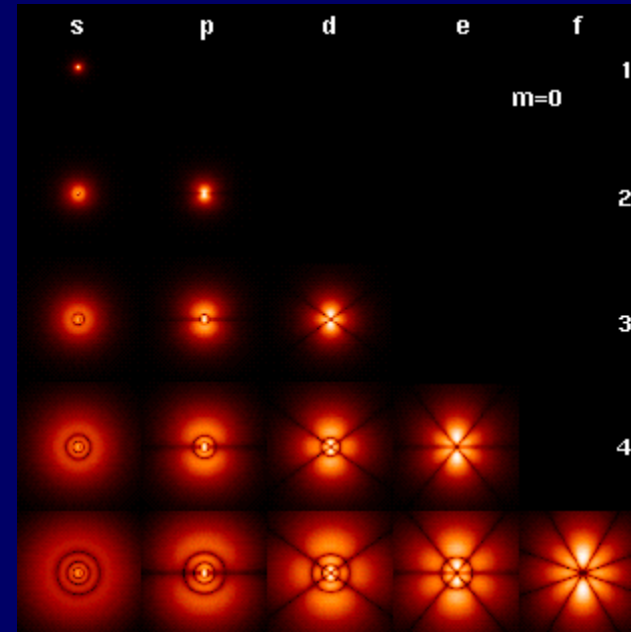


Physics 102: Lecture 25

Atomic Spectroscopy & Quantum Atoms



From last lecture – Bohr model

Angular momentum is quantized

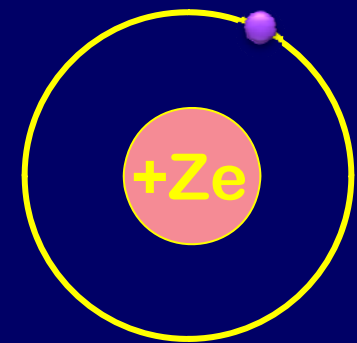
$$L_n = nh/2\pi \quad n = 1, 2, 3 \dots$$

Energy is quantized

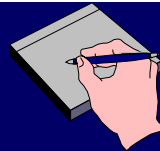
$$E_n = -\frac{mk^2e^4}{2\hbar^2} \frac{Z^2}{n^2} \approx -\frac{13.6 \cdot Z^2}{n^2} \text{ eV} \quad (\text{where } \hbar \equiv h/2\pi)$$

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! $E_n = -13.6 Z^2/n^2 = \frac{1}{2} mv_n^2$



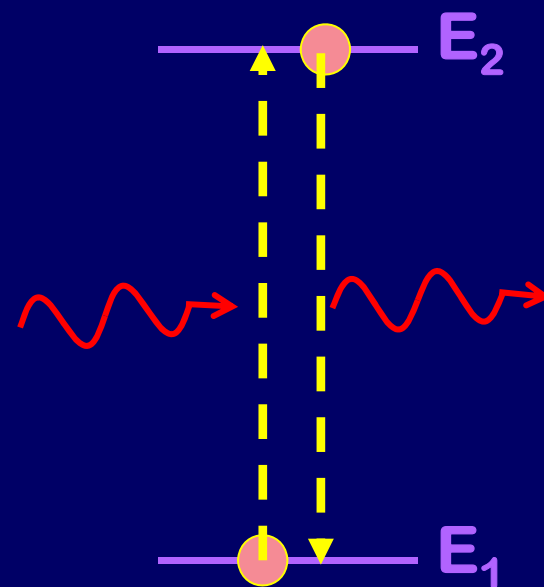
Transitions + Energy Conservation

- Each orbit has a specific energy:

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

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

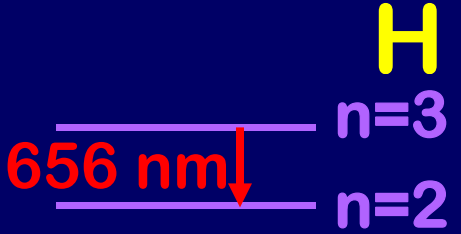
$$E_2 - E_1 = hf = hc/\lambda$$



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.

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



This is how neon signs & Na lamps work!

