

CHAPTER 6
Electronic Structure and
Periodic Properties of Elements

6

Chapter 06

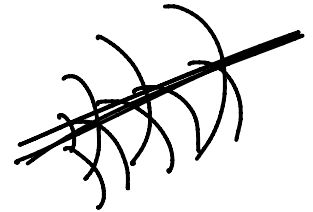
Electronic Structure and Periodic Properties of Elements

light (radiation) \rightarrow ^{sub-}atomic particles \rightarrow atom works

Electromagnetic Energy [6.1]

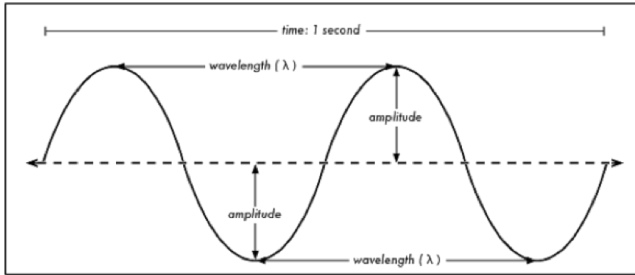
Light in Classical Mechanics vs. Classical Electromagnetism

- ① Issac NEWTON \rightarrow Prism \rightarrow ROYGBIV \rightarrow light is particles, explained by CLASSICAL MECHANICS
- ② Thomas YOUNG \rightarrow light interference patterns
- ③ James Clark MAXWELL \rightarrow light is part of EMR
 \downarrow
- ④ New Model: 2 Domains:
 - (i) Classical Mechanics \leftarrow particles
 - (ii) Classical Electromagnetism \leftarrow EMR waves



Waves

wave — oscillation that can transport energy



FM

AM

$$c = \lambda \nu = \text{wavelength} \cdot \text{frequency} = \frac{3.0 \times 10^8 \text{ m}}{\text{s}}$$

$$= \text{wavelength} \cdot \text{frequency}$$

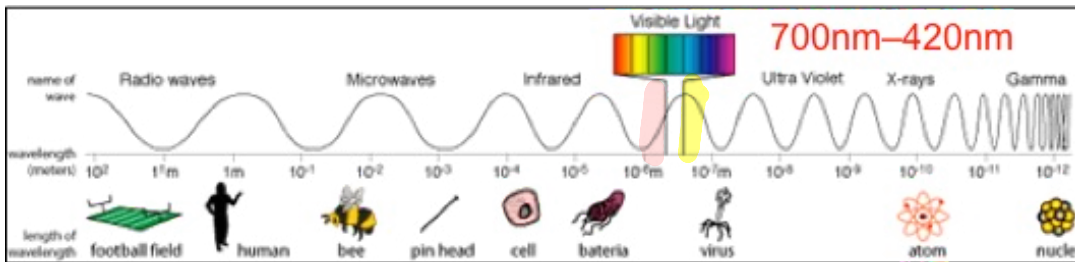
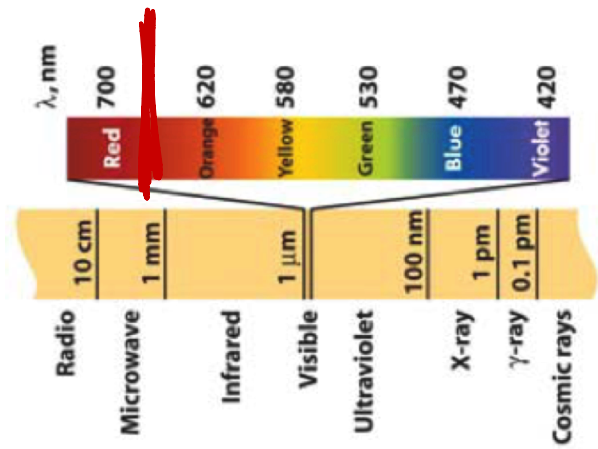
$$\rightarrow \frac{\text{m}}{\text{s}} = \frac{\text{m}}{\text{s}} \frac{1}{\text{s}}$$

(note: 1/s = Hz)

EMR Spectrum (EMR = ElectroMagnetic Resonance)

$$c = v\lambda ; v = \frac{c}{\lambda}$$

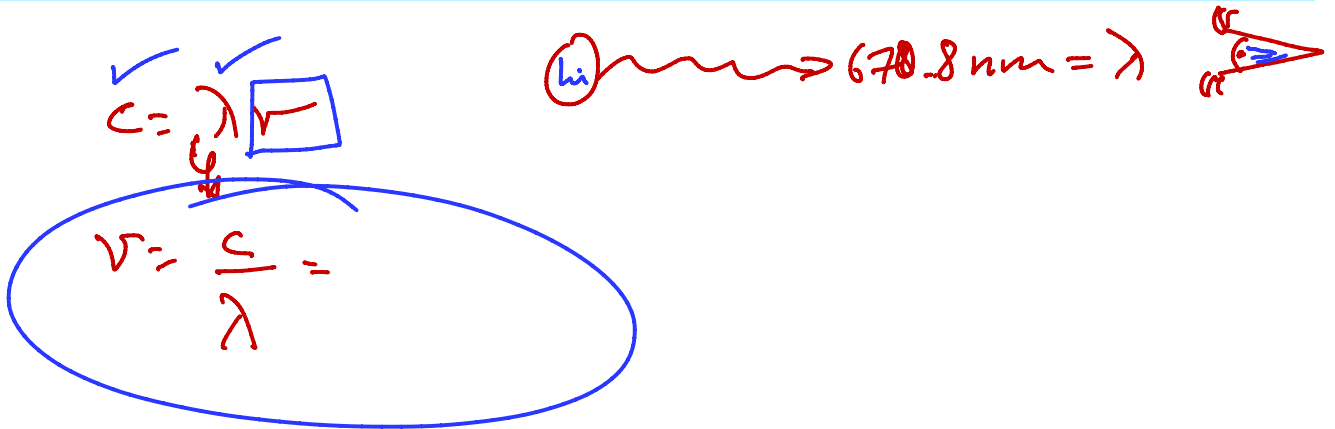
¿Do we want to talk about waves in terms of WAVELENGTH or FREQUENCY?



(EX) Calc λ from ν

[W 5.42 EOC]

Excited lithium ions emit radiation at a wavelength of 670.8 nm in the visible range of the spectrum. (This characteristic color is often used as a qualitative analysis test for the presence of Li.) Calculate the frequency of the yellow light?



$$\frac{\square}{\$} = \frac{670.8 \text{ nm}}{10^9 \text{ nm}} \times \frac{m}{2.998 \times 10^8 \text{ m}} \times \frac{s}{1} = \frac{2.236 \times 10^{-15} \text{ s}}{1} \rightarrow \boxed{\frac{4.472 \times 10^{14}}{\text{s}}}$$

* note: initial guess as to starting point was wrong, but didn't start over rather, merely fixed the answer based on target unit

Waves and the Guitar Analogy: Different Waves have Different Energies

Basic Terms

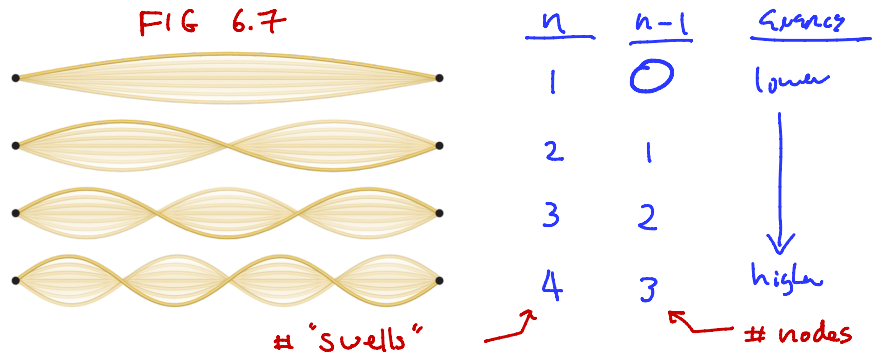
- interference patterns - can cancel or add to each other
- standing (stationary) wave - constrained w/ a region of space
- quantization - only discrete waves with an INTEGER number, n , of $\frac{1}{2}$ -wavelengths can form
- node - points of stationary wave not in motion

Thur, Oct 17

Fixed Waves: SWELLS, NODES, and ENERGY

- Fixed Waves are important because they mimic what happens at the atomic level, hence forming the basis for what is to come in this chapter.

