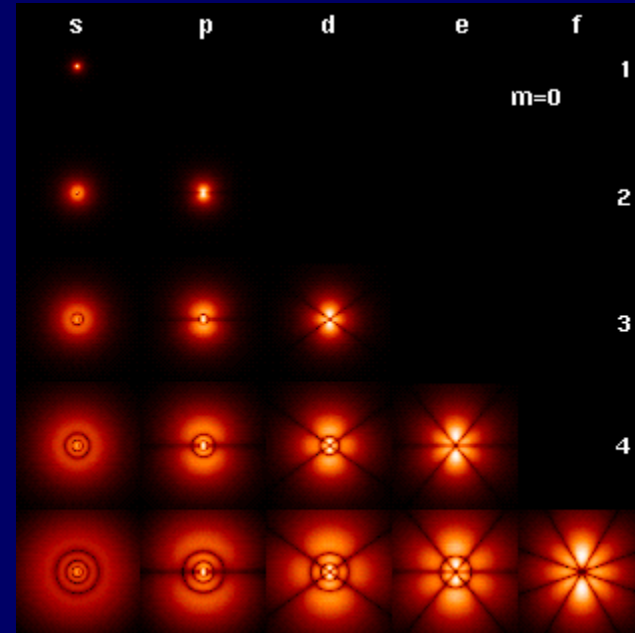


Physics 102: Lecture 25

Atomic Spectroscopy & Quantum Atoms



PICK UP A DIFFRACTION GRATING!

From last lecture – Bohr model

Angular momentum is quantized

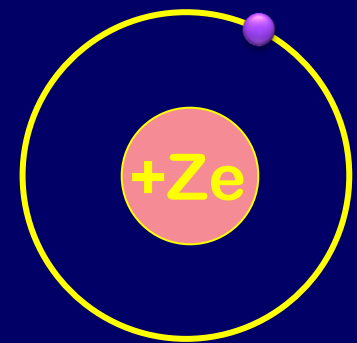
$$L_n = nh/2\pi \quad n = 1, 2, 3 \dots$$

Energy is quantized

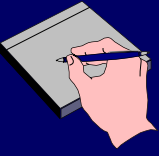
$$E_n = -\frac{mk^2e^4}{2\hbar^2} \frac{Z^2}{n^2} \approx -\frac{13.6 \cdot Z^2}{n^2} \text{ eV} \quad (\text{where } \hbar \equiv h/2\pi)$$

Radius is quantized

$$r_n = \left(\frac{h}{2\pi}\right)^2 \frac{1}{mke^2} \frac{n^2}{Z} = (0.0529 \text{ nm}) \frac{n^2}{Z}$$



Velocity too!



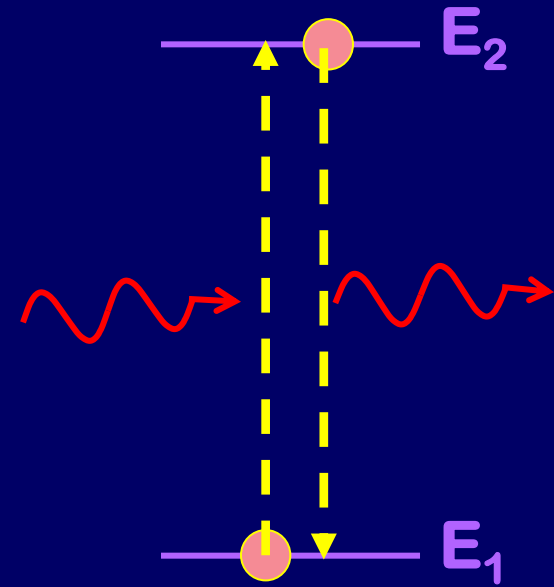
Transitions + Energy Conservation

- Each orbit has a specific energy:

$$E_n = -13.6 Z^2 / n^2$$

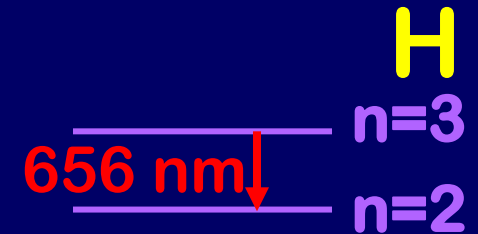
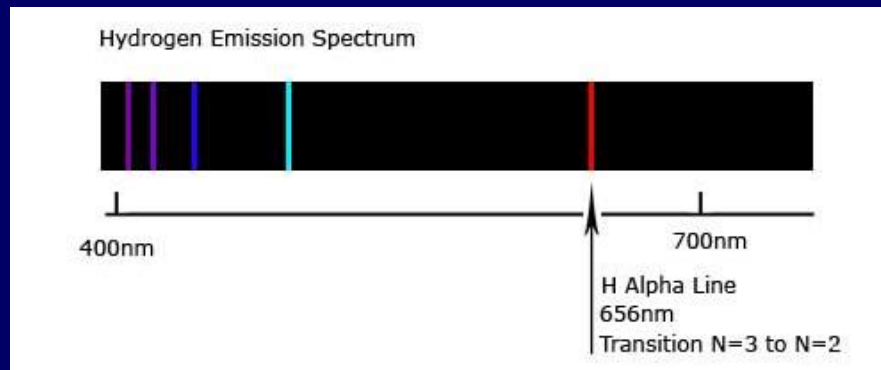
- Photon emitted when electron jumps from high energy to low energy orbit. Photon absorbed when electron jumps from low energy to high energy:

$$E_2 - E_1 = hf = hc / \lambda$$



Demo: Line Spectra

In addition to the continuous blackbody spectrum, elements emit a discrete set of wavelengths which show up as lines in a diffraction grating.



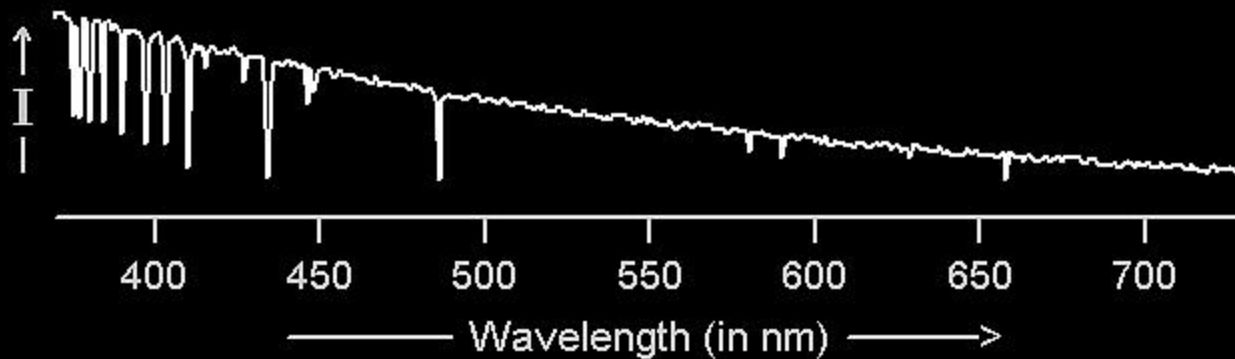
This is how neon signs & Na lamps work!

Spectra give us information on atomic structure

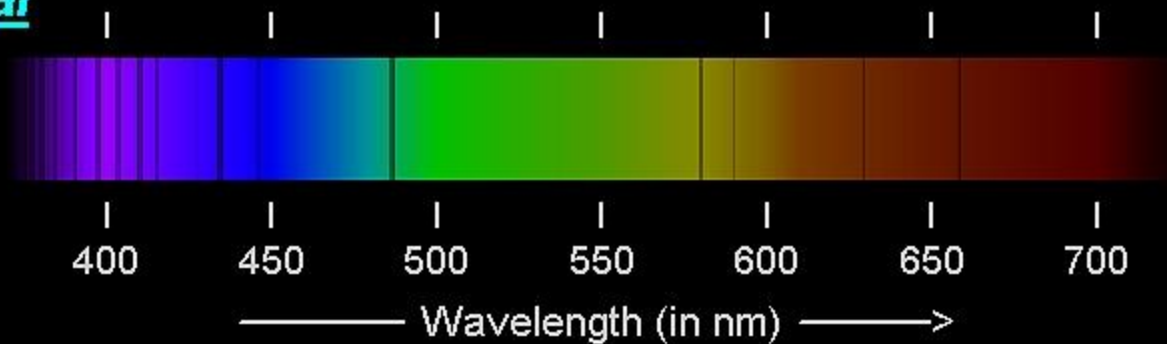


Solar spectrum!