Spectra give us information on atomic structure



Checkpoint 1.1

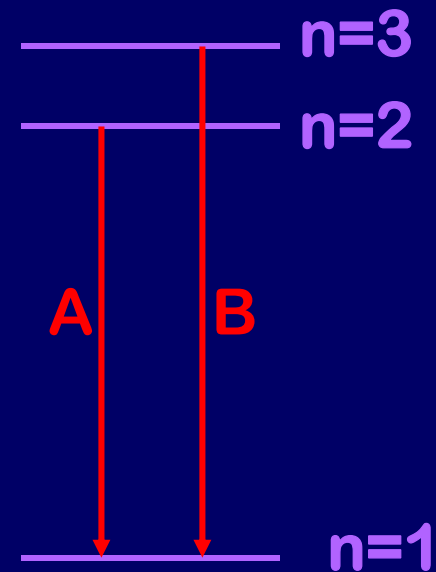
Electron A falls from energy level $n=2$ to energy level $n=1$ (ground state), causing a photon to be emitted.

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?

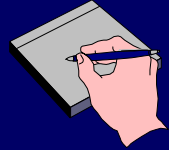
1) Photon A

2) Photon B

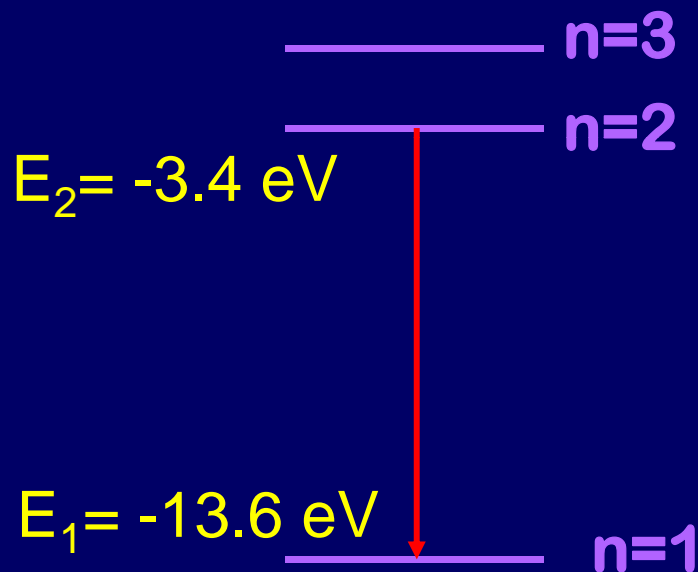


Example

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

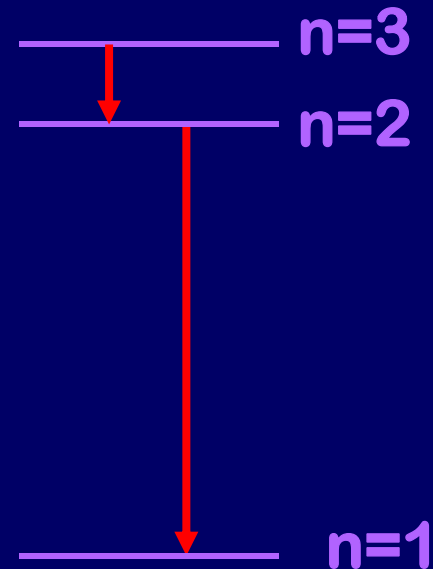
Compare the wavelength of a photon produced from a transition from $n=3$ to $n=2$ with that of a photon produced from a transition $n=2$ to $n=1$.

(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?

