Algebra-based Physics II
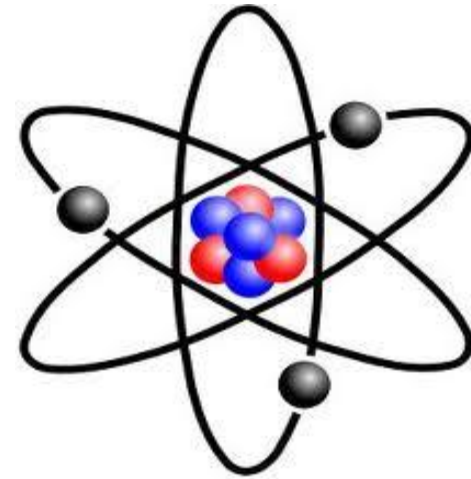
The Nature of Atom

Nov. 22th: Chap 30.1-2:

• Heisenberg uncertainty principle

$$\Delta x \Delta p_x \geq \frac{\hbar}{2}; \quad \Delta E \Delta t \geq \frac{\hbar}{2}$$

• Rutherford scattering

• Line spectra

• Bohr model

Bohr   Einstein

Bohr

Heisenberg

Another way to write the HUP is the following:

This is a statement of the <u>Heisenberg Uncertainty Principle for Energy and Time:</u>

$$\Delta E \Delta t \geq \frac{\hbar}{2}$$

We cannot know exactly the energy of a particle when it's in a particular state of a physical system and also know precisely the time interval that it remains in that state.

Or, the shorter the lifetime of a particle in a particular state, the greater the uncertainty in its energy.

Example:
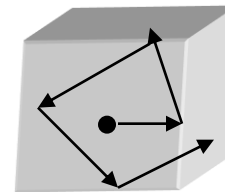
Suppose an electron is confined to a box that is roughly the size of an atom, say 0.5 A on each side. Take this distance to be equal to the uncertainty in the electron's position and calculate the minimum uncertainty in its momentum. Then, assume that this uncertainty in momentum is equal to the magnitude of the electron's momentum at some arbitrary time and calculate the electron's kinetic energy.

Solution: $\Delta y \Delta p_y \geq \dfrac{\hbar}{2}$ $\Rightarrow \Delta p_y = \dfrac{\hbar}{2\Delta y}$ $= \dfrac{6.626 \times 10^{-34}}{(4\pi)(0.5 \times 10^{-10})}$ $\boxed{= 1.06 \times 10^{-24} \text{ kg} \cdot \text{m/s}}$

Now assume $p = \Delta p_y$: $KE = \tfrac{1}{2} mv^2 = p^2 \Big/ 2m$ $= \dfrac{(1.06 \times 10^{-24})^2}{2(9.11 \times 10^{-31})} = 6.17 \times 10^{-19} \text{ J}$

$$= \boxed{4 \text{ eV}}$$

This is on the order of atomic energies! So the HUP tells us that an electron confined to a box the size of an atom must have an energy ~ 5 eV. Thus, it is bouncing around quite rapidly, ~1.2 × 10⁶ m/s.

What if we repeat this calculation for a tennis ball (m = 0.06 kg) confined to a cardboard box that is 0.5 m on each side?

$\Delta y \Delta p_y \geq \dfrac{\hbar}{2}$ $\Rightarrow \Delta p_y = \dfrac{\hbar}{2\Delta y}$ $= \dfrac{6.626 \times 10^{-34}}{(4\pi)(0.5)}$ $\boxed{= 1.06 \times 10^{-34} \text{ kg} \cdot \text{m/s}}$

Now assume $p = \Delta p_y$: $KE = \tfrac{1}{2} mv^2 = p^2 \Big/ 2m$ $= \dfrac{(1.06 \times 10^{-34})^2}{2(0.06)} = 9.28 \times 10^{-68} \text{ J}$

$$= \boxed{5.7 \times 10^{-49} \text{ eV}}$$

This is equivalent to a speed of ~1 × 10⁻³³ m/s!

In other words, the tennis ball just sits there!

30.1 Rutherford Scattering

We know there are two types of charge, + and -, and that matter is composed of both.

English physicist J.J. Thompson discovered the electron and measured its mass in 1897.

He then suggested the **Plum-Pudding Model** of the atom:

Negative electrons were scattered like plums in a pudding of positive charge that was <u>equally distributed</u> throughout the atom

To this point, no one had detected the positively-charged particles in an atom, but since they knew what the mass of the electron was, they knew most of the atom's mass was due to the positive charges.

electrons → Smeared-out positive charge
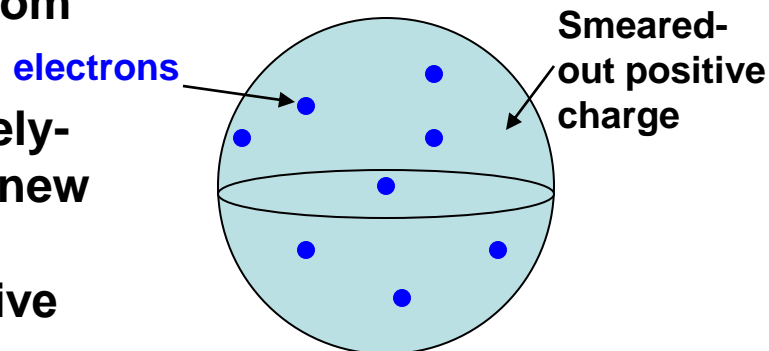
Then **Rutherford** comes along (a New Zealander), working in London in 1907.

He had been studying with Marie and Pierre Curie in Montreal who discovered radioactivity.

They observed two types of radiation. Rutherford called them α and β.
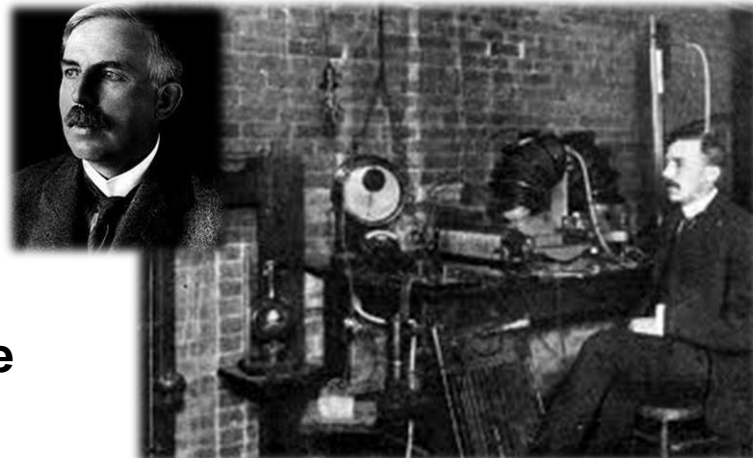
Rutherford soon realized that β-radiation or β-rays were really just electrons.

But α-particles were much **heavier and positively charged**.

(α-particles are really the nucleus of a helium atom. They consist of 2 protons and 2 neutrons. No one knew this at the time.)

Rutherford decided to use the α-particles to investigate the internal structure of atoms.

He shot the α-particles at a thin film of gold:

If Thompson's model of the atom was correct, very little should happen to the α-particles. They should basically travel straight thru the film. **WHY?**

Most of them did just that, but some of the a-particles were deflected at large angles. In some cases almost 180°!