Graphical



Visual





Checkpoint 1.1

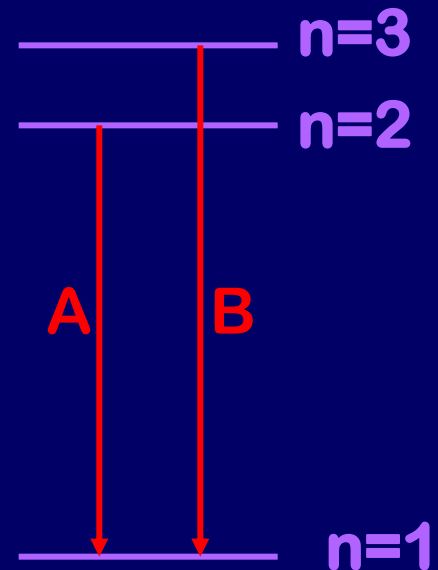
Electron A falls from energy level $n=2$ to energy level $n=1$ (ground state), causing a photon to be emitted.

Electron B falls from energy level $n=3$ to energy level $n=1$ (ground state), causing a photon to be emitted.

Which photon has more energy?

1) Photon A

2) Photon B

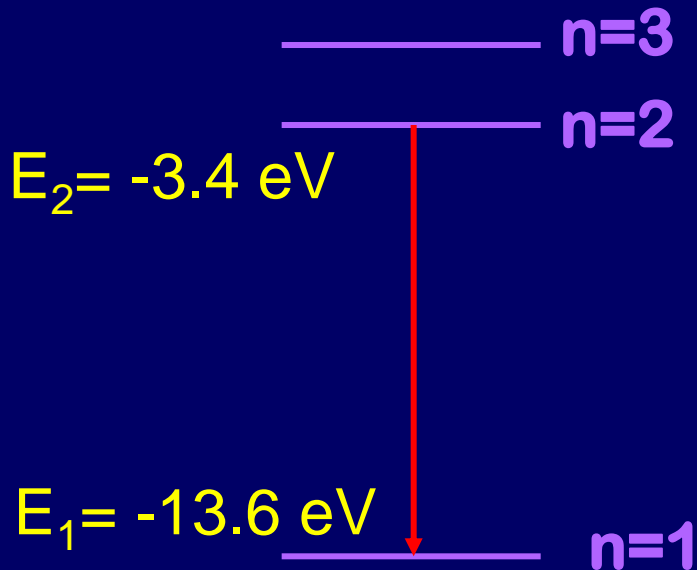


Example



Spectral Line Wavelengths

Calculate the wavelength of photon emitted when an electron in the hydrogen atom drops from the $n=2$ state to the ground state ($n=1$).



$$E_n = -13.6 \text{ eV} \frac{Z^2}{n^2}$$

$$hf = E_2 - E_1$$

$$= -3.4 \text{ eV} - (-13.6 \text{ eV}) = 10.2 \text{ eV}$$

$$E_{\text{photon}} = \frac{hc}{\lambda}$$

$$\lambda = \frac{hc}{10.2 \text{ eV}} = \frac{1240}{10.2} \approx 124 \text{ nm}$$



ACT: Spectral Line Wavelengths

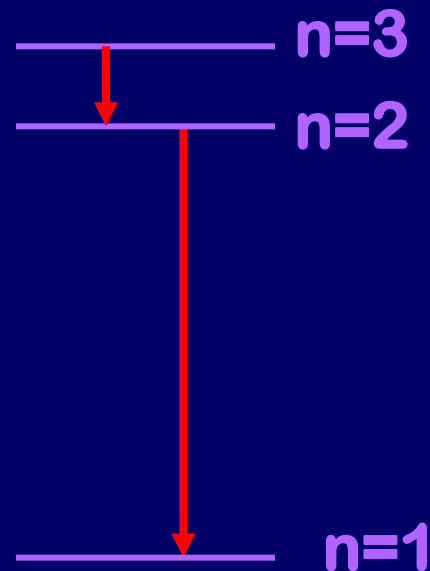
Compare the wavelength of a photon produced from a transition from $n=3$ to $n=2$ with that of a photon produced from a transition $n=2$ to $n=1$.