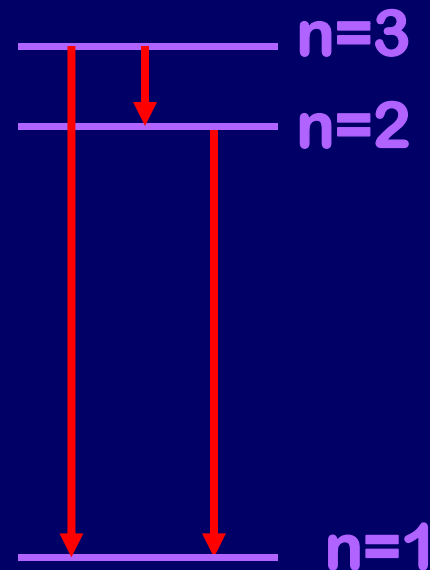
A. 1

B. 2

C. 3

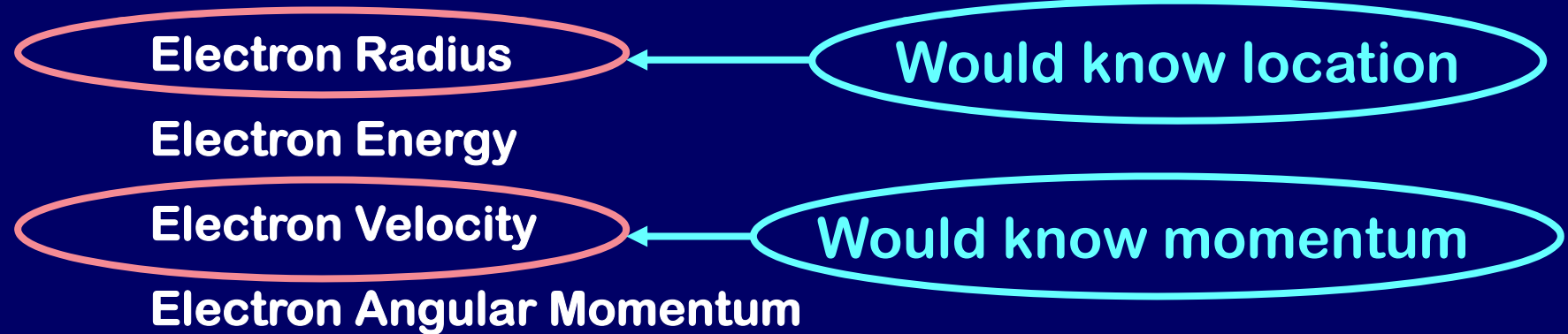
D. 4

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)?

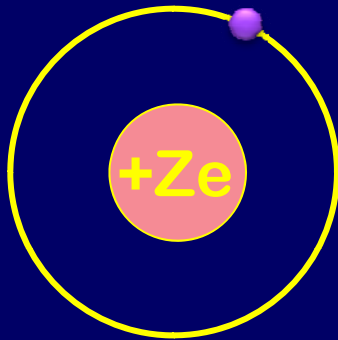


But, in the Bohr model:

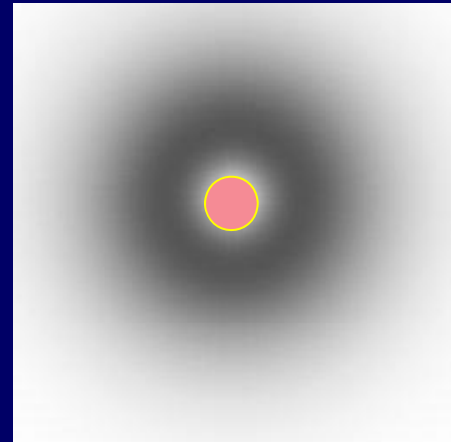
$$r_n = \left(\frac{h}{2\pi} \right)^2 \frac{1}{mke^2} \frac{n^2}{Z} = (0.0529 \text{ nm}) \frac{n^2}{Z}$$

**Quantized radii
and velocities for
electron orbitals**

Checkpoint 2



Bohr Model



Quantum Atom

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

Centripetal Acceleration

Pauli Exclusion Principle

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, ...)

