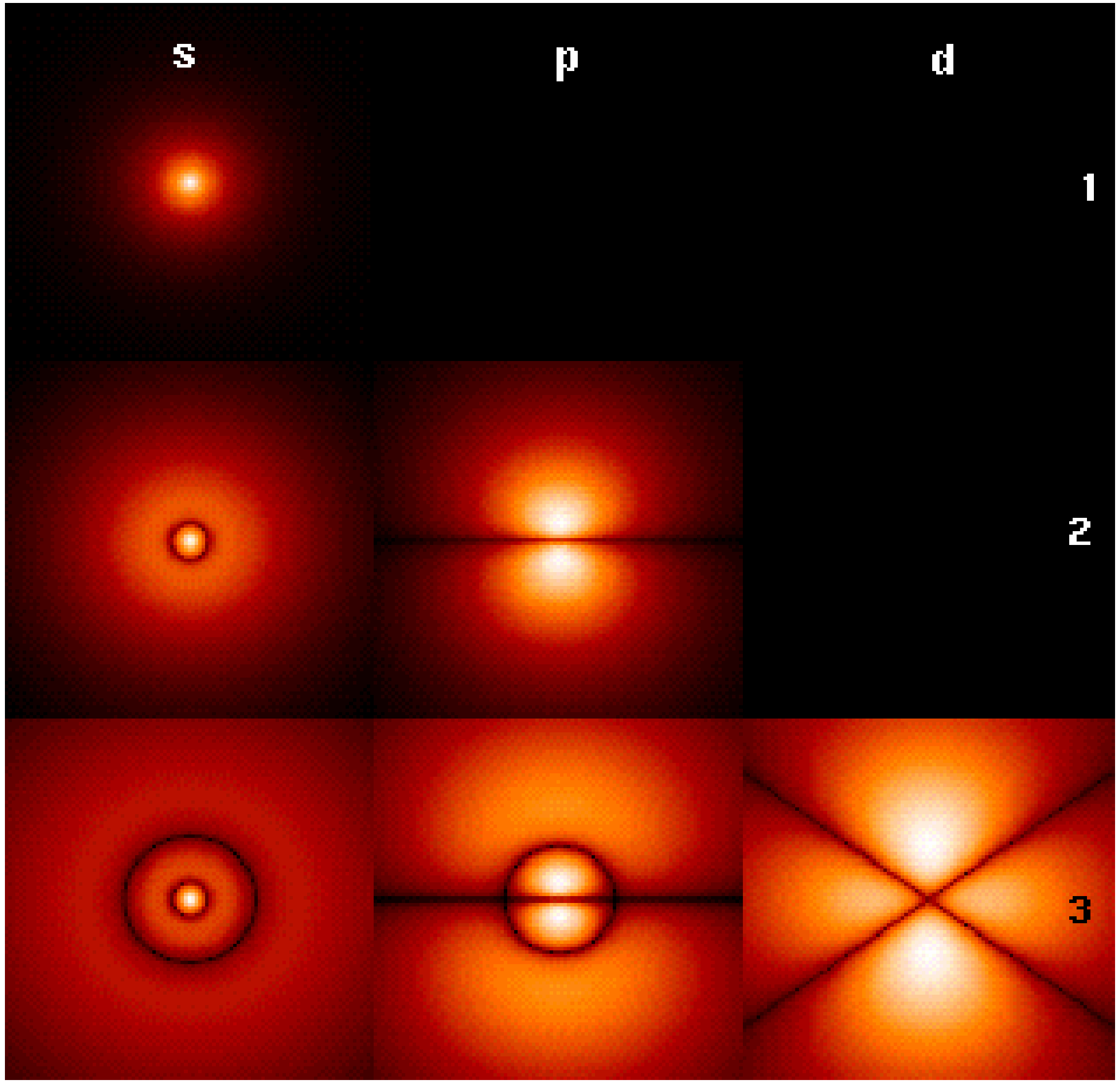
We expect you to know (memorize) the 3D shape of p orbitals and the number of nodal planes or surfaces

Hydrogen Atom

Based on Schrödinger's equation, how is the electron distributed around the nucleus?

Angular momentum quantum number (ℓ)

Probability densities through the *xz*-plane for the electron at different quantum numbers for $m_\ell = 0$.



Principal quantum number (n)

Source: https://en.wikipedia.org/wiki/Hydrogen_atom