(A) $\lambda_{32} < \lambda_{21}$

(B) $\lambda_{32} = \lambda_{21}$

(C) $\lambda_{32} > \lambda_{21}$

$E_{32} < E_{21}$ so $\lambda_{32} > \lambda_{21}$





ACT/Checkpoint 1.2

The electrons in a large group of hydrogen atoms are excited to the $n=3$ level. How many spectral lines will be produced?

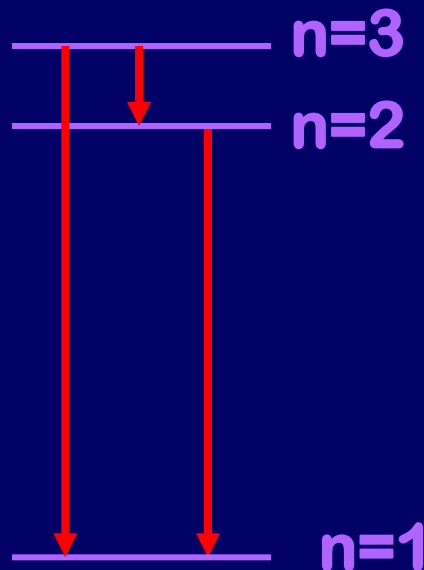
A. 1

B. 2

C. 3

D. 4

E. 5



The Bohr Model is incorrect!

To be consistent with the Heisenberg Uncertainty Principle, which of these properties cannot be quantized (have the exact value known)? (A=OK B= NOT)

Electron Radius

← **Would know location**

Electron Energy

Electron Velocity

← **Would know momentum**

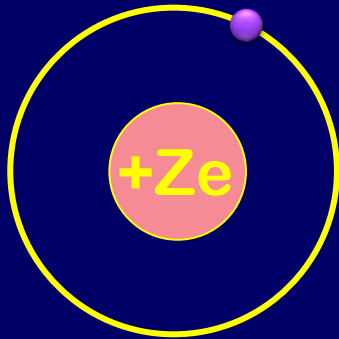
Electron Angular Momentum

But, in the Bohr model:

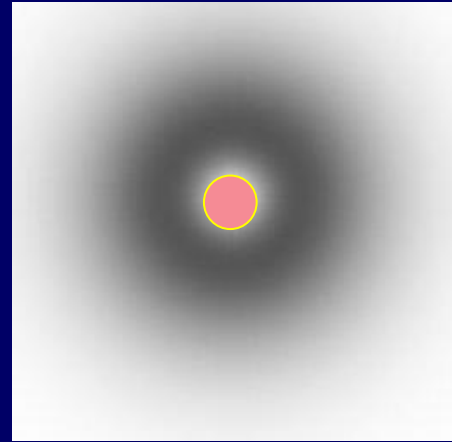
$$r_n = \left(\frac{h}{2\pi} \right)^2 \frac{1}{mke^2} \frac{n^2}{Z} = (0.0529 \text{ nm}) \frac{n^2}{Z}$$

**Quantized radii
and velocities for
electron orbitals**

Checkpoint 2



Bohr Model



Quantum Atom

So what keeps the electron from “sticking” to the nucleus?

- 21% **A) Centripetal Acceleration**
- 36% **B) Pauli Exclusion Principle**
- 42% **C) Heisenberg Uncertainty Principle**

Quantum Mechanics

Theory used to predict probability distributions



Quantum Mechanical Atom

- Predicts available energy states agreeing with Bohr.
- Don't have definite electron position, only a probability function.
- Each orbital can have 0 angular momentum!
- Each electron state labeled by 4 numbers:

n = principal quantum number (1, 2, 3, ...)