- The variables "n" and "n-1" and "energy" will come up many times



“Houston, we have a problem... two actually.”
Blackbody Radiation and the Ultraviolet Catastrophe

Problem #1: Blackbody Radiation

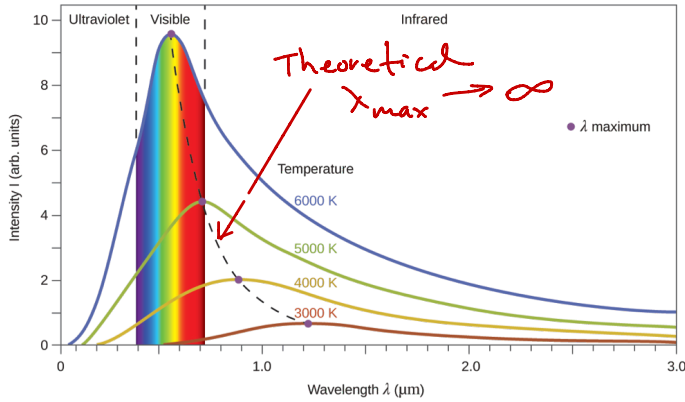


Figure 6.10 Blackbody spectral distribution curves are shown for some representative temperatures.

BLACKBODY

- a hypothetical body that completely absorbs all radiant energy falling upon it, reaches some equilibrium temperature, and then reemits that energy as quickly as it absorbs it

Problem #2: The UV Catastrophe

PROBLEM

↳ Black body models predicted that, at room temperature, everyday objects should emit large amount of UV radiation

REMEDY

↳ The dilemma was solved by Max Planck by assuming that atomic vibrational energies were restricted to discrete values

$$E = nh\nu \quad (n = 1, 2, 3, \dots, \quad h = \text{Planck constant} = 6.6E - 34 \text{ J} \cdot \text{s})$$

$$E = h\nu = \frac{hc}{\lambda} \quad (h = \text{Planck constant} = 6.6E - 34 \text{ J} \cdot \text{s})$$

In short: assumes the atoms, like guitar strings, vibrate only at quantized (discrete) energy levels

↓ ASIDE ↓

- Planck to explain the spectral-energy distribution of radiation emitted by a blackbody (a hypothetical body that completely absorbs all radiant energy falling upon it, reaches some equilibrium temperature, and then reemits that energy as quickly as it absorbs it).
- Planck assumed that the sources of radiation are atoms in a state of oscillation and that the vibrational energy of each oscillator may have any of a series of discrete values but never any value between.
- Planck further assumed that when an oscillator changes from a state of energy E_1 to a state of lower energy E_2 , the discrete amount of energy $E_1 - E_2$, or quantum of radiation, is equal to the product of the frequency of the radiation, symbolized by the Greek letter ν and a constant h , now called Planck's constant, that he determined from blackbody radiation data; i.e., $E_1 - E_2 = h\nu$.

—<https://www.britannica.com/science/Plancks-radiation-law#ref207605>

$$E = \frac{h\nu}{1} = \frac{hc}{\lambda}$$

- ↑ ASIDE ↑

(EX) Planck and Ionization Energy

To remove one electron from a Na atom, 8.22×10^{-19} J of energy is required. (That is, the 'first ionization constant' for Na is 8.22×10^{-19} J.) Calculate the maximum wavelength, in nm, needed to remove an electron from a sodium atom?

$$\lambda = \frac{hc}{E} = \frac{6.626 \times 10^{-34} \text{ J s} \cdot 3.00 \times 10^8 \text{ m}}{8.22 \times 10^{-19} \text{ J}} \cdot \frac{1 \times 10^9 \text{ nm}}{1 \text{ m}} = 242 \text{ nm}$$

Enter Albert Einstein: The Photoelectric Effect

(Einstein won his Nobel Prize for his work on The Photoelectric Effect, NOT Relativity)

EXPECTED: “Slow Boil”

① Low-energy radiation should cause current to flow, if irradiated long enough (cumulative effect)

↳ ANALOGY—slowly heating water: if heat water long enough with a low energy, it will eventually boil.

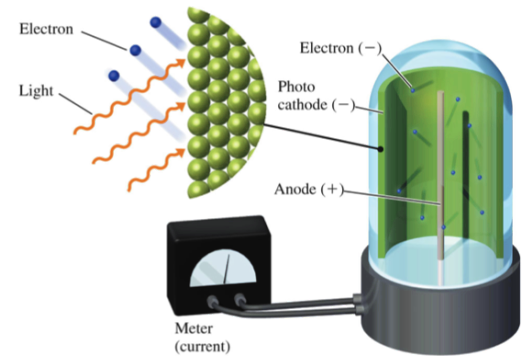
② Higher-energy radiation will cause the current to increase, even at intensity = k

↳ ANALOGY—higher heat will cause the water to boil at a greater rate

OBSERVED:

① THRESHOLD value must be reached

② Once reached: current (#electrons/sec) \propto f(intensity of light)



CONCLUSION:

- Einstein argued that the quantized energies that Planck had postulated in his treatment of blackbody radiation could be applied to the light in the photoelectric effect.
- Light consists of quantized packets of energy. ($E=h\nu$)
- Light energy is quantized, not continuum
- The “packet” of light energy, later dubbed photons, act like a particle—those particles (photons) strike the surface, and displace other particles (electrons)/

Each of Planck’s packet of quantized energy can transfer ALL of its energy to a single electron during a collision

How the work of Planck and Einstein distills out: The Dual Nature of Light



Planck — light is quantized
Einstein — light is particles



THE DUAL NATURE OF LIGHT

- Photoelectric Effect -- contrary to wave view
- Interference Patterns -- contrary to particle view

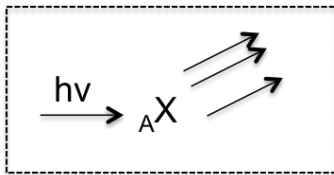
↳ Light can be described both wavelike (blackbody experiments) and particle-like (photoelectric effect).

RATIONALIZING THE PHOTOELECTRIC EFFECT

- Higher the frequency of light, the higher the KE energy of the photons
- Higher the amplitude of light (the brighter the light), the greater the number of photons

Absorbance and Emission Spectroscopy: Investigating how atoms interact with light

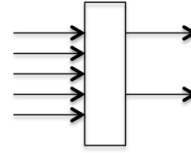
Emission



emission (emitted light)

¿what light is given off?

Absorbance



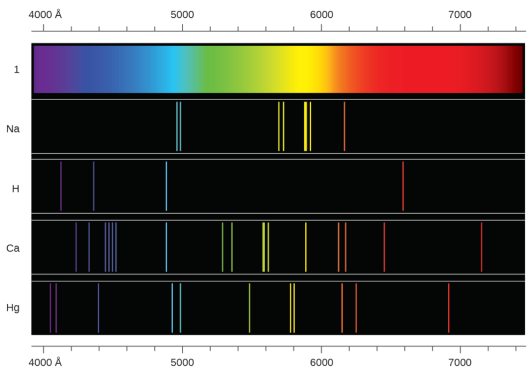
absorption (only certain λ absorbed)

¿what light is 'kept' by the sample?

PARADOX

- When an object, such as a piece of iron, is heated, excess may be given off as light—light in the form of a continuous spectrum (all of ROYGBIV)
- However, light can also be emitted as Discrete or Line Spectra—relatively few frequencies comprise the light. (PRISM analogy)

Line Spectra: taking a look at individual atoms, and how they differ

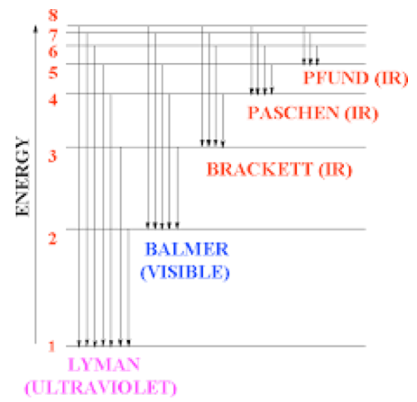


① Observation

FIG 6.13



② Model



③ Equations

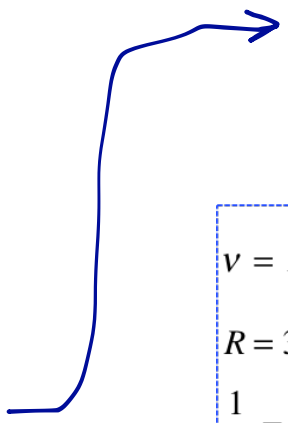
1/4 for Balmer

$$\nu = R \left(\frac{1}{n_L^2} - \frac{1}{n_H^2} \right)$$







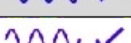




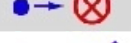
$$R = 3.3E15 \text{ Hz}$$

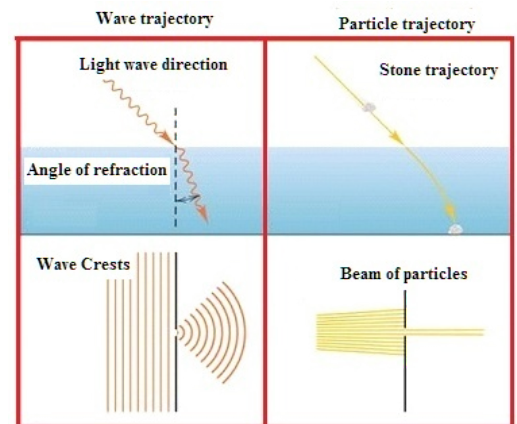
$$\frac{1}{\lambda} = R \left(\frac{1}{n_L^2} - \frac{1}{n_H^2} \right)$$

$$R = 1.097E7 \text{ m}^{-1}$$



Dual Nature of Light – Empirical Observation Summary

Phenomenon	Can be explained in terms of waves.	Can be explained in terms of particles.
Reflection	 ✓	 ✓
Refraction	 ✓	 ✓
Interference	 ✓	 ✗
Diffraction	 ✓	 ✗
Polarization	 ✓	 ✗
Photoelectric effect	 ✗	 ✓