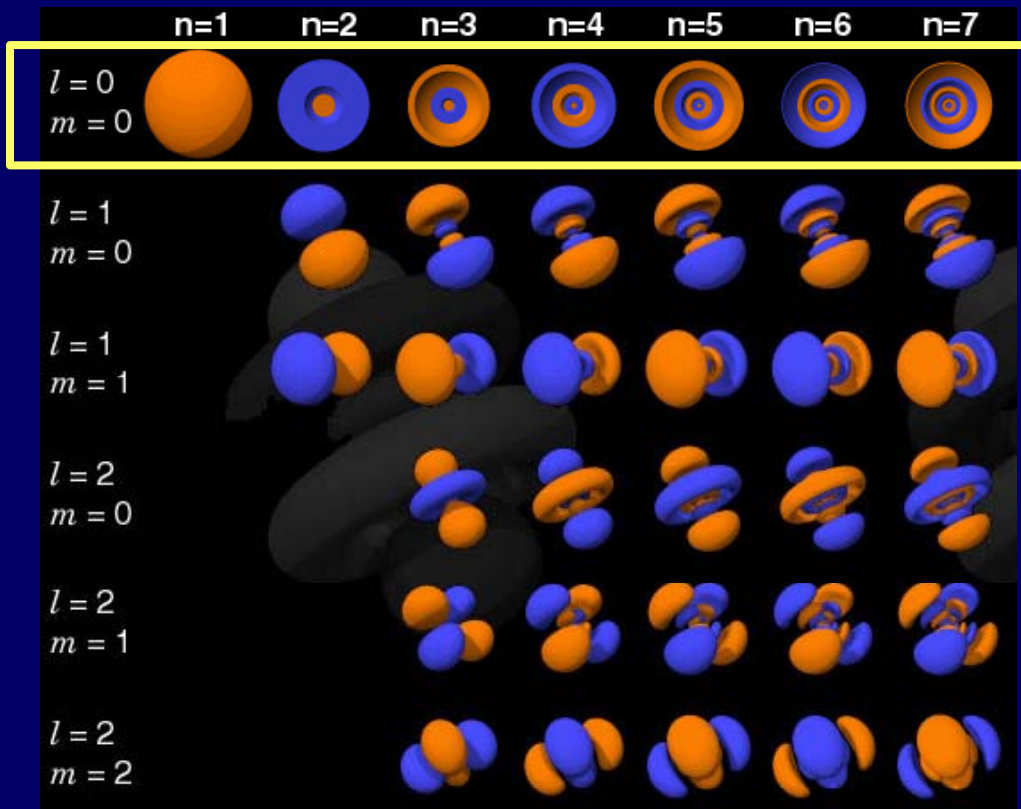
ℓ = angular momentum (0, 1, 2, ... $n-1$)

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

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

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!



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

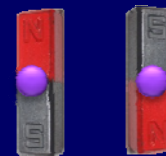
m_ℓ = Magnetic Quantum Number ($-\ell, \dots, 0, \dots, \ell$)

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

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

m_s = Spin Quantum Number ($-\frac{1}{2}, +\frac{1}{2}$)

- “Up Spin” or “Down Spin”





ACT: Quantum numbers

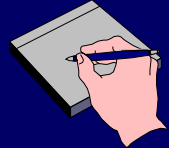
For which state of hydrogen is the orbital angular momentum **required** to be zero?

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**”

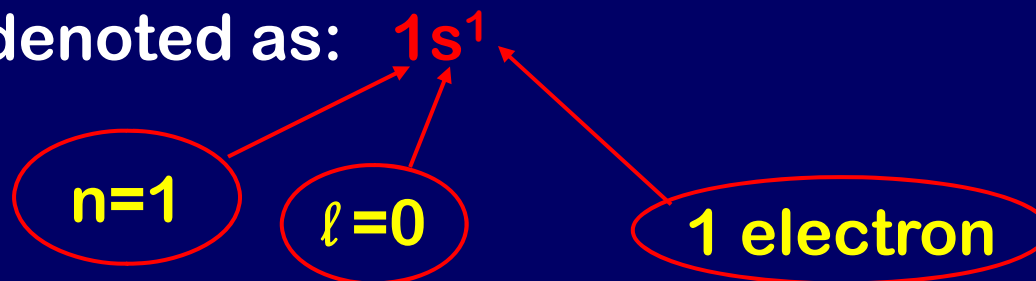
$\ell=3$ is “**f state**”

$\ell=4$ is “**g state**”