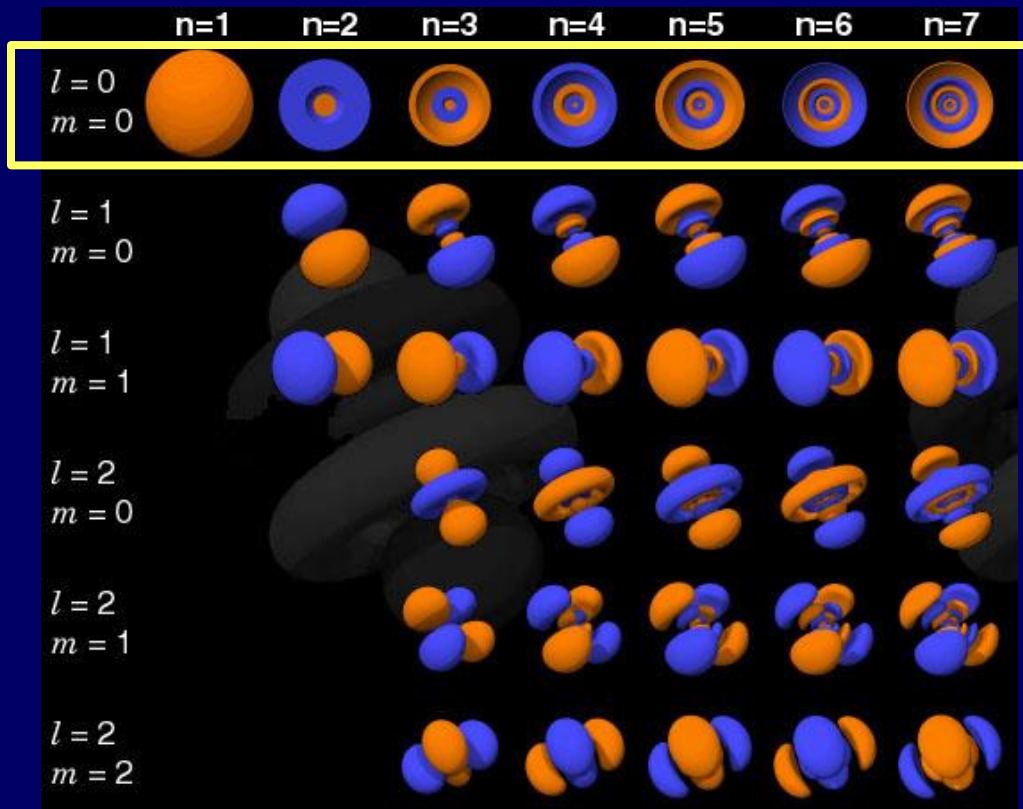
ℓ = angular momentum (0, 1, 2, ... $n-1$)

m_ℓ = component of ℓ ($-\ell < m_\ell < \ell$)

m_s = spin ($-1/2$, $+1/2$)

Quantum Mechanics (vs. Bohr)

Electrons are described by a probability function,
not a definite radius!



It takes 4 numbers to
describe the electron

Bohr: just n

Each orbital n can
have 0 angular
momentum

Bohr: $L_n = n \hbar$
 $n = 1, 2, 3 \dots$

Quantum Numbers

Each electron in an atom is labeled by 4 #'s

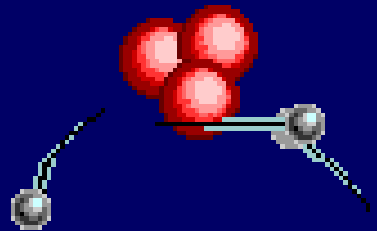
n = Principal Quantum Number (1, 2, 3, ...)

- Determines the Bohr energy

ℓ = Orbital Quantum Number (0, 1, 2, ... $n-1$)

- Determines angular momentum
- $\ell < n$ always true!

$$L = \sqrt{\ell(\ell + 1)} \frac{h}{2\pi}$$



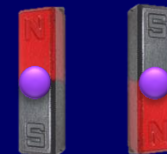
m_ℓ = Magnetic Quantum Number ($-\ell$, ... 0, ... ℓ)

- z-component of ℓ
- $|m_\ell| \leq \ell$ always true!

$$L_z = m_\ell \frac{h}{2\pi}$$

m_s = Spin Quantum Number ($-1/2$, $+1/2$)

- “Up Spin” or “Down Spin”





ACT: Quantum numbers

For which state of hydrogen is the orbital angular momentum **required** to be zero?

1. $n=1$

2. $n=2$

3. $n=3$

The allowed values of ℓ are 0, 1, 2, ..., $n-1$. When $n=1$, ℓ must be zero.