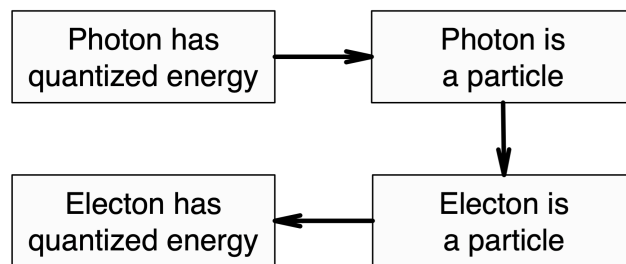
The Bohr Model [6.2]

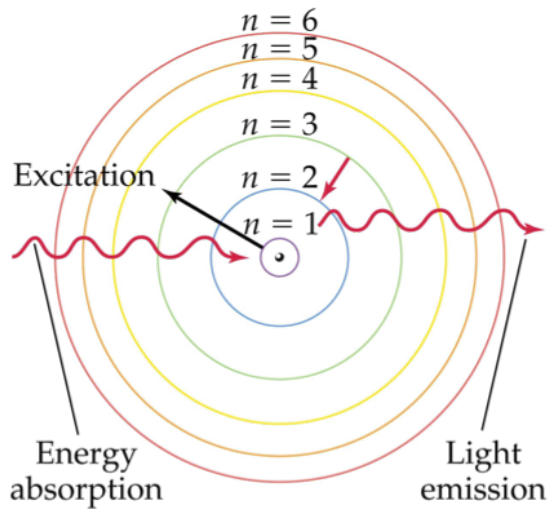
¿Who cares about photons anyways... atoms are made of electrons... how do you explain spectra based on electrons?

PARADOX

Classical mechanics → predicts Electron should fall into Nucleus, due to loss of energy of the orbiting electron

REMEDY





$$E_n = \frac{k}{n^2} \quad (k = \text{several fundamental constants combined})$$

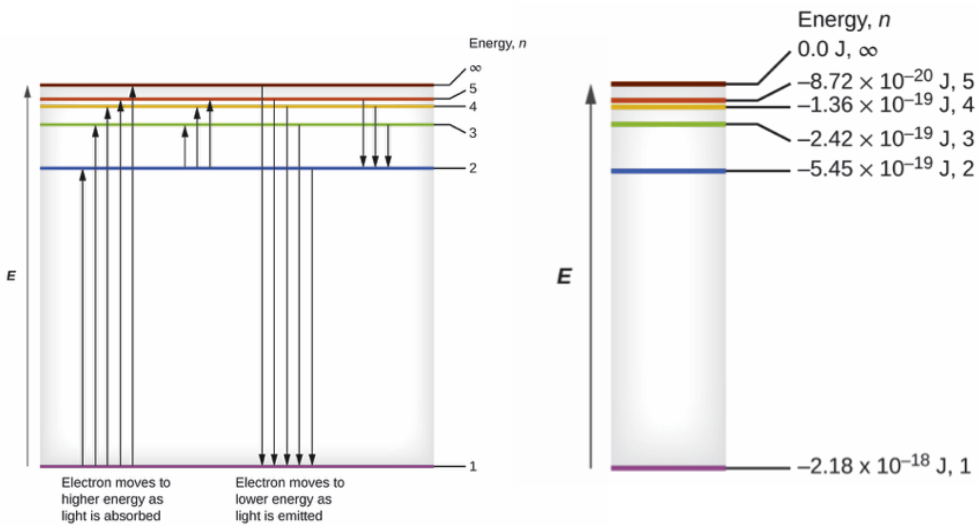
← Multiply by z^2 for other-than H

$$\Delta E_n = k \left(\frac{1}{n_L^2} - \frac{1}{n_H^2} \right) \quad (\text{Eq1 for a difference})$$

← Bohr derived Rydberg eq using his quantum model

$$\Delta E_n = h\nu = \frac{hc}{\lambda} \quad (\text{"Planck equation"})$$

$$\frac{1}{\lambda} = R \left(\frac{1}{n_L^2} - \frac{1}{n_H^2} \right) \quad (\text{substituting Planck Eq into Eq3, and rearranging})$$



$$E_n = \frac{kZ^2}{n^2} \text{ (single electron model)}$$

$$r = \frac{n^2}{Z} a_o \text{ (} a_o \text{ is the Bohr radius)}$$

$$\Delta E_n = E_{n \rightarrow \infty} - E_1 = 0 + k = k$$

$$E_0 = \text{ionization limit}$$

(EX) Calc Energy per Energy Level Change [6.5b]

(a) What is the energy (in Joules), and (b) the wavelength (in meters), of the photon produced when an electron falls from $n=5$ to $n=3$ level in a He^+ ion ($Z = +2$)?

(a) energy in Joules

3 Choices...

① $E = \frac{-kZ^2}{n^2}$ ② $\Delta E = k \left(\frac{1}{n_L^2} - \frac{1}{n_H^2} \right)$ ③ $E = h\nu = \frac{hc}{\lambda}$

Energy at distance from charge

Line Spectra

Eq 1

$$E_3 = \frac{-2.179 \text{E-18} \cdot 2^2}{3^2} = 9.684 \text{E-19}$$
$$E_5 = \frac{-2.179 \text{E-18} \cdot 2^2}{5^2} = 3.486 \text{E-19}$$

Δ } 6.198 E-19 J

$\therefore =$

Eq 2

$$\Delta E = -2.179 \text{E-18} \cdot \overbrace{\left(\frac{1}{3^2} - \frac{1}{5^2} \right)}^{0.0711} = 1.550 \text{E-19}$$

$\downarrow \times 4$

6.200 E-19 J

parallel ↗

<answer to (b) next page>

(b) wavelength in meters

$$\textcircled{b} \quad \epsilon = h \cdot \cancel{c / \lambda} = h \nu$$

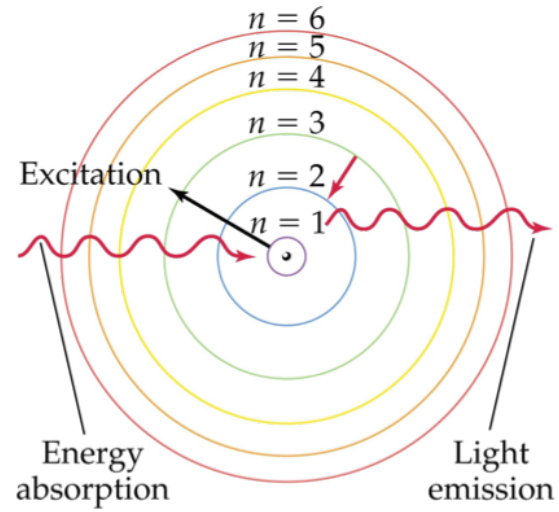
$$\begin{aligned} \text{243} \rightarrow \lambda &= \frac{2.998 \text{ E } 8 \text{ m} \cdot 6.626 \text{ E } -34 \text{ J}\cdot\text{s}}{6.188 \text{ E } -19 \text{ J}} \\ &= \boxed{3.205 \text{ E } -7 \text{ m}} \quad \leftarrow \text{wavelength} \end{aligned}$$

Bohr Model Conclusions

- Energy levels in an atom are quantized, described by Quantum Numbers
- Energy incr. with incr. distance from nucleus.
- The result is discrete energies (lines) in the spectra.

Oops! Bohr Model Flaw

- Does not work for ≥ 2 electrons



Development of Quantum Theory [6.3]

Unanswered Questions

- Why do electrons orbit at only fixed distances defined by a single quantum number $n = 1, 2, 3,$ and so on, but never in between?
- Why did the model work so well describing hydrogen and one-electron ions, but could not correctly predict the emission spectrum for helium or any larger atoms?

DeBroglie – Matter (electron) as a Wave

DeBroglie (1925)

If light can act like a particle, then a particle can act as a wave.

Broglie published his ideas that the electron in a hydrogen atom could be better thought of as being a circular standing wave instead of a particle moving in quantized circular orbits

(In his 1925 doctoral dissertation, de Broglie extended the wave-particle duality of light that Einstein used to resolve the photoelectric-effect paradox to material particles.)