Example

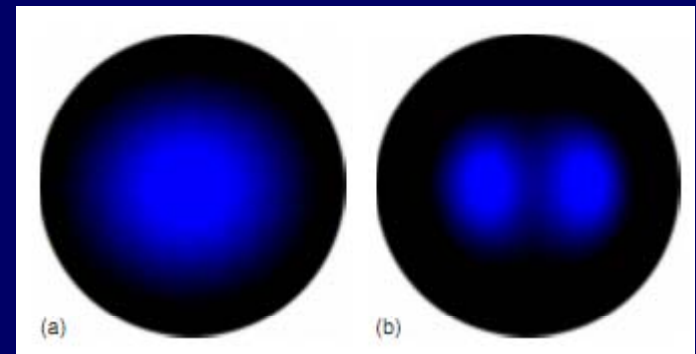
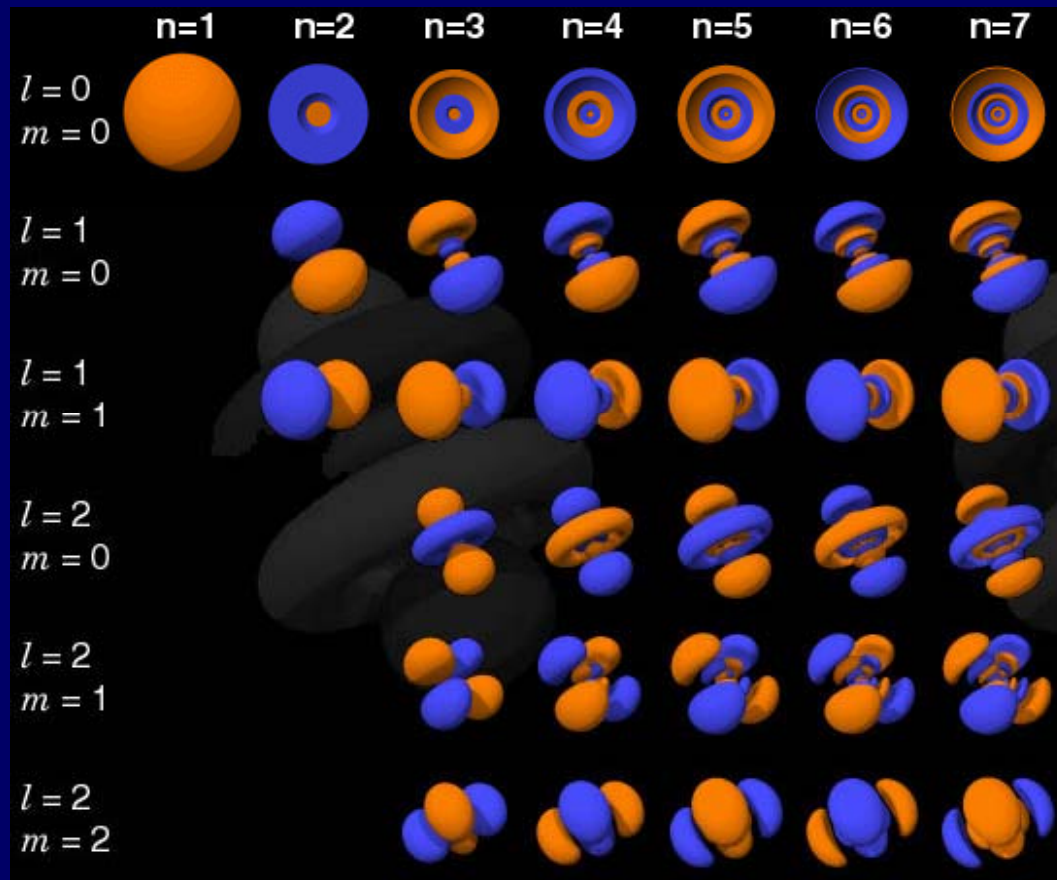
1 electron in ground state of Hydrogen:

$n=1, \ell=0$ is denoted as: **1s¹**



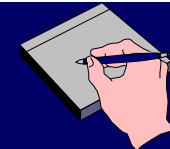
Electron orbitals

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



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

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 $n=2$



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).