Gold foil

Screen

Source of
α particles
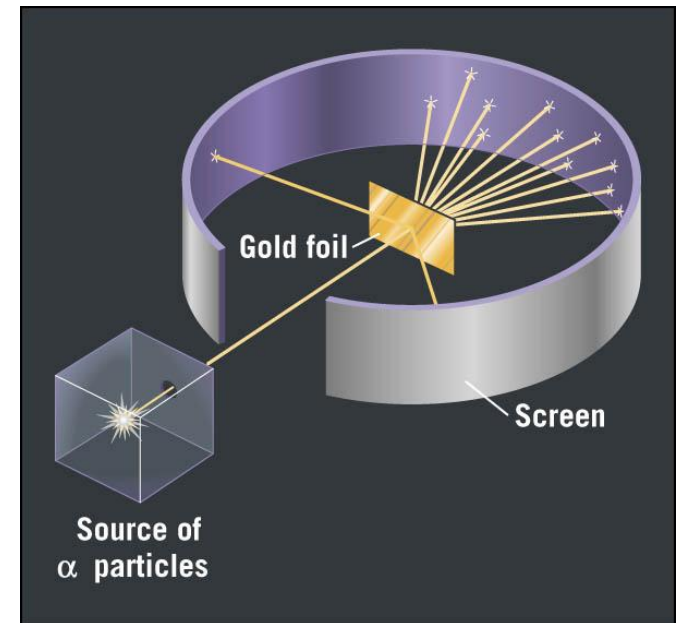
This was completely shocking! Rutherford would later say that, "*It was as if we were firing shells at tissue paper and having them bounce straight back at you*!"

So how could these large deflections occur?

Really only one solution presented itself, and that was to have all the positive charges in the atom concentrated in a very small region – called the <u>atomic nucleus.</u>

The nucleus was much smaller than the entire atom, but it accounted for almost all of the atom's mass.

Rutherford named the positively-charged particles in the nucleus <u>Protons</u>.

This led to the model of the atom that is still widely accepted today – the <u>nuclear model (planetary model).</u>

Negative electron
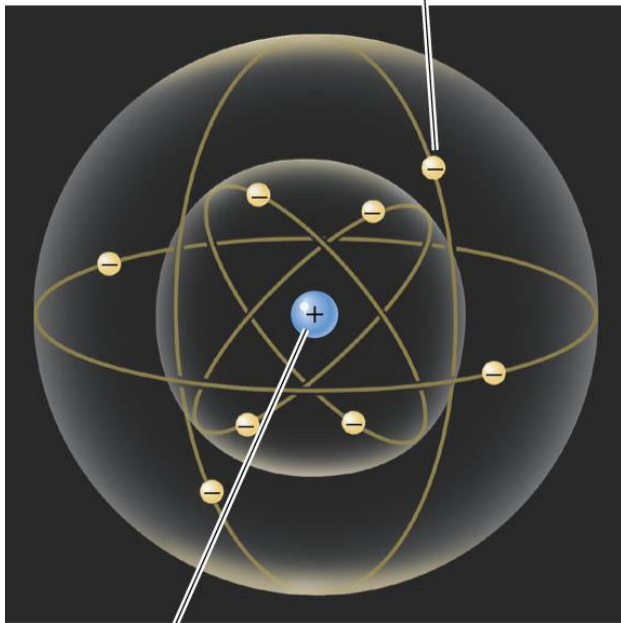
Positive nucleus

(The model is qualitatively accurate, although the electrons do not orbit the nucleus in pretty, constant, circular orbits. They actually exist in a cloud of probability.)
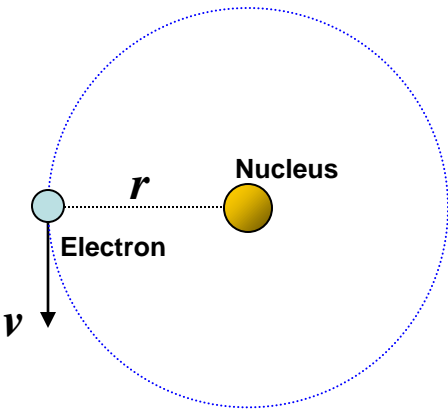
An atom is mostly empty space!!!

Nuclear radii ~1 × 10⁻¹⁵ m

Electron orbit ~1 × 10⁻¹⁰ m

But, there are problems with the <u>Planetary Model of the Atom</u>:

Consider an electron orbiting some nucleus at a radius r:

The electron has both KE and EPE.

Nucleus

r

Electron

v

And…..it is accelerating: $a = \dfrac{m_e v^2}{r}$

But we know from previous chapters that accelerating charges produce electromagnetic waves, and those waves carry energy.

This carries some of the electron's energy away, it slows down, its orbit decreases, since opposite charges attract, and the electron spirals into the nucleus……..The atom collapses!

The planetary model is <u>not</u> stable based on classical electrodynamics!

We'll come back to this soon, but first let's talk about <u>line spectra.</u>

<u>30.2 Line Spectra</u>

Remember, all objects emit EM radiation. Hot filaments in incandescent light bulbs emit a continuous range of wavelengths, some of which are in the visible spectrum.

Solid made of different atoms emits continuous energies of radiation

In contrast to this, single atoms only emit radiation at certain wavelengths.

Atoms emits discrete energies of photons rather than continuous ones!

We can use a diffraction grating to separate these wavelengths and produce a characteristic line spectra for those atoms.
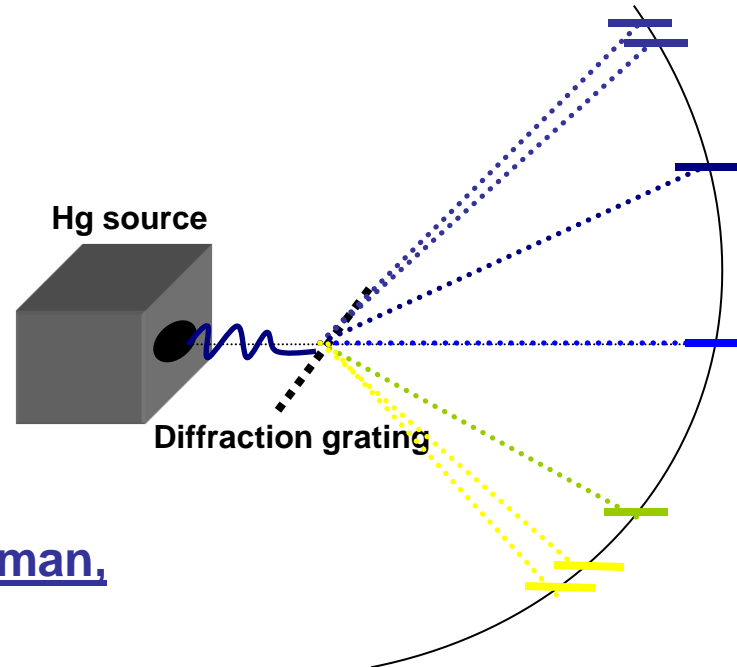
Take mercury (Hg) for example:

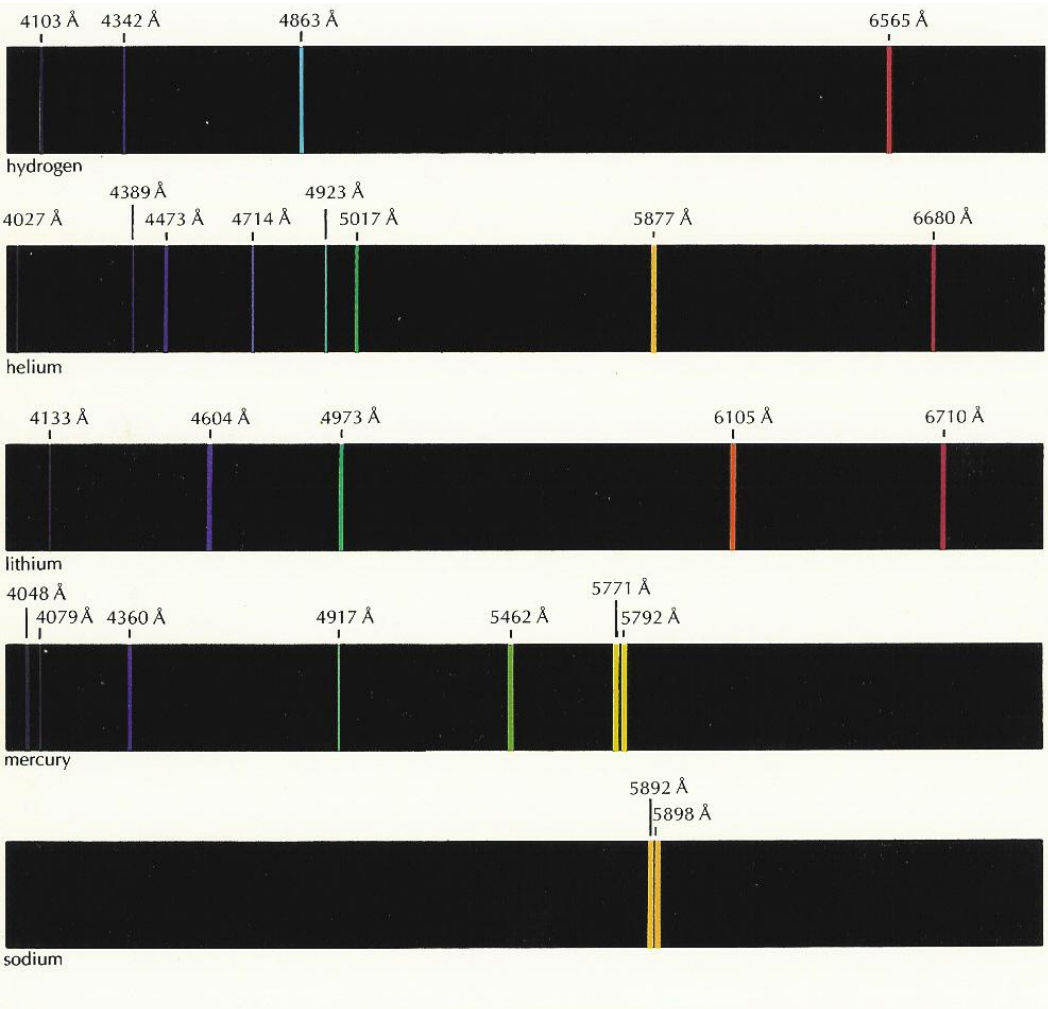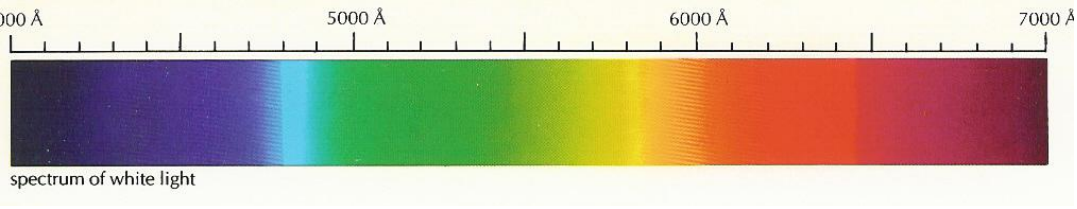**This is mercury's line spectra.**

Hydrogen gas, being the simplest element, also has the simplest line spectra.

It forms 3 groups of lines, called the Lyman, Balmer, and Paschen Series.

Only the Balmer series lies in the visible spectrum.

Hg source

Diffraction grating

spectrum of white light

4103 Å 4342 Å   4863 Å   6565 Å

hydrogen

Balmer series for hydrogen gas.

4389 Å   4923 Å
4027 Å   4473 Å 4714 Å   5017 Å   5877 Å   6680 Å

helium

4133 Å   4604 Å   4973 Å   6105 Å   6710 Å

lithium

Lyman, Balmer, and Paschen discovered relationships between the different wavelengths of light in the line spectra.

4048 Å   5771 Å
   4079 Å 4360 Å   4917 Å   5462 Å   5792 Å

mercury

                                     5892 Å
                                        5898 Å

sodium

Lyman Series:

$$\frac{1}{\lambda} = R\left(\frac{1}{1^2} - \frac{1}{n^2}\right), \; n = 2,3,4,...$$

Balmer Series:

$$\frac{1}{\lambda} = R\left(\frac{1}{2^2} - \frac{1}{n^2}\right), \; n = 3,4,5,...$$

Paschen Series:

$$\frac{1}{\lambda} = R\left(\frac{1}{3^2} - \frac{1}{n^2}\right), \; n = 4,5,6,...$$

$$\boxed{R = \text{Rydberg Constant} = 1.097 \times 10^7 \text{ m}^{-1}}$$

General Formula:

$$\boxed{\frac{1}{\lambda} = R\left(\frac{1}{m^2} - \frac{1}{n^2}\right), \; m, \; n \; = \; 4,5,6,...; \; m < n}$$

Algebra-based Physics II

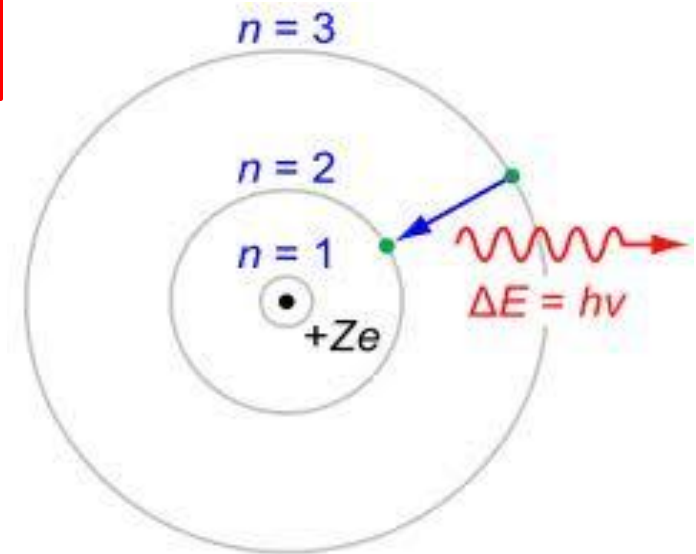**Nov. 24th: Chap 30.3-4:**

• Atomic line spectra

$$\frac{1}{\lambda} = R\left(\frac{1}{m^2} - \frac{1}{n^2}\right), \ \ m, \ n \ = \ 4,5,6,...; \ \ m < n$$

