OK, let's bring it back to atoms (but keep Coulomb's Law fresh... it's important!)

If we heat an atom up (give it energy), we can force an electron to be ejected!

this is where stuff gets <u>REALLY</u> cool!

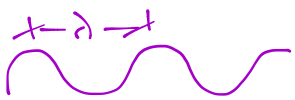
Even though Coulomb's Law can describe some behaviors of electrons interacting with nuclei... it fails to describe <u>ALL</u> observations scientists can make.

This is the basis of the field of quantum mechanics: Electrons have the properties of a <u>wave</u> as they interact with the nucleus of an atom.

<u>Properties of a wave</u>

wavelength $\xrightarrow{(\lambda)}$ this is a length and has a distance unit (m or nm)

frequency → Hz (1/s) ν



ν = how many times a peak of the wave passes by a point in one second

these two are related through the speed of light ($c = 2.9979 \times 10^8 \frac{m}{s}$)

$$c = \lambda * \nu$$
$$\frac{m}{s} \quad m \quad \frac{1}{s}$$

so if you know the λ, you can easily calculate ν and vice versa

- ν + λ can vary over huge ranges.

The energy of any wave can be calculated if you know λ <u>or</u> ν

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

h = Planck constant = 6.626×10^{-34} J·s

hugely important!

And as it turns out, energy in this form also has the properties of a particle: Particle Wave Duality

Photon = energy particle (which also has the property of a wave when it is in motion)

Proof that photons can have the properties of a particle:

Photoelectric Effect (think metal in the microwave)

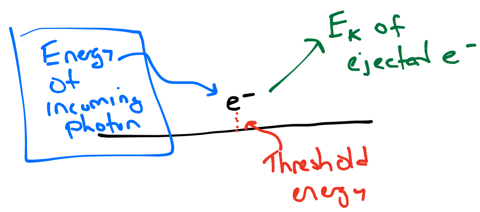
Photons can interact with a surface. If they have enough energy, an e^- will be ejected

same thing as ionization energy!

$$M \longrightarrow M^+ + e^-$$

the electron that is ejected will have a certain amount of Kinetic

Conservation of energy: The energy of the incoming photon must be equal to the energy required to release the e^- (threshold energy) plus the kinetic energy of the e^- that gets ejected



energy of photon

$$E_{photon} = \phi + E_K$$

ϕ: Threshold energy

E_K: ← Kinetic Energy of electron

Sample problem: Calculate E_K ejected e^- when 210 nm light hits a Cu surface

Threshold Energy of copper is $\underbrace{7.1296 \times 10^{-19} J}_{\text{energy necessary to eject the } e^-}$

$$E_{photon} = \frac{hc}{\lambda} = \frac{6.626 \times 10^{-34} J \cdot s \,(2.998 \times 10^8 m/s)}{210 \times 10^{-9} m} = 9.459 \times 10^{-19} J$$

$$E_{photon} - E_{Cu} = KE = 2.329 \times 10^{-19} J$$

Further, we can calculate the velocity of the ejected electron

$$KE = \frac{1}{2} m v^2 \qquad m_{e^-} = 9.109 \times 10^{-31} kg$$

$$2.329 \times 10^{-19} \frac{kg\, m^2}{s^2} = \frac{9.109 \times 10^{-31} kg}{2} v^2$$

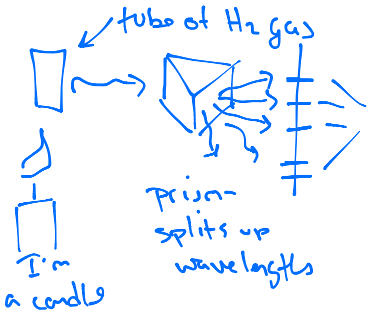
$$v^2 = 2.556 \times 10^{11} \frac{m^2}{s^2}$$

$$v = 5.056 \times 10^5 \, m/s$$

So if we heat up a hydrogen atom, we expect to eject one e^- that has characteristic $\lambda + \nu$. However, when we do an experiment that explores this, we actually see 5 distinct wavelengths in the visible region + LOTS more in the UV + IR.

This is our first clue about the "quantization of energy"

- an electron can exist in very well defined energy states within an atom



for H_2, these λ are:
397.0 nm, 410.2 nm,
434.0 nm, 486.1 nm
653.3 nm

We could try to explain this based on KE of "ejected" e^- + it's deBroglie wavelength, but we would be wasting our time.