For WAVE: $E \propto \text{wavelength}$
For PARTICLE: $E \propto \text{momentum/mass}$

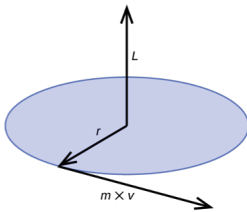
$$\lambda = \frac{h}{m v} \text{ (deBroglie)}$$

note: "v" = velocity, not frequency

CAUTION !!! do NOT confuse
v (velocity) with ν (frequency)

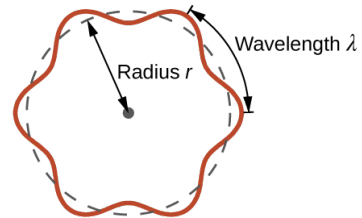
$$L = \frac{n h}{2 \pi} = n \hbar$$

ANGULAR MOMENTUM



$$2 \pi r = n \lambda$$

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



(EX) Calc DeBroglie Wavelength [6.6b]

¿Calculate the wavelength of a softball with a mass of 100 g traveling at a velocity of 35 m s⁻¹, assuming that it can be modeled as a single particle

$$\lambda = \frac{h}{m v} = \frac{6.626E-34 \text{ Kg } m^2}{s} \cdot \frac{1}{0.100 \text{ Kg}} \cdot \frac{s}{35 m} = 1.9E-34 m$$

WHY WE DON'T SEE QUANTIZED MOTION IN THE MACRO-WORLD

We never think of a thrown softball having a wavelength, since this wavelength is so small it is impossible for our senses or any known instrument to detect (strictly speaking, the wavelength of a real baseball would correspond to the wavelengths of its constituent atoms and molecules, which, while much larger than this value, would still be microscopically tiny).

The de Broglie wavelength is only appreciable for matter that has a very small mass and/or a very high velocity.

Tue Oct 22



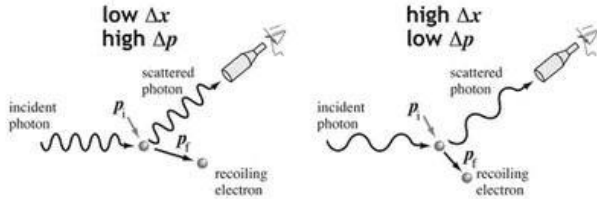
Heisenberg Uncertainty Principle

Cannot know the Position and Particle of particle at same time

The Heisenberg Uncertainty Principle

$$\Delta x \Delta p \geq \hbar$$

Δx = uncertainty in position
 Δp = uncertainty in momentum
 $\hbar = h / 2\pi$

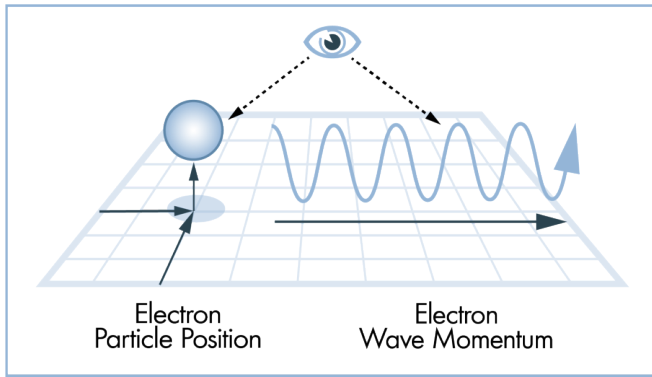


$$\Delta x \cdot \Delta p_x = \Delta x \cdot m \Delta v \geq \frac{\hbar}{2} = \frac{h}{4\pi}$$

... the larger (smaller) this uncertainty.
 The smaller (larger) this uncertainty ...

- Heisenberg's principle imposes ultimate limits on what is knowable in science.
- The value of \hbar is not large, so the uncertainty in the position or momentum of a macroscopic object like a baseball is too insignificant to observe. However, the mass of a microscopic object such as an electron is small enough that the uncertainty can be large and significant.
- A light wave hitting a baseball will reflect, allowing the observer to see the baseball. But light will go over an electron. To get small enough for a wave to reflect from an electron, one needs a short wavelength (hence high energy) such as a gamma ray. This high energy actually affects the path and momentum.

Heisenberg's principle imposes ultimate limits on what is knowable in science.



(EX) Heisenberg Uncertainty

Example: Uncertainty Principle

An electron is confined to a region of width $5.00 \times 10^{-11} \text{ m}$, which is its uncertainty in position Δx . Estimate the minimum uncertainty in its momentum.

$$\Delta x \Delta p_x \geq h$$

so

$$\Delta p_x \geq \frac{h}{\Delta x} = \frac{6.626 \times 10^{-34} \text{ J s}}{5.00 \times 10^{-11} \text{ m}} = 1.33 \times 10^{-23} \text{ kg m s}^{-1}$$

(EX) Heisenberg Uncertainty

[OpenStax textbook]

For example, if we improve our measurement of an electron's position so that the uncertainty in the position (Δx) has a value of, say, 1 pm (10^{-12} m, about 1% of the diameter of a hydrogen atom), then our determination of its momentum must have an uncertainty with a value of at least:

$$\left[\Delta p = m\Delta v = \frac{h}{(2\Delta x)} \right] = \frac{(1.055 \times 10^{-34} \text{ kg m}^2/\text{s})}{(2 \times 1 \times 10^{-12} \text{ m})} = 5 \times 10^{-23} \text{ kg m/s.}$$

Mathematically:

$$\Delta x \cdot \Delta p \geq \frac{h}{4\pi}$$

Where Δx = Uncertainty or error in position
and Δp = Uncertainty or error in momentum

$$\therefore p = mv$$

$$\Delta p = m\Delta v$$

$$\therefore \Delta x \cdot \Delta v \cdot m \geq \frac{h}{4\pi}$$

$$\text{or } \Delta x \cdot \Delta v \geq \frac{h}{4\pi m}$$

Where Δv = uncertainty in velocity

The Quantum–Mechanical Model of an Atom: Electrons are waves traveling in 3d's

Schrodinger and the wave equation

Developed a 3D stationary wave, called a Wavefunction, ψ

- Schrodinger accepted deBroglie's idea of electron as wave, and was influenced by Bohr's idea that hydrogen could be thought of as a Standing Wave.
- Noted deBroglie eq only works in force-free environment, not one in which electrons subject to pull of proton.
- Rejected deBroglie's/Bohr's idea of circular orbits, and developed a 3D stationary wave, called a Wavefunction, ψ .

$$\psi(r,\theta,\phi) = R_{n,\ell}(r) \cdot Y_{\ell,m}(\theta,\phi)$$

Max Born

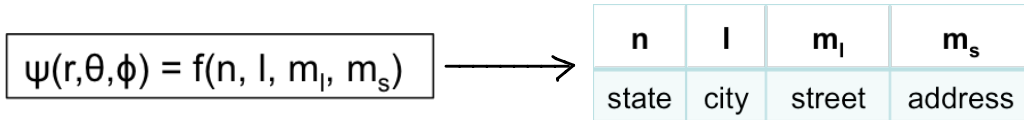
- ① Electrons are still particles, and so the waves represented by ψ are not physical waves but, instead, are complex probability amplitudes.
- ② The square of the magnitude of a wavefunction $|\psi|^2$ describes the probability of the quantum particle being present near a certain location in space

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

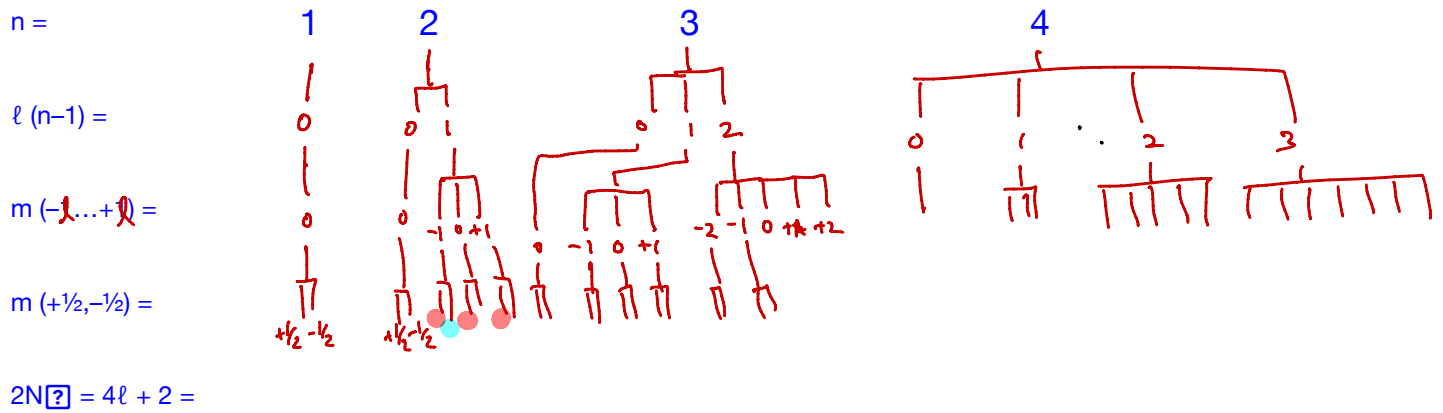
$$\psi(r, \theta, \phi) = f(n, \ell, m_l, m_s)$$