• Bohr model of atom

$$hf = E_i - E_f = \frac{hc}{\lambda}$$

• de Broglie explanation on quantized angular momentum

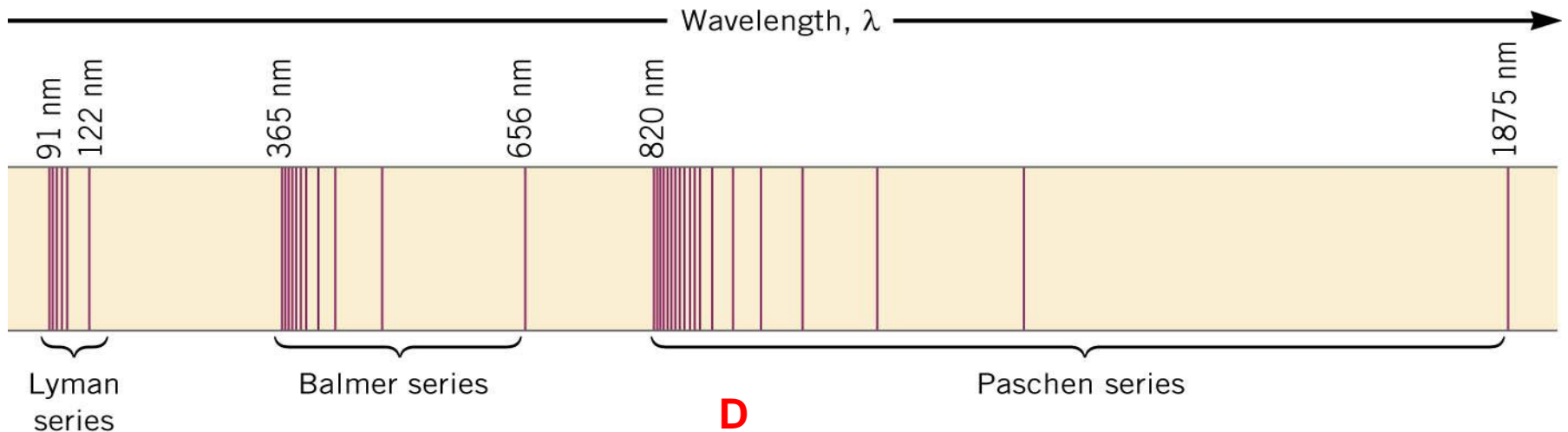$$L_n = mv_n r_n = n\hbar, \ \ n = 1,2,3,...$$

For n = 3, the Balmer series is:
$$\frac{1}{\lambda} = R\left(\frac{1}{2^2} - \frac{1}{3^2}\right) \Rightarrow \frac{1}{\lambda} = R\left(\frac{1}{4} - \frac{1}{9}\right)$$

$$\Rightarrow \lambda = \frac{7.2}{R} = 656 \text{ nm} \longrightarrow \textbf{Red part of visible spectrum}$$

For n = ∞, the Balmer series is:
$$\frac{1}{\lambda} = R\left(\frac{1}{2^2} - \frac{1}{\infty^2}\right) \Rightarrow \frac{1}{\lambda} = R\left(\frac{1}{4}\right)$$

$$\Rightarrow \lambda = \frac{4}{R} = 365 \text{ nm} \longrightarrow \textbf{UViolet part of visible spectrum}$$

Wavelength, λ

91 nm 122 nm 365 nm 656 nm 820 nm 1875 nm

Lyman series Balmer series **D** Paschen series

30.3 Bohr Model of the Atom

Niels Bohr died in 1962. He was a native of Denmark who went to England on scholarship to work with J.J. Thompson. He and Thompson didn't get along, so Bohr went to work for Rutherford.

He worked on the planetary model and tried to understand how matter could be stable if electrons are accelerating around the nucleus.

Hydrogen atom

Proton

r

Electron

v
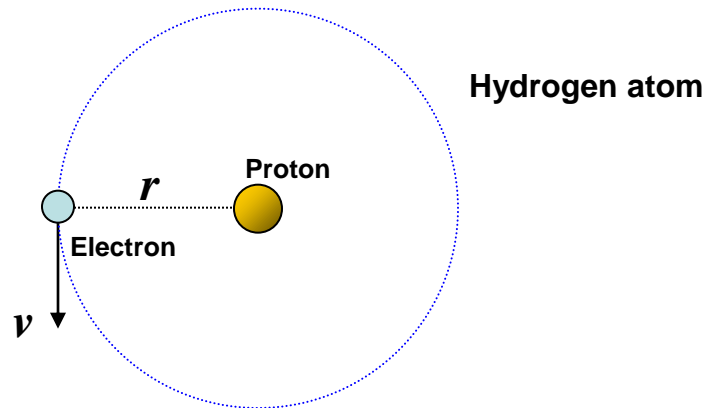
Bohr started with hydrogen, since it is the simplest of all elements. We have just 1 electron orbiting 1 proton.

Like Einstein did with the photoelectric effect, Bohr adopted Planck's idea of quantized energy levels, and assumed that the electron in the hydrogen atom could only have certain values of energy, i.e. they are quantized.

Each of these energy levels corresponds to a unique orbit that the electron moves in around the proton. The larger the orbit, the larger the energy.

So here are Bohr's assumptions:

1. Electrons travel in fixed orbits around the proton, each orbit being defined by a unique radius and energy. These orbits are called stationary orbits or states, and while in these orbits, the electrons do not emit radiation.

How can we have radiationless orbits??? This goes against classical physics!!!!!

Furthermore, we know that all matter absorbs and emits radiation, so how do Bohr's atoms do this??

To explain this, Bohr incorporated Einstein's photon model:

2. An electron in an atom emits radiation (emits photons) when and only when it moves from a higher energy level to a lower one, i.e. it moves from a larger radius orbit to a smaller one.
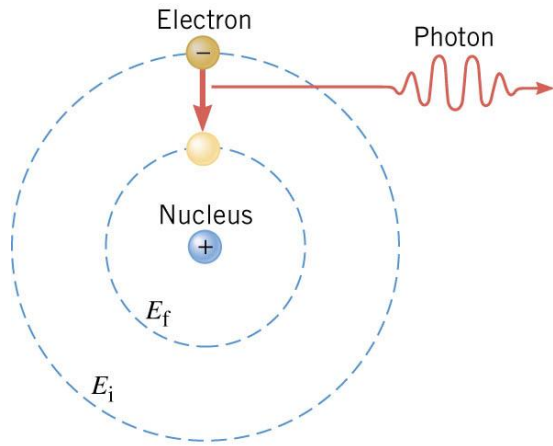
As the electron makes a transition from a higher energy level to a lower one, it emits a photon.

By conservation of energy, the energy of the photon must be equal to the difference in the energies between the two stationary states E_i and E_f:

$$\text{Photon Energy} = E_i - E_f \Rightarrow \boxed{hf = E_i - E_f = \frac{hc}{\lambda}}$$

Remember, this is all theoretical, and Bohr could use this equation to calculate the wavelengths (colors) of light emitted by a hydrogen atom.

But first, he needed a way to calculate the energies, E_i and E_f.

**To do this, he ends up using both classical and quantum physics.**

An electron sitting in the n = 2 energy level of a hydrogen atom has an energy of -3.4 eV. This electron makes a transition to the n=1 state by emitting a photon. The n=1 state has an energy of -13.6 eV. What is the energy of the emitted photon?

✓1.   10.2 eV

2.   17.0 eV

3. -10.2 eV

4. -17.0 eV

$$\text{Photon Energy} = E_i - E_f$$

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

0%   0%   0%   0%

10.2 eV   17.0 eV   3. ...   4. ...
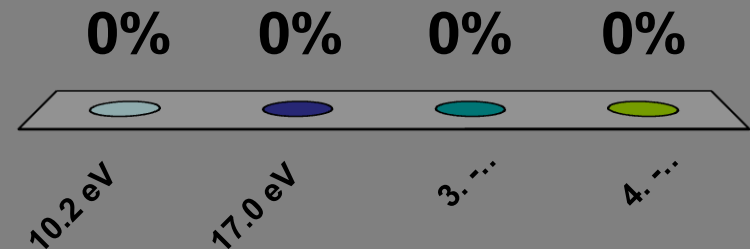
In order to predict the wavelengths of light emitted by hydrogen, he first had to come up with an expression for the energy levels.