Swedish Physicist Johannes Rydberg came up with an expression that can explain these wavelength for Hydrogen (and only H_2)

$$\frac{1}{\lambda} = (1.097 \times 10^7 \, m^{-1})\left(\frac{1}{4} - \frac{1}{n^2}\right)$$ where n is an integer $n = 3, 4, 5, 6 ..$

observed wavelength

if $n = 7$

$$\underbrace{\left(\frac{1}{4} - \frac{1}{7^2}\right)}_{0.2296} 1.097 \times 10^7 m^{-1} = 2.519 \times 10^6 m^{-1} = \frac{1}{\lambda}$$

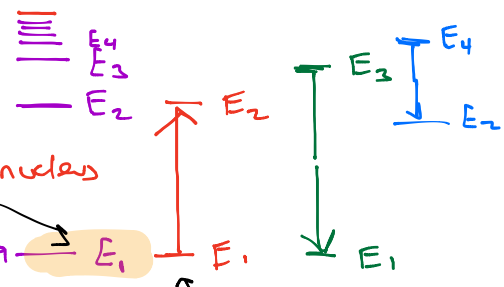
$$\lambda = 3.97 \times 10^{-7} m \left| \frac{1\,nm}{10^{-9} m} \right. = 397\,nm$$

this is one of the observed lines

This type of experiment can allow scientists to unambiguously identify an element because each atom has a unique

Energy Level Diagram

E_∞ →



$E_\infty = \emptyset$ → NO attraction of the e- to the nucleus

ground state = the lowest energy state (so most stable)

Energy is absorbed & the e- gets "excited"

So the idea here is that an e- can move between energy levels. To move UP, energy is needed, to move down energy is released

ΔE = change in energy = $E_{final} - E_{initial}$

$E_2 - E_1 = -0.54 - {}^{-}2.18 = 1.64\,aJ$

this value is (+) because energy is required

$E_n \rightarrow E_1$ = Lyman Series

$E_n \rightarrow E_2$ = Balmer Series

$E_n \rightarrow E_3$ = Paschen Series

$E_1 - E_3 = -2.18 - {}^{-}0.24 = -1.94\,aJ$ → (-), so Energy is released

This energy is released in the form of a Photon with 1.94 aJ of energy

If we calculate the λ of the emitted photon

$$1.94 \times 10^{-19}\,J = \frac{6.626 \times 10^{-34}\,J \cdot s\,(2.998 \times 10^8\,m/s)}{\lambda}$$

$$\lambda = \frac{1.986 \times 10^{-25}\,J \cdot m}{1.94 \times 10^{-18}\,J} = 1.024 \times 10^{-7}\,m = 102.4\,nm$$

this is the UV

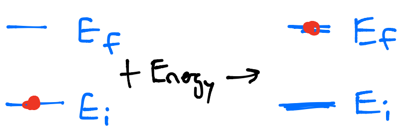
Lyman Series

$E_2 - E_4 = {}^-0.54\,aJ - {}^-0.13\,aJ = {}^-0.41\,aJ$

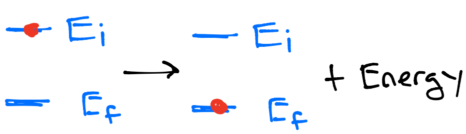
$0.41 \times 10^{-18} J = \frac{hc}{\lambda}$ $\qquad \lambda = \frac{1.986 \times 10^{-25} J \cdot m}{0.41 \times 10^{-18}} = 4.86 \times 10^{-7} m$

486 nm → this is one of the lines in the Balmer Series

Generalized Equation: $\Delta E = -2.1799 \times 10^{-18} J \left(\frac{1}{n^2_{final}} - \frac{1}{n^2_{initial}} \right)$



If this is a (+) number, energy is being absorbed by the electron → it moves to an Excited State



If $\Delta E < 0$, the electron is moving to a lower energy state. It gives off energy in the form of a photon

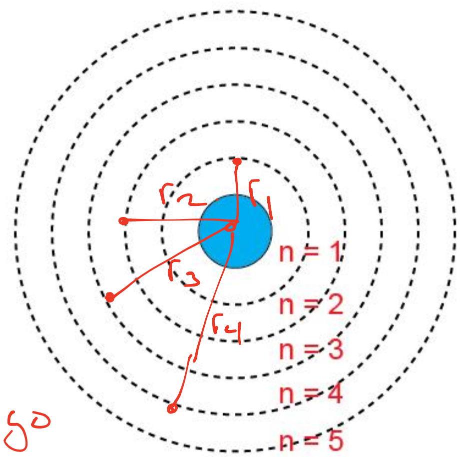
Today we are going to work toward understanding why e⁻ go into an atom in the specific way that they do. ($1s^2\ 2s^2, 2p^6 \ldots$)

- let's start by thinking about the Bohr model of the atom:

  - Each shell is represented by a single circle surrounding the nucleus. Each <u>shell</u> is a specific distance (r) from the nucleus.