➔ You will NOT need to solve the Schrodinger Equation, but you WILL need to understand, in detail, what the solutions—what the 4 variables: n , ℓ , m_l , m_s —mean

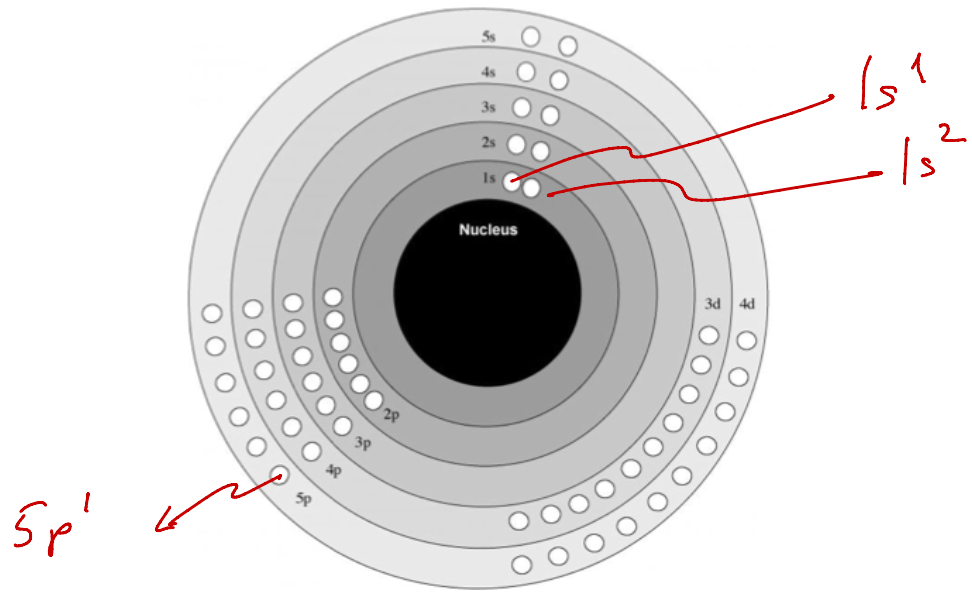
Placing Meaning to Quantum Theory of Electrons in Atoms



“The Comb” Mnemonic Device



$n =$	1	2	3	4
$l(n-1) +$	0 ^s	0 ^s 1 ^p	0 ^s 1 ^p 2 ^d	0 ^s 1 ^p 2 ^d 3 ^f
$m(-1...+1)$	0	0 -1 0 1	0 -1 0 1 -2 -1 0 1 2	-3 -2 -1 0 1 2 3
$m(+1/2, -1/2)$	↑↓	↑↓ ↑↓ ↑↓ ↑↓	↑↓ ↑↓ ↑↓ ↑↓ ↑↓ ↑↓ ↑↓ ↑↓	↑↓ ↑↓ ↑↓ ↑↓ ↑↓ ↑↓ ↑↓ ↑↓
$2N_{\square} = 4l + 2$	2	8	18	32



Quantum Number (QN) Name	Defines	Label	Symbol	QN Values	Comment	Letters	Comment 2
Principal QN	energy	level	n	1,2,3,4,5,6,7	There are 7 possible energy levels (There are 7 periods in the periodic chart)	n	
Angular Momentum QN	shape	sublevel	l	0...(n-1)	EACH <u>energy level</u> has n number of sublevels. For example, the 3rd level (n=3) has three sublevels. Those sublevels are "0" (for n=1 -> n-1=0), "1" (for n=2 -> n-1=1), and "2" (n=3 -> n-1=2)	s (l = 0) p (l = 1) d (l = 2) f (l = 3)	
Magnetic QN	orbit	orbital	m_l	-l...0...+l	EACH <u>sublevel</u> has 2l+1 number of orbitals. For example, the l = 3 sublevel (i.e., the f-sublevel) has 7 orbitals with the QN's: -3,-2,-1,0,+1,+2,+3	p-orbitals = x, y, z d-orbitals = xy,yz,xz, x ² -y ² ,z ² f-orbitals <look up>	The 2l+1 rule provides that: s-sublevels have 1 orbital p-sublevels have 3 orbitals d-sublevels have 5 orbitals f-sublevels have 7 orbitals
Spin QN	spin	spin	m_s	+1/2, -1/2	EACH <u>orbital</u> carries a maximum of two electrons. One carries a spin of +1/2; the other carries a spin of -1/2.		+1/2 spin referred to as "up" -1/2 spin referred to as "down"

Rules		
Aufbau Principal	filling order	Fill in way that gives the lowest TOTAL energy. Fill periodic chart as if reading a book, noting the 'd' level is displaced one row, and the 'f' level is displaced two rows.
Hund's Rule	sublevel filling priority	Fill sublevel orbitals singly, then begin pairing. Relative Stability: Full sublevel > 1/2-filled sublevel > "unevenly" filled sublevel
Pauli Exclusion Principle	unique address	No two electron may have the exact same set of four QN's.

The Pauli Exclusion Principle

- no two electrons may have the exact set of QN'a
- i.e., each electron has a UNIQUE "n- l - m_l - m_s " address
- i.e., there are no twins

Bucket (Graphical) Approach to solving n- l - m_l - m_s problems

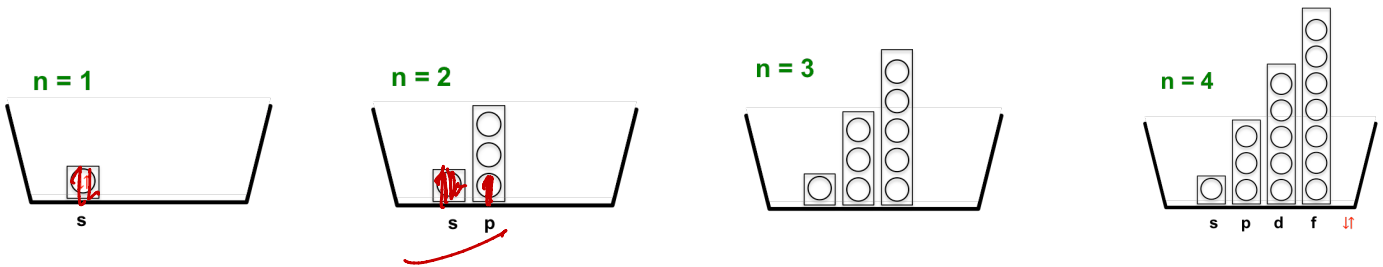
Represent each of the quantum number with a graphical element

n = bucket;

l = box,

m_l = circle,

m_s = arrow



(EX) Det'n # Electrons [w eoc70]

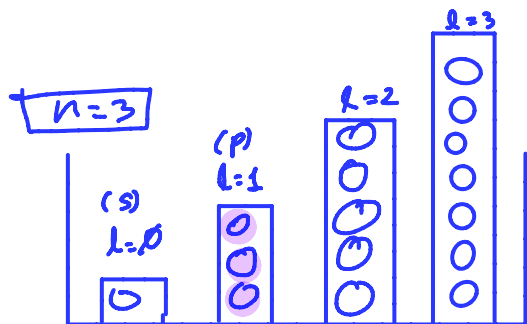
¿What is the maximum number of electrons in an atom that can have the quantum numbers:

(a) $n = 3, l = 1$ → "p"

(b) $n = 2$

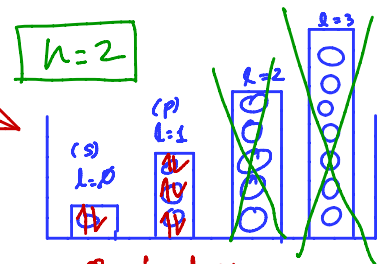
Ⓐ $n = 3, l = 1 = 6$

TOTAL # elect
in a
single
energy level
 $= 2n^2$



6 elect
3 orbitals
1 subshell

Ⓑ $n = 2 = 8$



8 electrons
4 orbitals
2 subshells

(EX) Det'n Value of 'n' and 'l'

¿What are the values of 'n' and 'l' for the following:

(a) 1s = $\frac{n}{1} \frac{l}{0}$

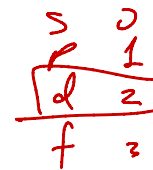
(b) 3p = $\frac{3}{3} \frac{1}{1}$

(c) 4f = $\frac{4}{4} \frac{3}{3}$

$n=1, l=0$

$n=3, l=1$

$n=4, l=3$



(EX) ID incorrect 'n, l, m_l, m_s' sets

¿Which of the following are incorrect, and why?