Periodic Table of the Elements

- hydrogen
- alkali metals
- alkali earth metals
- transition metals
- poor metals
- nonmetals
- noble gases
- rare earth metals

1 H																	2 He														
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne														
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	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

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)

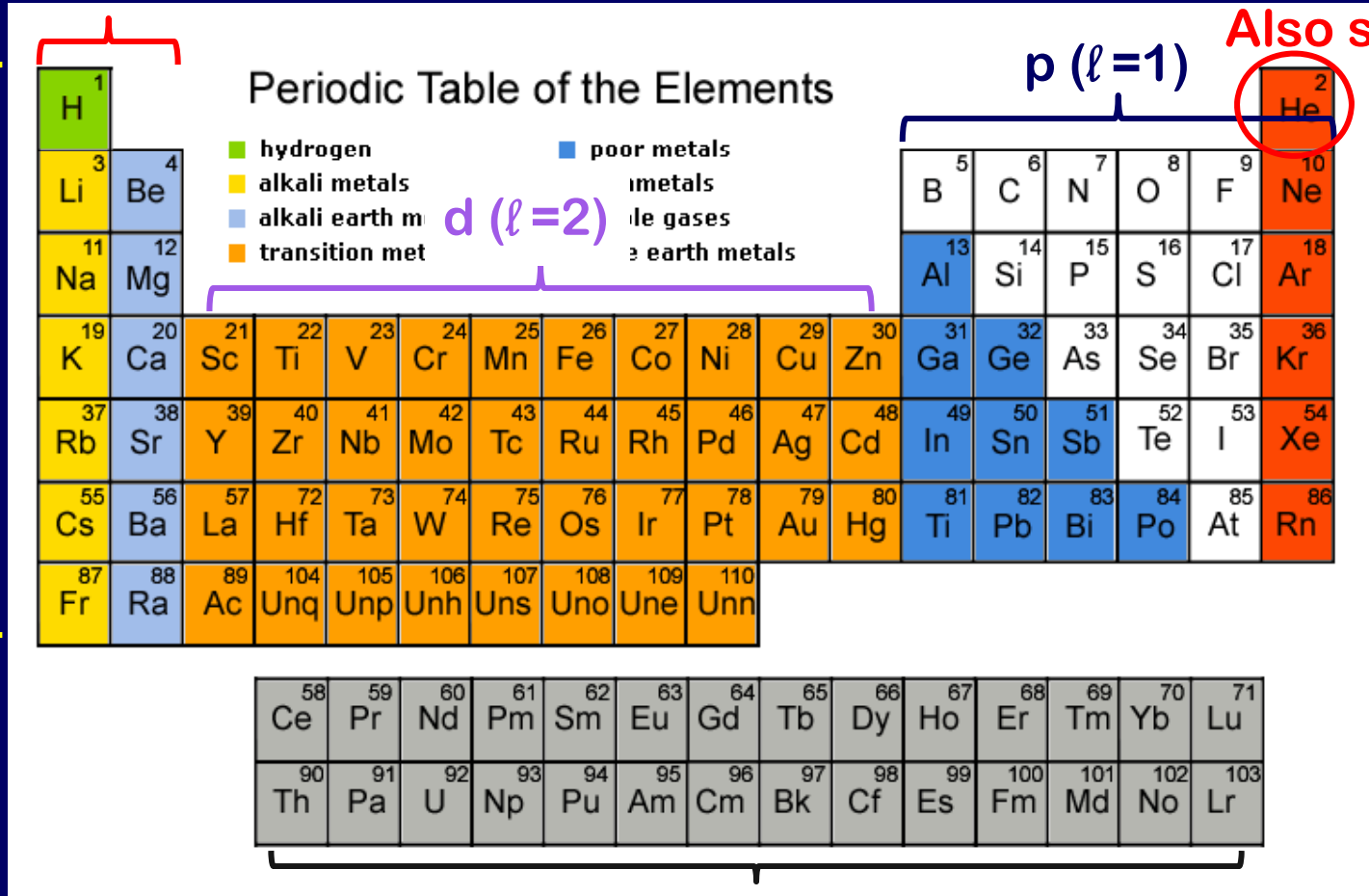
s shells hold up to 2 electrons

p shells hold up to 6 electrons

The Periodic Table

$s (\ell=0)$

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



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 ($-\frac{1}{2}$, $+\frac{1}{2}$)
- Pauli Exclusion Principle explains periodic table
- Shells fill in order of lowest energy.