Here is his simple model, where Z represents the # of protons in the nucleus.
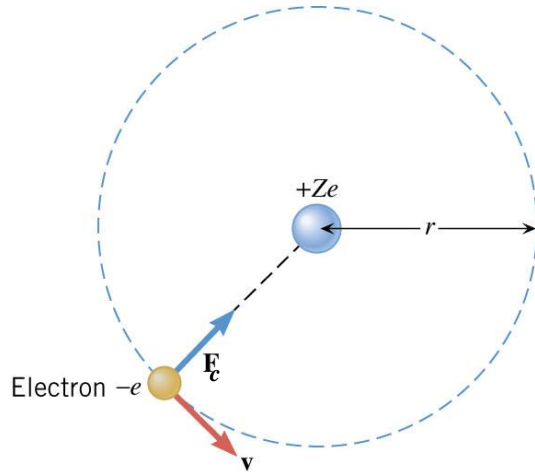
There is an electrostatic force – attractive Coulomb force – between the proton and electron.

+Ze

Electron −e

F_c

v

r

This is directed in toward the center of motion and thus provides the centripetal force.

$$E_{Tot} = KE + EPE = \tfrac{1}{2}mv^2 + k\frac{Q_1 Q_2}{r}$$

Here, $Q_1 = +Ze,$ and $Q_2 = -e$,**so:**

$$E_{Tot} = \tfrac{1}{2}mv^2 - k\frac{Ze^2}{r}$$

But from forces, we know that: $\left|F_c\right| = \left|F_E\right| \Rightarrow \dfrac{mv^2}{r} = k\dfrac{Ze^2}{r^2}$

Solve for mv^2 and plug into the energy equation:

$$E = -k\frac{Ze^2}{2r}$$

This is a classical result for the total energy in a hydrogen atom. It is negative, because the magnitude of the negative EPE is larger than the KE.

But what about the radius? Here's where the quantum physics comes in.

r not only defines a unique orbit, but also a unique <u>angular momentum</u>.

Remember from Physics 1, $L = I\omega$, where $I = mr^2$ for the electron, since it is a point particle, and $\omega = v/r$.

Thus, $L = (mr^2)(\tfrac{v}{r}) = mvr$ **<u>Angular Momentum</u>**

This is the classical result for angular momentum.

But since Bohr assumed the energy of the electron in the hydrogen atom was quantized, that meant r was quantized, which means the <u>angular momentum must be quantized.</u>

Thus, L can only assume discreet values of angular momentum.

But what would those discreet values be???? A clue is given if we look at the units of angular momentum: $\left[\dfrac{\text{kg} \cdot \text{m}^2}{\text{s}}\right]$

What else has these units??? Well, oddly enough, look at $\hbar$:

$$\hbar \left[\text{J} \cdot \text{s} \right] = \left[\text{N} \cdot \text{m} \cdot \text{s} \right] = \left[\frac{\text{kg} \cdot \text{m}^2 \cdot \text{s}}{\text{s}^2} \right] = \left[\frac{\text{kg} \cdot \text{m}^2}{\text{s}} \right]$$

Thus, $\hbar$ has the same units as angular momentum!!!

In other words, $\hbar$ is the fundamental quantum value of angular momentum.

This led to Bohr's third assumption: $\boxed{L_n = mv_n r_n = n\hbar, \ n = 1,2,3,...}$

In the quantum world, angular momentum comes in little packets of $\hbar$.

Solve the above for v and plug into the force equation:

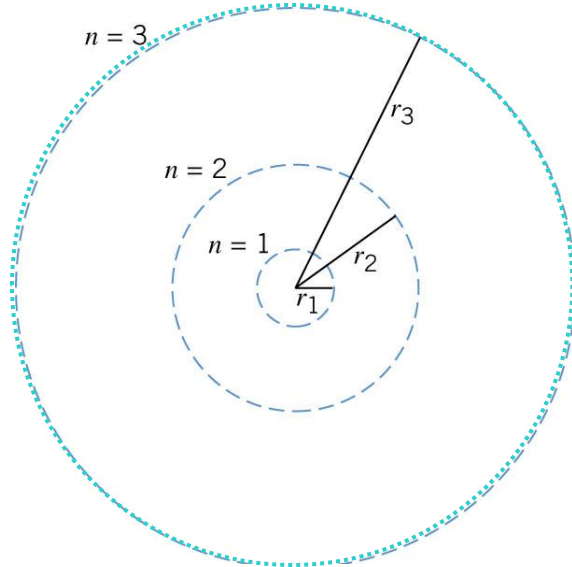$$\boxed{r_n = \left(\frac{h^2}{4\pi^2 mke^2} \right) \frac{n^2}{Z} = \left(5.29 \times 10^{-11} \text{ m} \right) \frac{n^2}{Z}, \ n = 1,2,3,...}$$

So here is the equation that gives us the different <u>quantized orbits.</u>

For the hydrogen atom, $Z = 1$, and for the lowest quantized orbit ($n = 1$) we find that:

$$r_1 = 5.29 \times 10^{-11} \text{ m}$$

This is the first <u>Bohr radius</u> for hydrogen.

Remember, each n-level will correspond to a different Bohr radius.

Now that we have our expression for r, we can plug it into our equation for the total energy:

$$E_n = -\left(\frac{2\pi^2 m k^2 e^4}{h^2} \right) \frac{Z^2}{n^2}, \quad n = 1,2,3,...$$

This represents the <u>quantized Bohr energy levels</u> of the hydrogen atom.

The stuff in parentheses is just a constant:

$$E_n = -(2.18 \times 10^{-18} \text{ J}) \frac{Z^2}{n^2}$$
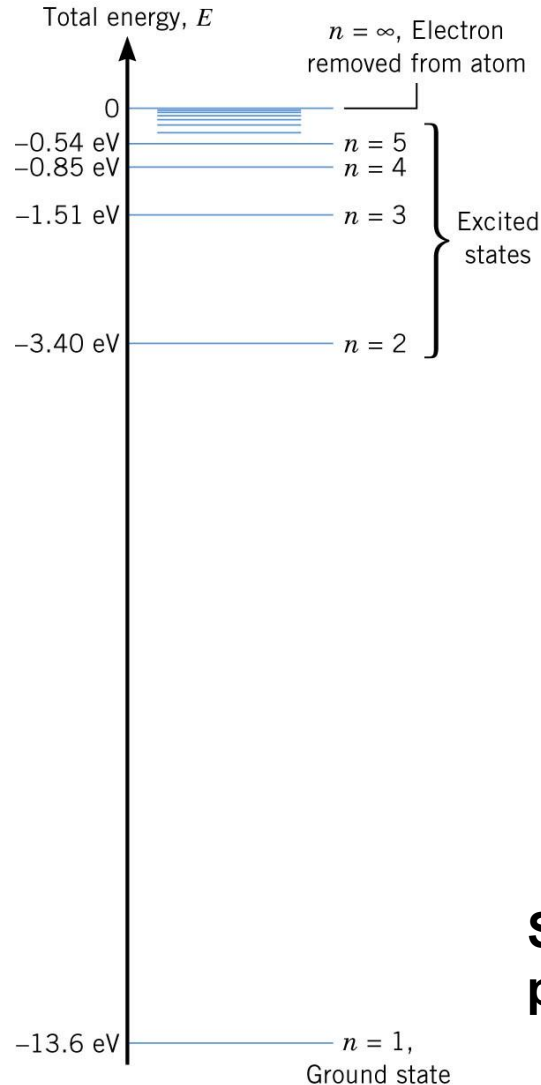
Bohr energy levels in Joules.

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

Bohr energy levels in electron volts.

Again for hydrogen, $Z = 1$, and $n = 1$:

$$E_1 = -13.6 \, \text{eV}$$

This is the energy of the electron in the first Bohr level. It is also called the <u>ground-state energy.</u>

Notice, because of the $1/n^2$ dependence, the spacing between higher and higher energy levels decreases.