GO \longrightarrow 2d'

(a) 2, 2, 1, +1/2

(b) 3, 2, 3, +1/2

(c) 3, 1, 1, -1/2

- (a) 2, ~~2~~, 1, 1/2
- (b) 3, 2, ~~3~~, 1/2
- (c) 3, 1, 1, -1/2

if $n=2, l=0, 1$

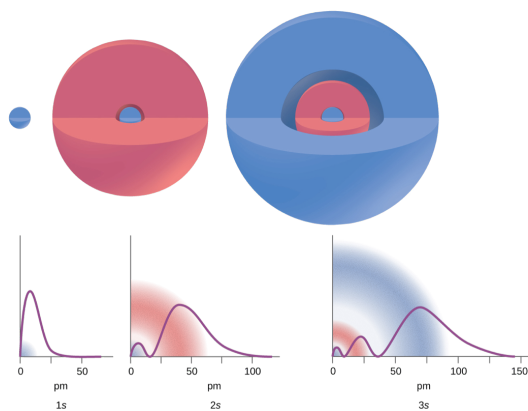
if $l=2, m_l = -2, -1, 0, 1, 2$

Thurs Oct 24

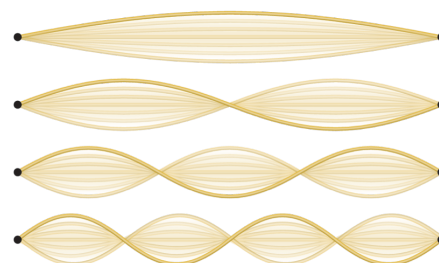
Radial Nodes

- Distances from the nucleus at which the probability density of finding an electron located at a particular orbital is zero.
- In other words, the value of the wavefunction ψ is zero at this distance for this orbital.

$$\# \text{ Radial nodes} = n - \ell - 1$$



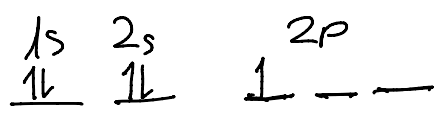
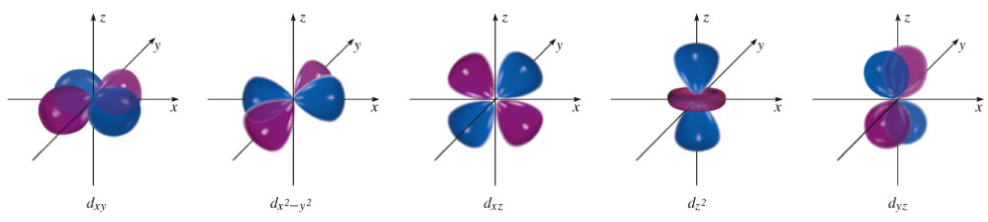
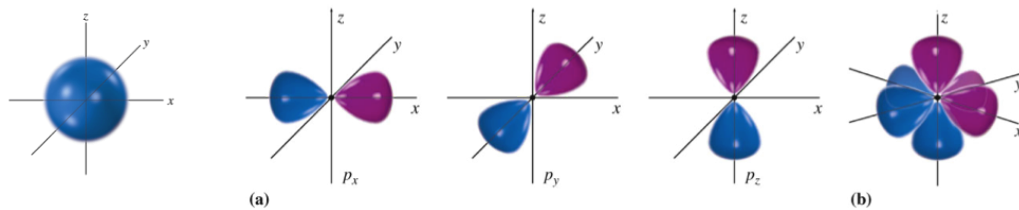
Recall: modes in 2d wave



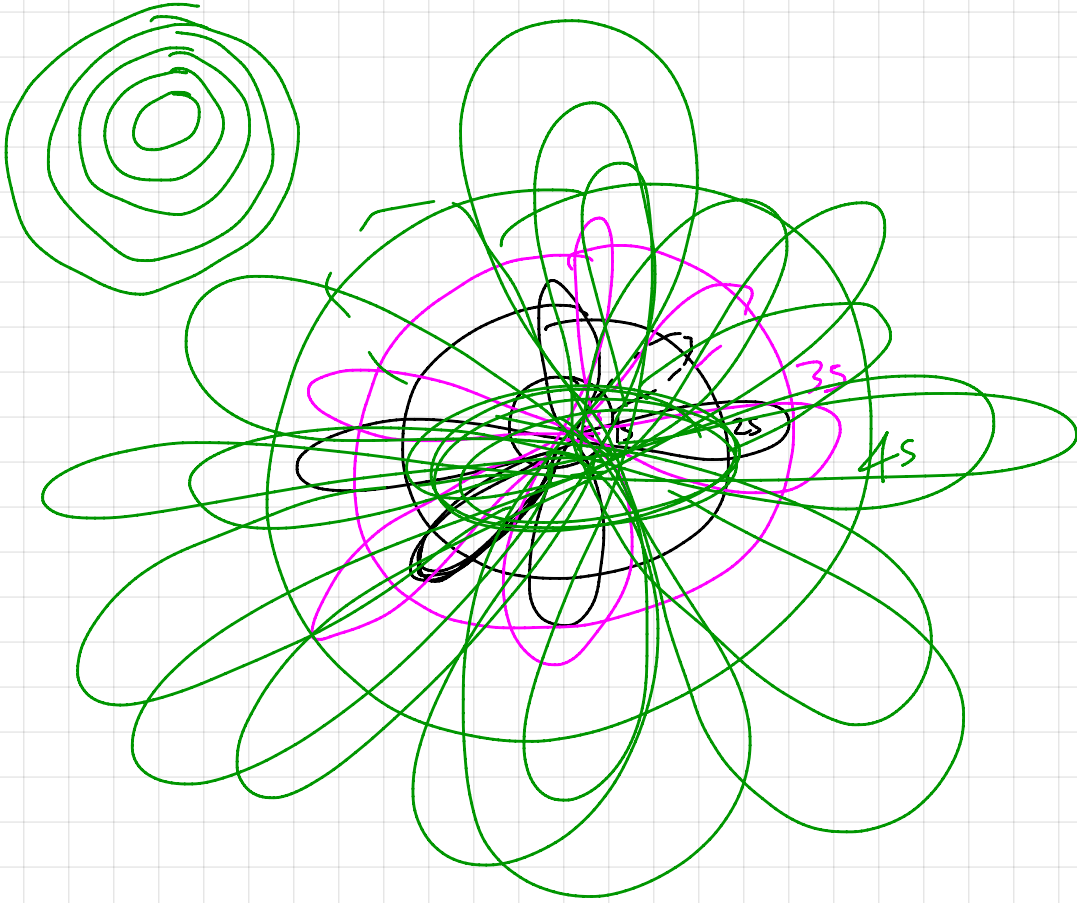
Orbital Shapes

Recall Schrodinger rejected deBroglie's/Bohr's idea of circular orbits, and developed a 3D stationary wave, called a Wavefunction, ψ .

If not circular orbits... then what?



11e



(EX) Write Electronic Configuration

Give the electronic configuration for the following:

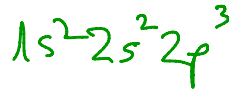
(a) N

(b) V

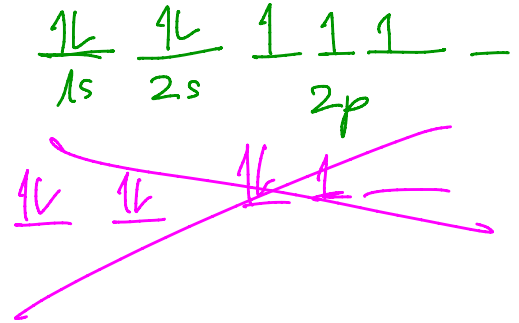
(c) Cr

(d) Cs

(e) Mg $\boxed{2}$ $\rightarrow 2+$



7e



(a) N $1s^2 2s^2 2p^3$

(b) V $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^3$ or $[Ar] 4s^2 3d^3$

(c) Cr $[Ar] 4s^1 3d^5$

(d) Cs $[Xe] 6s^1$

(e) Mg $\boxed{2}$ $\rightarrow 2+$ $1s^2 2s^2 2p^6$ (isoelectronic w noble gas)
 \uparrow
 Mg

Orbital Diagrams

- Similar to Electronic Configurations, only (a) orbitals are represented as blank underlines, and (b) electrons are represented with up and down arrows with each orbital

(EX) Draw orbital diagram

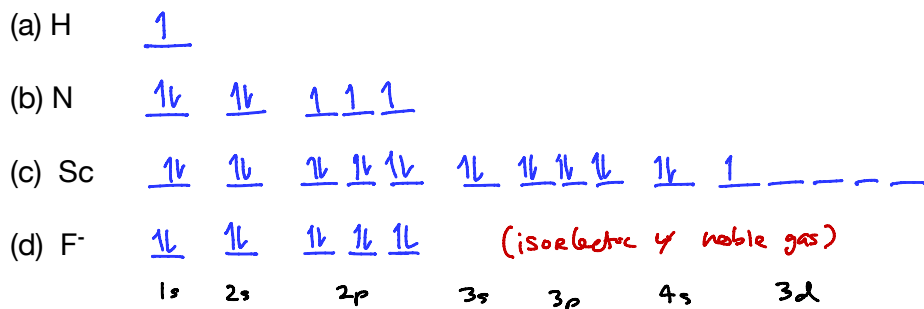
¿ Draw orbital diagrams for the following:

(a) H

(b) N

(c) Sc

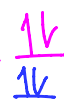
(d) F⁻



Rules Wrapup: Aufbau Principle, Hund's Rule, Pauli Exclusion Principle

Rules		
Aufbau Principal	filling order	Fill in way that gives the lowest TOTAL energy. Fill periodic chart as if reading a book, noting the 'd' level is displaced one row, and the "f" level is displaced two rows.
Hund's Rule	sublevel filling priority	Fill sublevel orbitals singly, then begin pairing. Relative Stability: Full sublevel > 1/2-filled sublevel > "unevenly" filled sublevel
Pauli Exclusion Principle	unique address	No two electron may have the exact same set of four QN's.

d-Orbital Anomalies



- 4 & 9 d-electrons" borrow from the "s-orbital" and fill the "d-orbital"
- Fill sublevel orbitals singly, then begin pairing.
- Relative Stability: Full sublevel > 1/2-filled sublevel > "unevenly" filled sublevel

Electron Configurations and the Periodic Table

Classifications according to VALANCE SHELL configuration

<u>ELEMENT</u>	<u>LAST ELECTRON INTO</u>
① MAIN GROUP (REPRESENTATIVE) ELEMENTS	s, p
② TRANSITION ELEMENTS (METALS)	d
③ INNER TRANSITION ELEMENTS	f

Electron Configurations of Ions

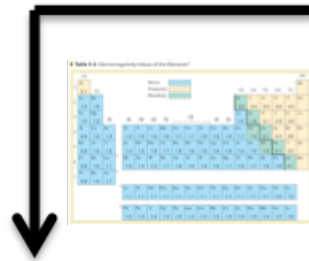
For ions, follow the AUFBAU principle... same as for an element, but taking into account lost electrons (makes a cation) and gained electrons (makes anion)

5 periodic variations

- (1) covalent radius
 - (2) ionic radius
 - (3) ionization energy
 - (4) electron affinity
 - (5) electronegativity
- ⇒ trend problems

(1) Variation in Covalent Radius

1A	2A	3A	4A	5A	6A	7A	8A
H 0.37		Atomic radii					He 0.31
Li 1.52	Be 1.12	B 0.85	C 0.77	N 0.75	O 0.73	F 0.72	Ne 0.71
Na 1.86	Mg 1.60	Al 1.43	Si 1.18	P 1.10	S 1.03	Cl 1.00	Ar 0.98
K 2.27	Ca 1.97	Ga 1.35	Ge 1.22	As 1.20	Se 1.19	Br 1.14	Kr 1.12
Rb 2.48	Sr 2.15	In 1.67	Sn 1.40	Sb 1.40	Te 1.42	I 1.33	Xe 1.31
Cs 2.65	Ba 2.22	Tl 1.70	Pb 1.46	Bi 1.50	Po 1.68	At 1.40	Rn 1.41



Down
























- incr n = incr R (Schrodinger)

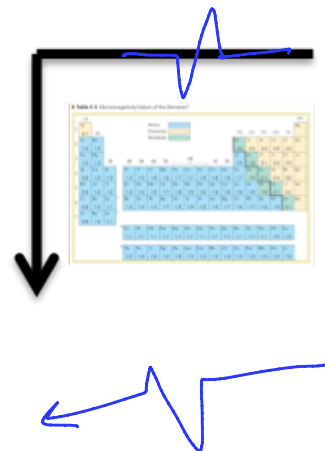
Across (L → R)

- shielding = $k \dots \uparrow$ Nu (+)... \uparrow
 $Z_{\text{eff}} \dots \downarrow$ size

(2) Variation in Ionic Radii

Comparison of Atomic and Ionic Radii

1A	2A	3A	5A	6A	7A
Li 1.52 	Be 1.12 		N 0.75 	O 0.73 	F 0.72 
Na 1.86 	Mg 1.60 	Al 1.43 		S 1.03 	Cl 1.00 
K 2.27 	Ca 1.97 	Ga 1.35 		Se 1.19 	Br 1.14 
Rb 2.48 	Sr 2.15 	In 1.67 		Te 1.42 	I 1.33 
Cs 2.65 	Ba 2.22 	Tl 1.70 			



Down

- incr n (incr R)

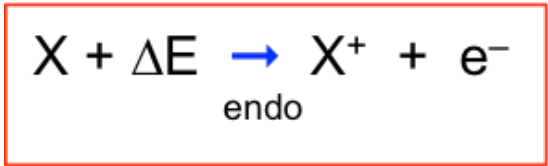
Across (L \rightarrow R)

- CATION isoelectrics (+1>+2>+3): shielding = $k \dots \uparrow \text{Nu} (+) \dots \uparrow Z_{\text{eff}} \dots \downarrow \text{size}$
(also, number of electrons in outer shell)
- ANION isoelectrics (-3,-2,-1): shielding = $k \dots \uparrow \text{Nu} (+) \dots \uparrow Z_{\text{eff}} \dots \downarrow \text{size}$

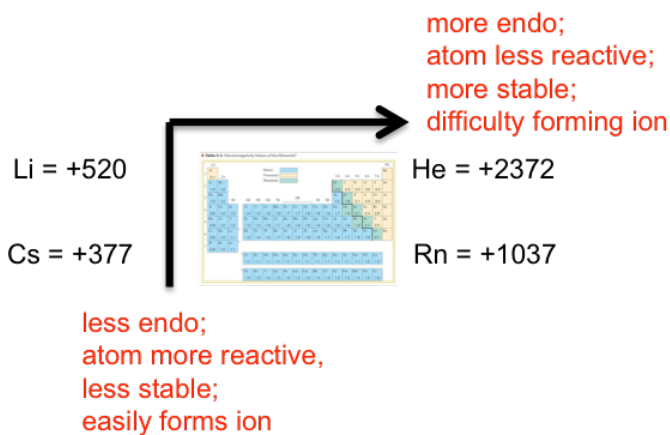
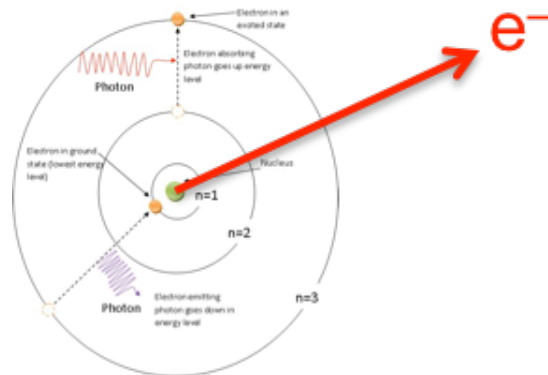
Cations vs. Anions

- Cations smaller than parent (fewer electrons)
- Anions larger than parent (more electrons)
- for given period: Anions (excess of neg. chg) larger than Cations (deficit of neg. chg)

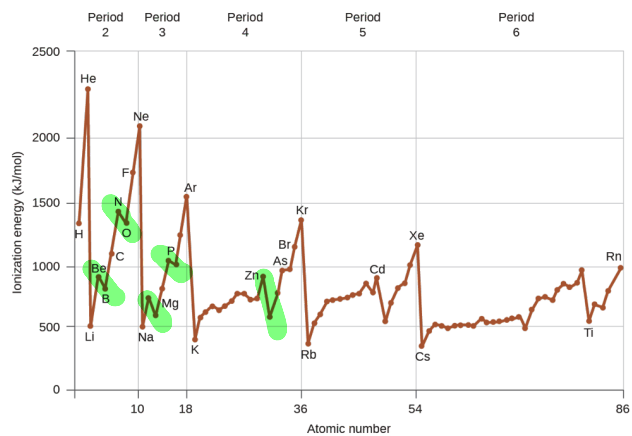
(3) Variation in Ionization Energies



- ① Don't confuse with EA
- ② always ENDOTHERMIC
- ③ MNEMONIC: Bohr/Rydberg model in which e^- breaks orbit
- ④ for POYLATOMICS: $IE_{1st} < IE_{2nd} < IE_{nth}$



- If you understand IE in terms of QM, you should be able to recognizing the anomalies



\uparrow \uparrow
 \downarrow \downarrow
1L 1L 1 1
 2s 2p

(EX) Order of Increasing IE

¿Arrange the following in order of increasing IE: Na, Mg, Al, Si?