  - Apply Coulomb's law:

$$E_1 = \text{constant}\ \frac{(+1)(-1)}{r_1}$$



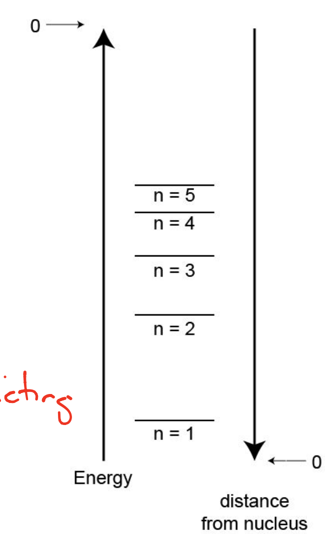
$E_1 < E_2$ (more negative)

which means that the e^- in the 1st shell are more attracted to the nucleus. This is why they go "in" 1st

$E_1 < E_2 < E_3 < E_4 \ldots$

Another way of looking @ this:

Energy level diagram:



Coulomb's Law can get us close to predicting those energies, but the next equation will let you calculate it exactly!

$$\text{The energy of the } n^{th} \text{ wavelength} \equiv E_n = \frac{-2.1799 \times 10^{-18}\,J}{n^2}(Z^2)$$

Hydrogen Atom

$E_1 = -2.18\ aJ$

$E_2 = -0.54$

$E_3 = -0.24$

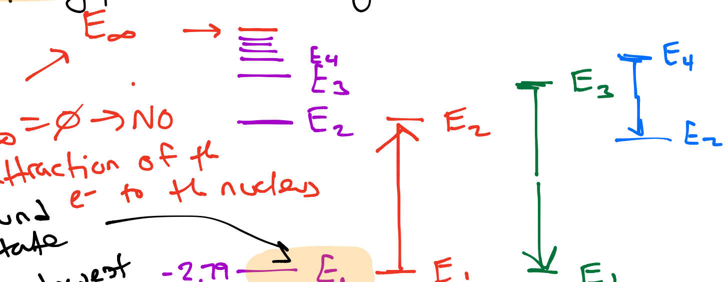
$E_4 = -0.13$

$E_5 = -0.09$

This Equation holds true ONLY for single electron atoms!

(H, He^{+}, Li^{2+}, Be^{3+}, etc)

Energy Level Diagram



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486 nm → this is one of the lines in the Balmer Series

OK, so why is this so important?

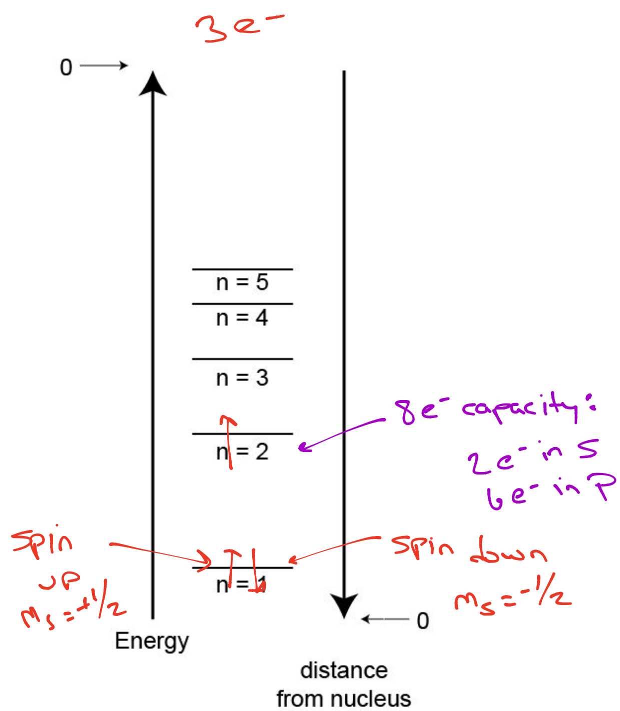
Experimental evidence that e⁻ can <u>only</u> exist @ very specific energies - <u>NOT</u> between the calculated levels.