So, if I add 13.6 eV to an electron in the ground state of a hydrogen atom, then it will have zero total energy and no longer be bound to the proton → **The electron is removed.**

This process is called <u>ionization.</u>

So the Bohr theory predicts that the first ionization energy of hydrogen is 13.6 eV. This was in excellent agreement with experiment.

So clearly he was on the right track, but did his theory predict the correct emission wavelengths for hydrogen???

From his second assumption:

$$\frac{hc}{\lambda} = E_i - E_f \implies \frac{1}{\lambda} = \left(\frac{2\pi^2 mk^2 e^4}{h^3 c}\right)(Z^2)\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right), \quad n_f, n_i = 1,2,3,...$$
$$n_i > n_f$$

$$\implies (\text{Constant})\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right) \quad \text{So what is this constant:} \quad \left(\frac{2\pi^2 mk^2 e^4}{h^3 c}\right)$$
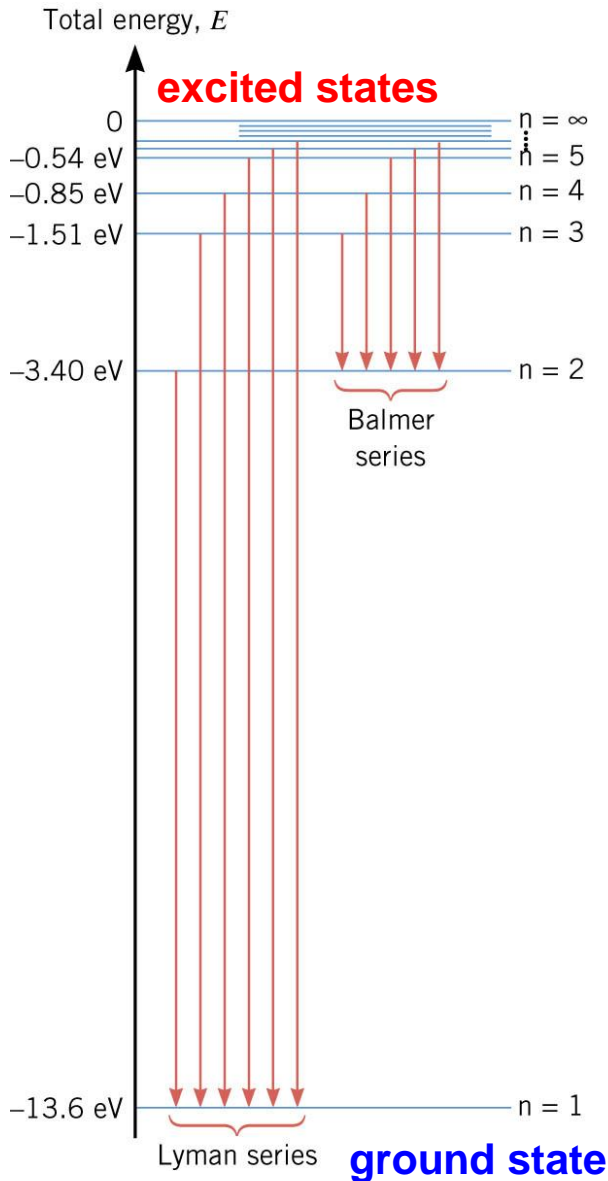
$$\left(\frac{2\pi^2 mk^2 e^4}{h^3 c}\right) = 1.097 \times 10^7 \text{ m}^{-1} = R \qquad \text{Holy crap!!! This is just:}$$

$$\boxed{\frac{1}{\lambda} = R\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right), \quad n_i = 2,3,4,...} \quad \underline{\text{Lyman Series!!!}}$$

Bohr's theory reproduces the experimental result!!!

The Lyman series consists of transitions to the ground state ($n = 1$) starting with the first excited state ($n = 2$):

Total energy, E

excited states

0	$n = \infty$
−0.54 eV	$n = 5$
−0.85 eV	$n = 4$
−1.51 eV	$n = 3$
−3.40 eV	$n = 2$

Balmer series

−13.6 eV	$n = 1$

Lyman series   **ground state**

The Balmer series consists of transitions to the first excited state ($n = 2$) starting with the 2nd excited state ($n = 3$).

The wavelengths we observe from hydrogen are called <u>emission lines</u>.

Atoms can also absorb photons (<u>absorption lines</u>).

If a photon is incident on an atom and has an energy equal to the energy difference between two quantum energy levels of the atom, then the electron can get "bumped up" to that higher energy level, called an <u>excited state.</u>

The lifetime of the electron in the excited state is finite and rather short. It quickly drops back down to a lower energy state and emits a photon whose energy is equal to the difference in the energies of the two levels.

Turkey can in excited states!

Happy Holiday!

Algebra-based Physics II

Nov. 29th: Chap 30.4-5:

• de Broglie explanation on quantized

angular momentum
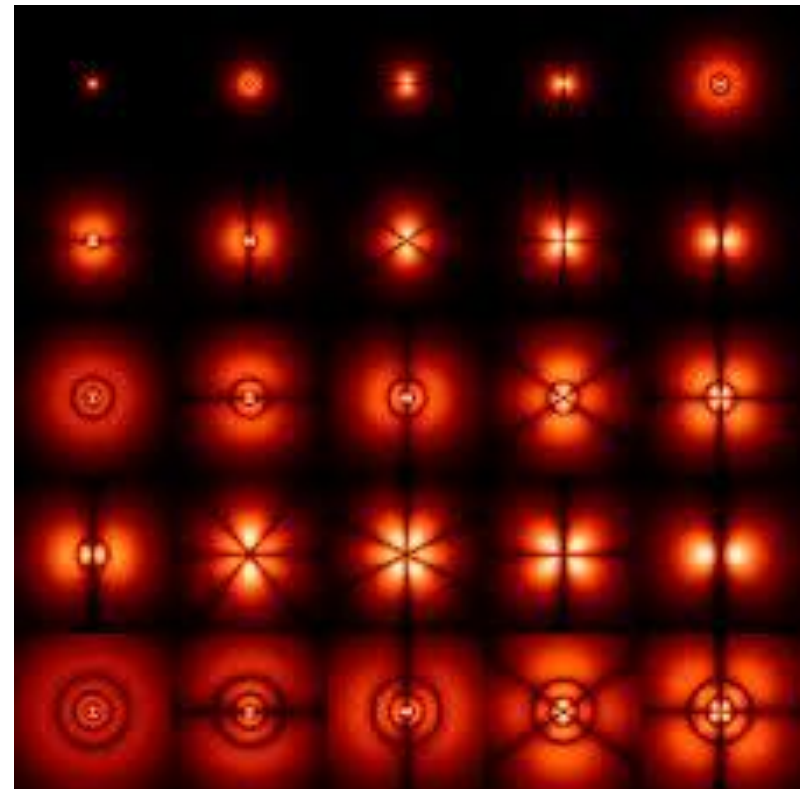
$$L_n = mv_n r_n = n\hbar, \; n = 1,2,3,...$$

• Quantum mechanics of the atom:

1. angular momentum of orbit

$$L = \sqrt{l(l+1)}\,\hbar$$

2. spin
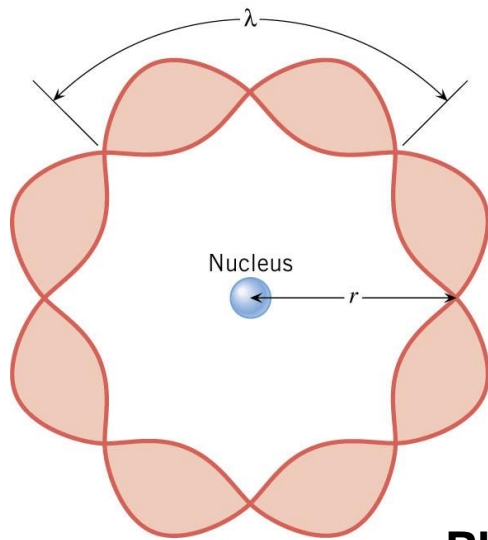
$$m_s = \pm \tfrac{1}{2}$$

Electron wave cloud in different orbits

30.4 deBroglie's Explanation of Bohr's Angular Momentum Assumption

Based on Bohr's work, deBroglie pictured the electron orbiting the proton as a particle-wave.