Spectroscopic Nomenclature

“Shells”

$n=1$ is “**K shell**”

$n=2$ is “**L shell**”

$n=3$ is “**M shell**”

$n=4$ is “**N shell**”

$n=5$ is “**O shell**”

“Subshells”

$\ell=0$ is “**s state**”

$\ell=1$ is “**p state**”

$\ell=2$ is “**d state**”

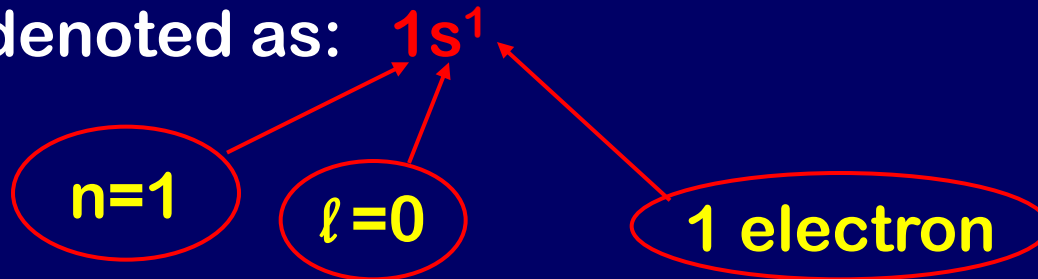
$\ell=3$ is “**f state**”

$\ell=4$ is “**g state**”

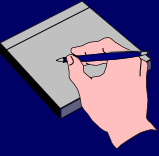
Example

1 electron in ground state of Hydrogen:

$n=1, \ell=0$ is denoted as: **$1s^1$**



Example



Quantum Numbers

How many unique electron states exist with $n=2$?

$$\ell = 0 : 2s^2$$

$$m_\ell = 0 : m_s = \frac{1}{2}, -\frac{1}{2} \quad 2 \text{ states}$$

$$\ell = 1 : 2p^6$$

$$m_\ell = +1 : m_s = \frac{1}{2}, -\frac{1}{2} \quad 2 \text{ states}$$

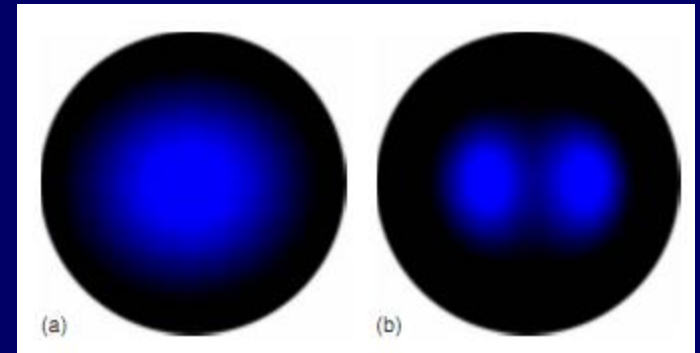
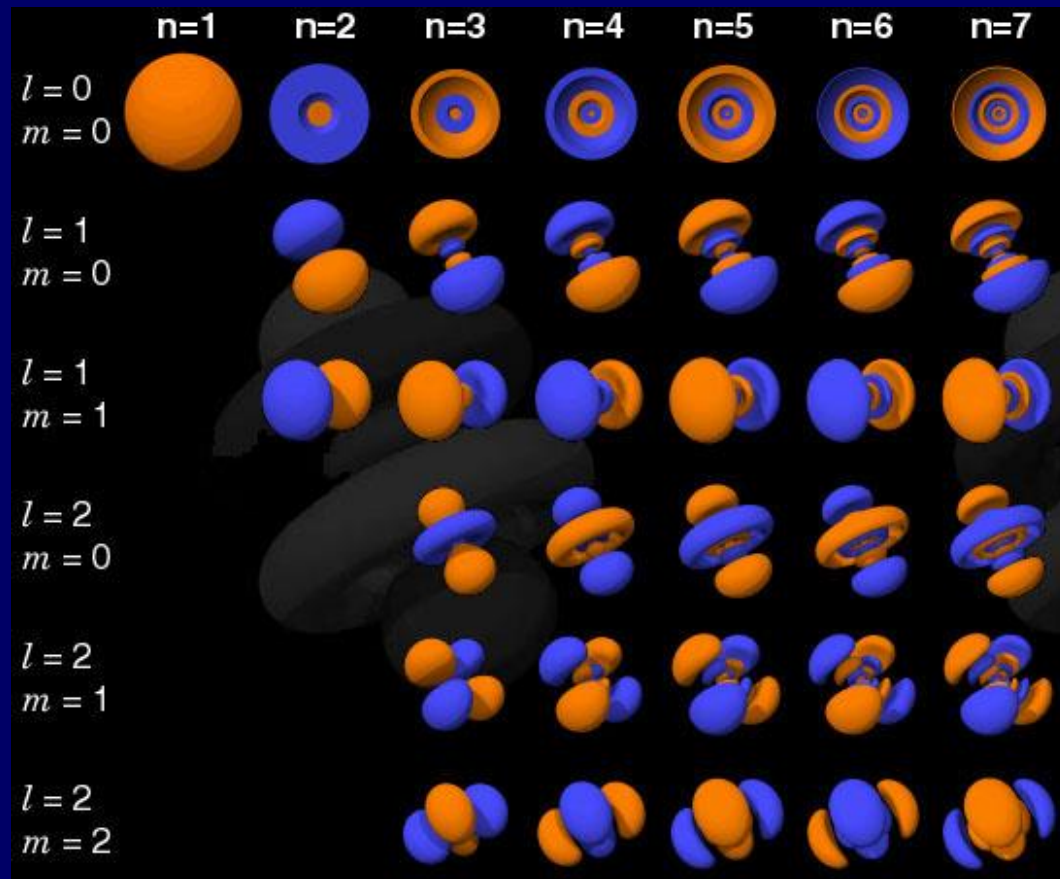
$$m_\ell = 0 : m_s = \frac{1}{2}, -\frac{1}{2} \quad 2 \text{ states}$$