Quantization of energy: e⁻ around an atom are confined to discrete energy states

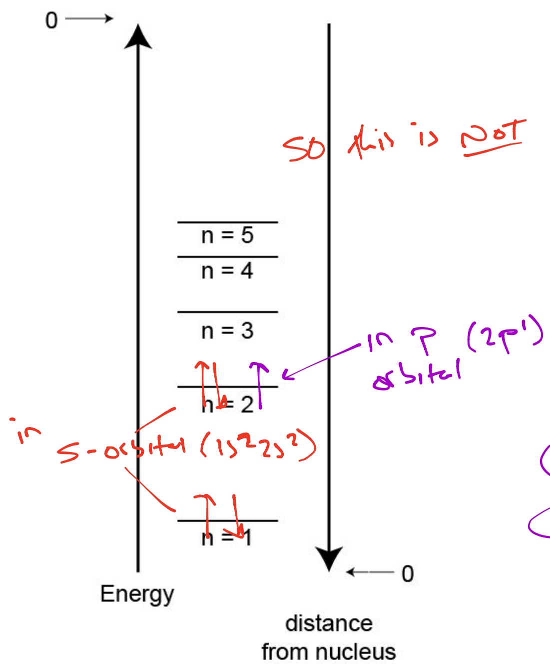
This concept gets deeper + more profound (Quantum Mechanics), but we will leave this for another class:

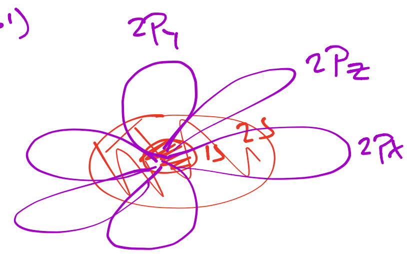
-punchline — Electrons are confined to specific energy states which actually confine the regions of space that they can exist!

What happens when more than one e^- gets put on an atom?

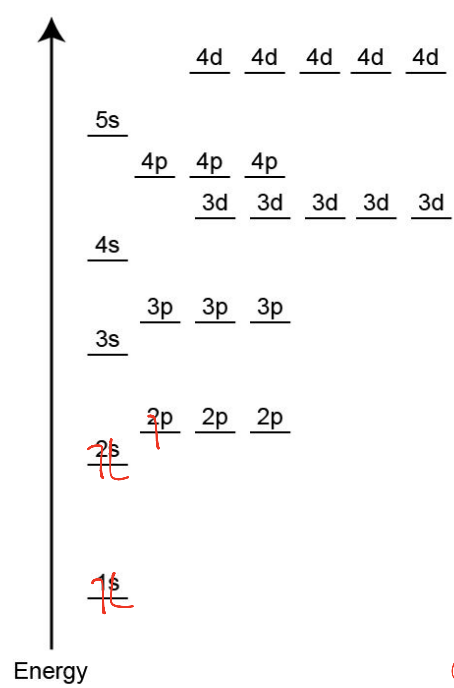


So this is NOT accurate!





P-orbitals are further away from the nucleus, so they are higher in energy.



Rules for filling an energy level diagram

1. Lowest energy 1st
2. In degenerate (equal energy) orbitals, one e^- per orbital before making a pair
3. Add e^- until you've run out

Things we can learn:

- # of unpaired e^- (diamagnetic $= \emptyset$; paramagnetic ≥ 1)
- ground state e^- config (lowest energy e^- config)
- excited state predictions (move $\underline{1}$ e^- up to the next energy level)

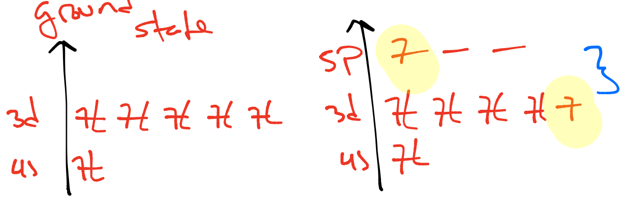
Consider the ground state & 1st excited state of Zn.

(1) Which of these states is paramagnetic? $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10}$

(2) Upon relaxation to the ground state, a photon ($\lambda = 200$ nm) is emitted

- What is the energy difference between the two orbitals?
- Which orbitals have this energy gap?

ground state



} paramagnetic

$$100\,\text{nm} \left| \frac{10^{-9}\,\text{m}}{1\,\text{nm}} \right. = 1\times10^{-7}\,\text{m}$$

$$E = \frac{hc}{\lambda}$$

$$E = \frac{6.626\times10^{-34}\,\text{Js}\,(2.998\times10^{8}\,\text{m/s})}{1\times10^{-7}\,\text{m}}$$

$E = 1.986\times10^{-18}$ J difference between 4p & 3d