For certain wavelengths, the electron will form standing waves around the nucleus:

A standing wave occurs when the distance the wave travels is an integral number of its wavelength.

For this condition, $\qquad 2\pi r = n\lambda, \ \ n = 1,2,3,...$

But, $\qquad \lambda = \dfrac{h}{p} = \dfrac{h}{mv}$

Plug in above $2\pi r = \dfrac{nh}{mv} \Rightarrow mvr = \dfrac{nh}{2\pi} = n\hbar$

$\Rightarrow L_n = n\hbar$ **Which is just the Bohr assumption on angular momentum!!!**

So Bohr's assumption of quantized angular momentum is exactly equivalent to a standing-wave condition for electron waves around the nucleus.

I believe de Broglie's hypothesis is the first feeble ray of light on this worst of our physical enigmas. It may look crazy, but it is really sound!

-Albert Einstein

30.5 The Quantum-Mechanical Description of the Atom

Considering the scope of the problem, Bohr's achievements with such a simple model were remarkable. The electron states in the hydrogen atom were denoted by one unique number, n.

But, it was later determined that for more complicated atoms (and hydrogen too) quantum mechanics would rely on **4 quantum numbers** to describe the electron states in an atom.

1. **Principle Quantum #, n:** Similar to the Bohr model. It gives the total energy of the atom.

2. **Orbital Quantum #, l:** This # determines the angular momentum of the orbit. The values of l depend on n: $l = 0,1,2,…,(n-1)$. Notice, there are n values of l.

Example: What would be the values of l for $n = 3$? $l = 0,1,$ and 2

The magnitude of L (the angular momentum) of the electron is then given by:

$$L = \sqrt{l(l+1)}\ \hbar$$

3. Magnetic Quantum #, m_l: This becomes important when we place the atom in a magnetic field. The field alters the electron energy levels. This is known as the **Zeeman Effect.** If $B = 0$, then m_l plays no role. The value of m_l depends on l:

m_l = -l, -l+1,....,-1,0,1,...+l, in integer steps.

Notice, there are (2l+1) total values of m_l.

If an atom is placed in a magnetic field pointing in the z-direction, then the component of the angular momentum which would arise along the z-direction due to the Zeeman effect is:

$$L_z = m_l \hbar$$

Example: What would be the values of m_l if l=3?

m_l =-3, -2, -1, 0, 1, 2, and 3

4. Spin Quantum #, m_s: An electron has the intrinsic property of **spin**. The orbital and spin motions of the electron combine to produce magnetism in materials. The spin quantum # can only take two possible values:

$$m_s = \pm\tfrac{1}{2}$$

The m_s = +1/2 is often called the **"spin-up" state**, and m_s = -1/2 is referred to as the **"spin-down" state**.

Spin, like mass and charge, is an **intrinsic property** of all electrons. Each electron has the same spin.

Example: Determine completely the number of electronic states in a hydrogen atom for $n = 2$.

Solution: $n = 2 \rightarrow l = 0,1$

$$l = 0 \rightarrow m_l = 0, \quad m_s = \pm\tfrac{1}{2}$$

$$l = 1 \rightarrow m_l = -1,0,1 \quad \begin{array}{l} m_l = -1, \ m_s = \pm\tfrac{1}{2} \\ m_l = 0, \ m_s = \pm\tfrac{1}{2} \\ m_l = 1, \ m_s = \pm\tfrac{1}{2} \end{array}$$

**Thus, there are 8 total states (in general, the total # of states is ($2n^2$).**

	n	l	m_l	m_s
1.	2	0	0	+1/2
2.	2	0	0	-1/2
3.	2	1	-1	+1/2
4.	2	1	-1	-1/2
5.	2	1	0	+1/2
6.	2	1	0	-1/2
7.	2	1	1	+1/2
8.	2	1	1	-1/2

**Total #
Of states** $=$ **$2n^2$**

According to the Bohr model, the nth energy level is defined by the orbit whose radius is r_n. Each time we make a measurement of the position of the electron, it is always in a circular orbit at a distance r_n from the nucleus.

This picture is not correct. The quantum mechanical picture dictates that due to the HUP, the position of the electron is uncertain. If we were to take many measurements of the electron's position, sometimes it would be very close to the nucleus, and sometimes it would be far away.

So the electron exists as a particle-wave in a **probability cloud** around the nucleus.
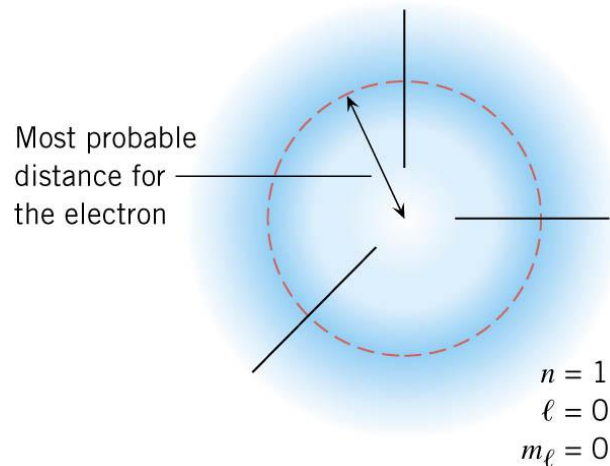
If the electron is in the $n=1$ state, then after many measurements, the most probable distance for the electron would be at $r_1 = 5.29×10^{-11}$ m.

Most probable
distance for
the electron

$n = 1$
$\ell = 0$
$m_\ell = 0$

The higher-density cloud regions indicate areas of higher probability.

There are different probability clouds for different quantum states.

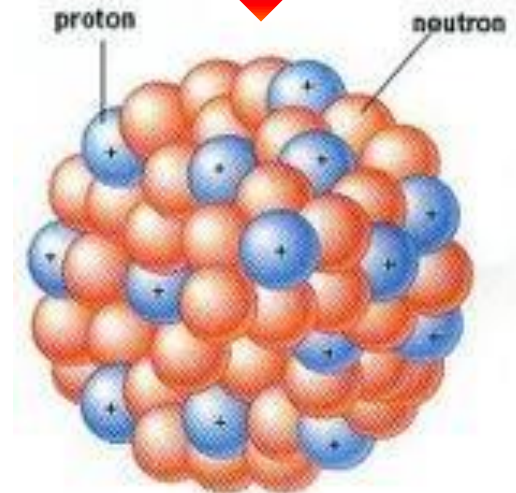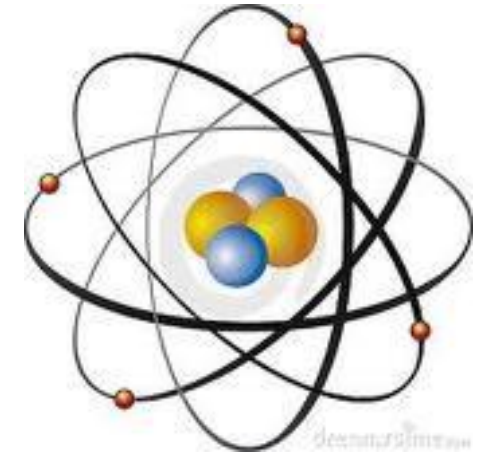# Algebra-based Physics II