$$m_\ell = -1 : m_s = \frac{1}{2}, -\frac{1}{2} \quad 2 \text{ states}$$

There are a total of 8 states with $n=2$

Electron orbitals

In correct quantum mechanical description of atoms, positions of electrons not quantized, orbitals represent probabilities



**Carbon orbitals
imaged in 2009 using
electron microscopy!**



ACT: Quantum Numbers

How many unique electron states exist with $n=5$ and $m_\ell = +3$?

- A) 0 **B) 4** C) 8 D) 16 E) 50

$$\ell = 0 : m_\ell = 0$$

$$\ell = 1 : m_\ell = -1, 0, +1$$

$$\ell = 2 : m_\ell = -2, -1, 0, +1, +2$$

$$\ell = 3 : m_\ell = -3, -2, -1, 0, +1, +2, +3$$

$$m_s = \frac{1}{2}, -\frac{1}{2}$$

2 states

$$\ell = 4 : m_\ell = -4, -3, -2, -1, 0, +1, +2, +3, +4$$

$$m_s = \frac{1}{2}, -\frac{1}{2}$$

2 states

Only
 $\ell = 3$ and $\ell = 4$
have $m_\ell = +3$

There are a total of 4 states with $n=5$, $m_\ell = +3$

Pauli Exclusion Principle

In an atom with many electrons only one electron is allowed in each quantum state (n, ℓ, m_ℓ, m_s).

[illegible]

Electron Configurations

#

electrons Atom

Configuration

1 H $1s^1$

2 He $1s^2$ **1s shell filled** (n=1 shell filled - noble gas)

3 Li $1s^2 2s^1$

4 Be $1s^2 2s^2$ **2s shell filled**

5 B $1s^2 2s^2 2p^1$

etc

10 Ne $1s^2 2s^2 2p^6$ **2p shell filled** (n=2 shell filled - noble gas)

s shells hold up to 2 electrons

p shells hold up to 6 electrons

The Periodic Table

S ($\ell=0$)

p ($\ell=1$)

Also s

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

Periodic Table of the Elements

■ hydrogen
■ alkali metals
■ alkali earth m
■ transition met

■ poor metals
■ metalloids
■ noble gases
■ earth metals

$d (\ell=2)$
 $p (\ell=1)$

Also s

1 H																	2 He	
3 Li	4 Be																	10 Ne
11 Na	12 Mg																	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr	
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe	
55 Cs	56 Ba	57 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn	
87 Fr	88 Ra	89 Ac	104 Unq	105 Unp	106 Unh	107 Uns	108 Uno	109 Une	110 Unn									
58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu					
90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr					

f ($\ell=3$)

What determines the sequence? Pauli exclusion & energies

Summary

- Each electron state labeled by 4 numbers:
 - n = principal quantum number (1, 2, 3, ...)
 - ℓ = angular momentum (0, 1, 2, ... $n-1$)
 - m_ℓ = component of ℓ ($-\ell < m_\ell < \ell$)
 - m_s = spin ($-1/2$, $+1/2$)
- Pauli Exclusion Principle explains periodic table
- Shells fill in order of lowest energy.