TREND: ↑ IE, ↑ endo, L→R on PC

[1] Note obvious trends:
• Na < Mg < Al < Si

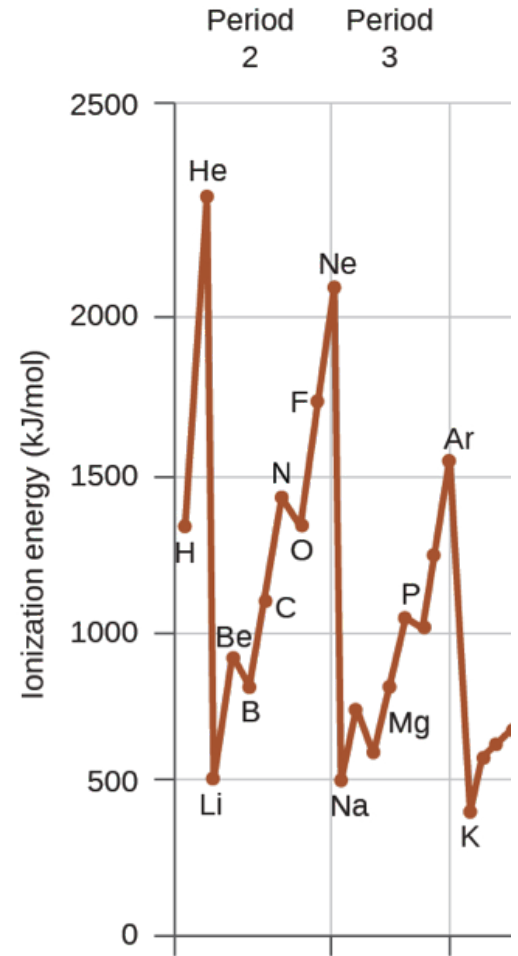
[2] Check for Exceptions:
here, Al unusually stable...
swaps with Mg

Al more reactive (lower IE):
given it gains a full outer sublevel
if it can lose an electron.

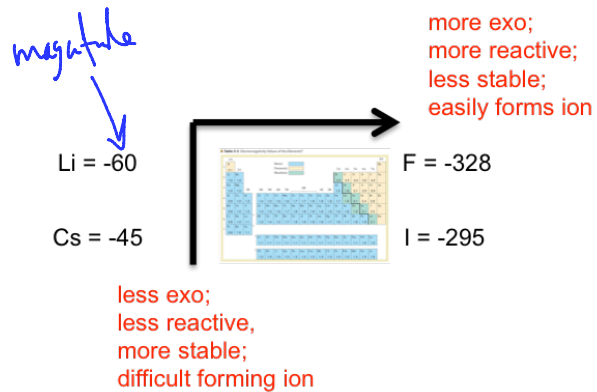
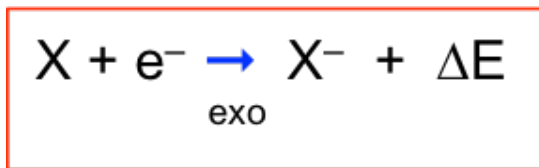
• Na < **Al** < **Mg** < Si



hydrogen 1 1.0079																	helium 2 4.0026	
lithium 3 6.941	beryllium 4 9.0122																	neon 10 20.180
sodium 11 22.990	magnesium 12 24.305																	argon 18 39.948
potassium 19 39.098	calcium 20 40.078	scandium 21 44.956	titanium 22 47.867	vanadium 23 50.942	chromium 24 51.996	manganese 25 54.938	iron 26 55.845	cobalt 27 58.933	nickel 28 58.693	copper 29 63.546	zinc 30 65.38	gallium 31 69.723	germanium 32 72.64	arsenic 33 74.922	seelenium 34 78.96	bromine 35 79.904	krypton 36 83.798	
rubidium 37 85.468	strontium 38 87.62	yttrium 39 88.906	zirconium 40 91.224	niobium 41 92.906	molybdenum 42 95.96	technetium 43 [98]	ruthenium 44 101.07	rhodium 45 102.91	palladium 46 106.42	silver 47 107.87	cadmium 48 112.41	indium 49 114.82	tin 50 118.71	antimony 51 121.76	tellurium 52 127.60	iodine 53 126.90	xenon 54 131.29	
cesium 55 132.91	barium 56 137.33	lanthanum 57 138.91	hafnium 72 178.49	tantalum 73 180.95	tungsten 74 183.84	rhenium 75 186.21	osmium 76 190.23	iridium 77 192.22	platinum 78 195.08	gold 79 196.97	mercury 80 200.59	thallium 81 204.38	lead 82 207.2	bismuth 83 208.98	polonium 84 [209]	astatine 85 [210]	radon 86 [222]	
francium 87 [223]	radium 88 [226]	actinium 89 [227]	rutherfordium 104 [261]	dubnium 105 [262]	seaborgium 106 [266]	bohrium 107 [264]	hassium 108 [277]	meitnerium 109 [268]	darmstadtium 110 [271]	roentgenium 111 [272]								



(4) Variation in Electron Affinities

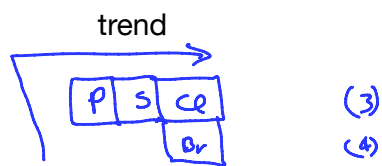


EXO — It always takes energy to move an electron away from the nucleus

EA = the energy change when an electron is added to an isolated gaseous atom to form an ion with a -1 charge

NOTE: Addn of a 2nd electron to a 1- anion is always ENDO—it takes energy to bring a neg. chg. into a neg. chg. species ∴ EA's for anions are always (+) positive

¿Arrange the following in order of increasing negative values of EA: P, S, Cl, Br?



i) $P < S < Cl$

ii) $Br < Cl$ $P < S < Cl$

iii) Br vs S $ES = 0$
TABLE

(ANSWER) Cannot solve w/ information given.

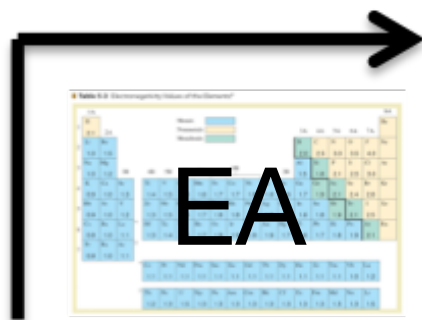


if specific EA data given...

iv) $P < S < Br < Cl$

(5) Variation in Electronegativity

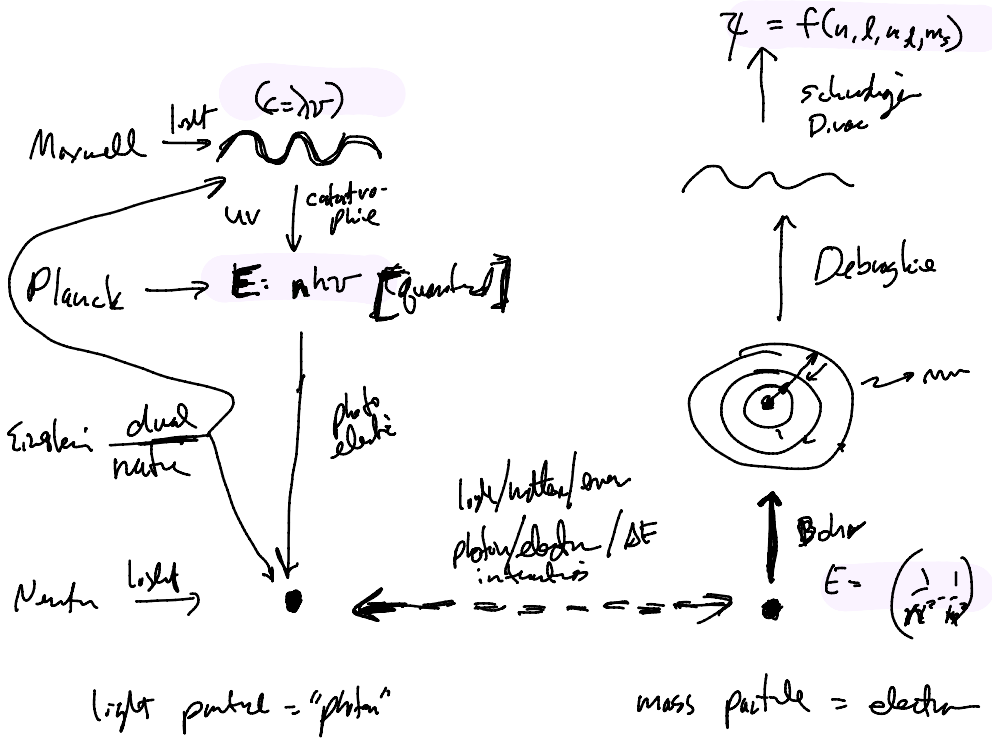
- Introduced early in next chapter, “Chemical Bonding and Molecular Geometry”
- But to give the punchline early, EN increases in the same direction as IE and EA: it’s magnitude increases from bottom-to-top, and left-to-right



↓ SCRATCH ↓

Photon

Electron



↑ SCRATCH ↑