Dec. 1ˢᵗ: Chap 30.6-7:

• **Atomic state is determined by**

$$\{n, l, m_l, m_s\}$$

• **Maximum # of electrons in any shell (*n*) is 2*n*²**

• **X-ray**

• **Nuclear Physics and Radioactivity**
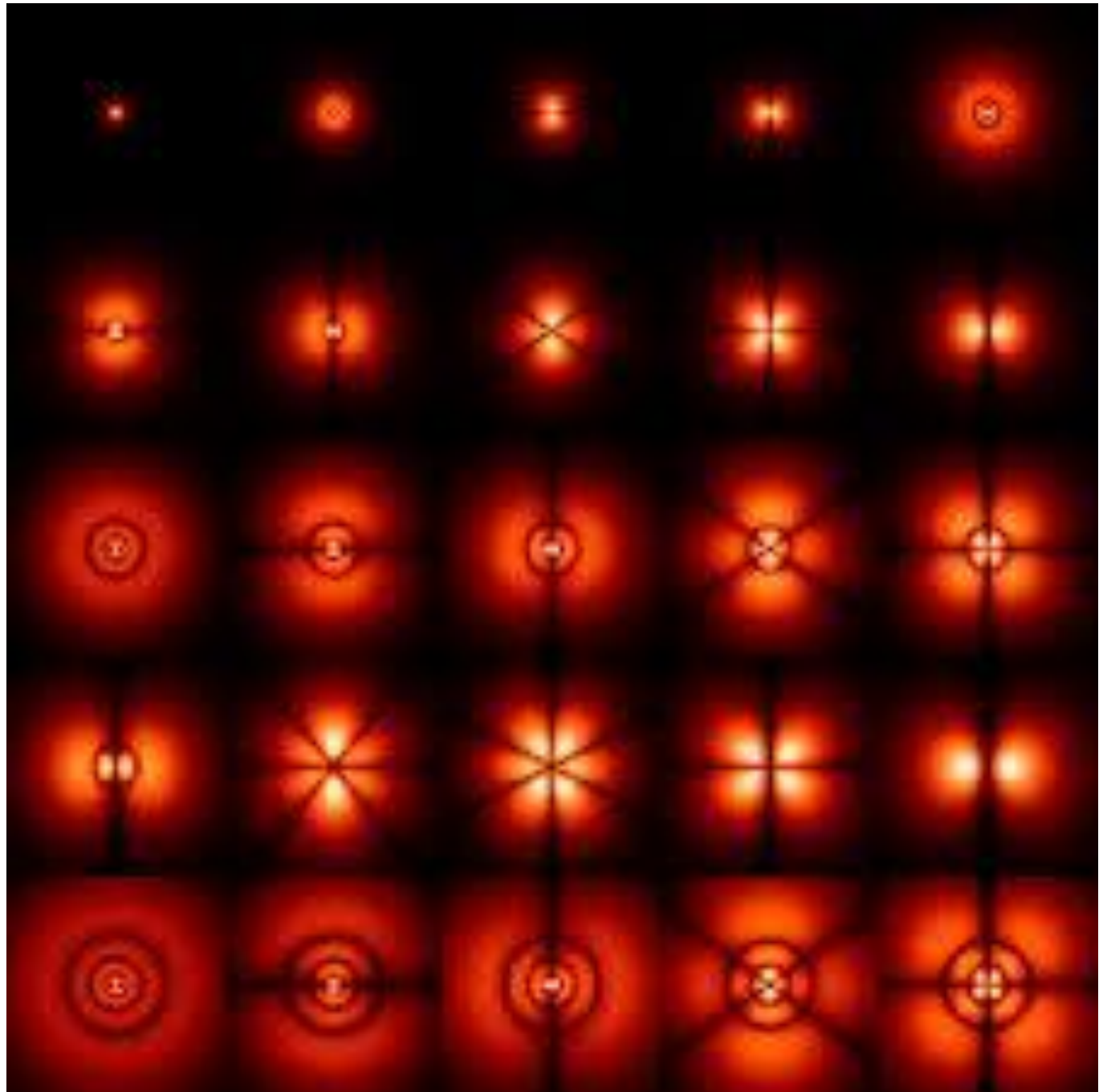

proton   neutron

Density clouds of a electron at different orbits in an atom labeled as {*n, l, m_l, m_s*}

Different orbits have different symmetry!

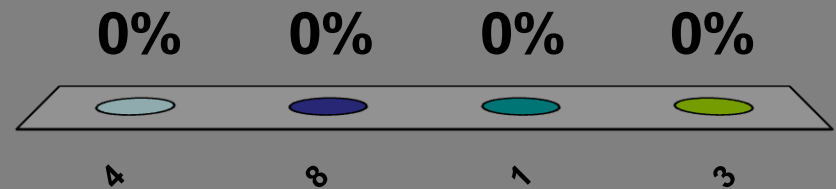**Atomic state is determined by both orbit and spin degrees of freedom**

For the hydrogen atom, how many total electron states exist for n = 4?

1.   4
2.   8
3.   16
✔ 4.   32

0%   0%   0%   0%

4   8   ^   3

30.6 The Pauli Exclusion Principle (PEP)

The Bohr model was derived explicitly for one electron and one proton. Will the energy levels apply to atoms with more than one electron?

The answer is NO!

Quantum mechanics does describe the energy levels correctly in multi-electron atoms, and it uses the 4 quantum #'s:

$$\{n, l, m_l, m_s\}$$

The energy of the electrons depends on n and l, and in general, the energy increases as n and l increase, but there are exceptions.
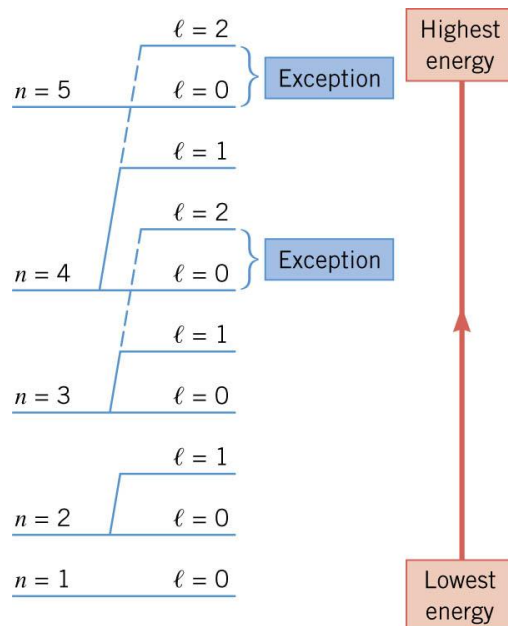
So how do we categorize the energy levels of electrons in multi-electron atoms?

Each value of n corresponds to a single "shell", called the K-shell for n = 1, L-shell for n = 2, and the M-shell for n =3.

Each shell has <u>subshells</u> defined by the orbital quantum #, l.

Example, the K-shell is the $n = 1$, and it has one subshell, $l = 0$.

The L-shell is the $n = 2$, and it has two subshells defined by $l = 0,1$

When atoms are not subjected to violent collisions, high temperature, or high electric fields, characteristics of say room temperature, then the electrons in the atoms tend to spend most of their time in the low energy levels of the atom. The lowest energy state is called the ground state.

However, when a multi-electron atom is in its ground state, not every electron can be in the $n = 1$ level. They must obey a rule known as the Pauli Exclusion Principle (PEP).

No two electrons in an atom can have the same set of values for their 4 quantum numbers: n, l, m_l, and m_s. In other words, no two electrons can be in the same quantum state.

Because of the PEP, there is a maximum # of electrons that can fit into each energy level and subshell:
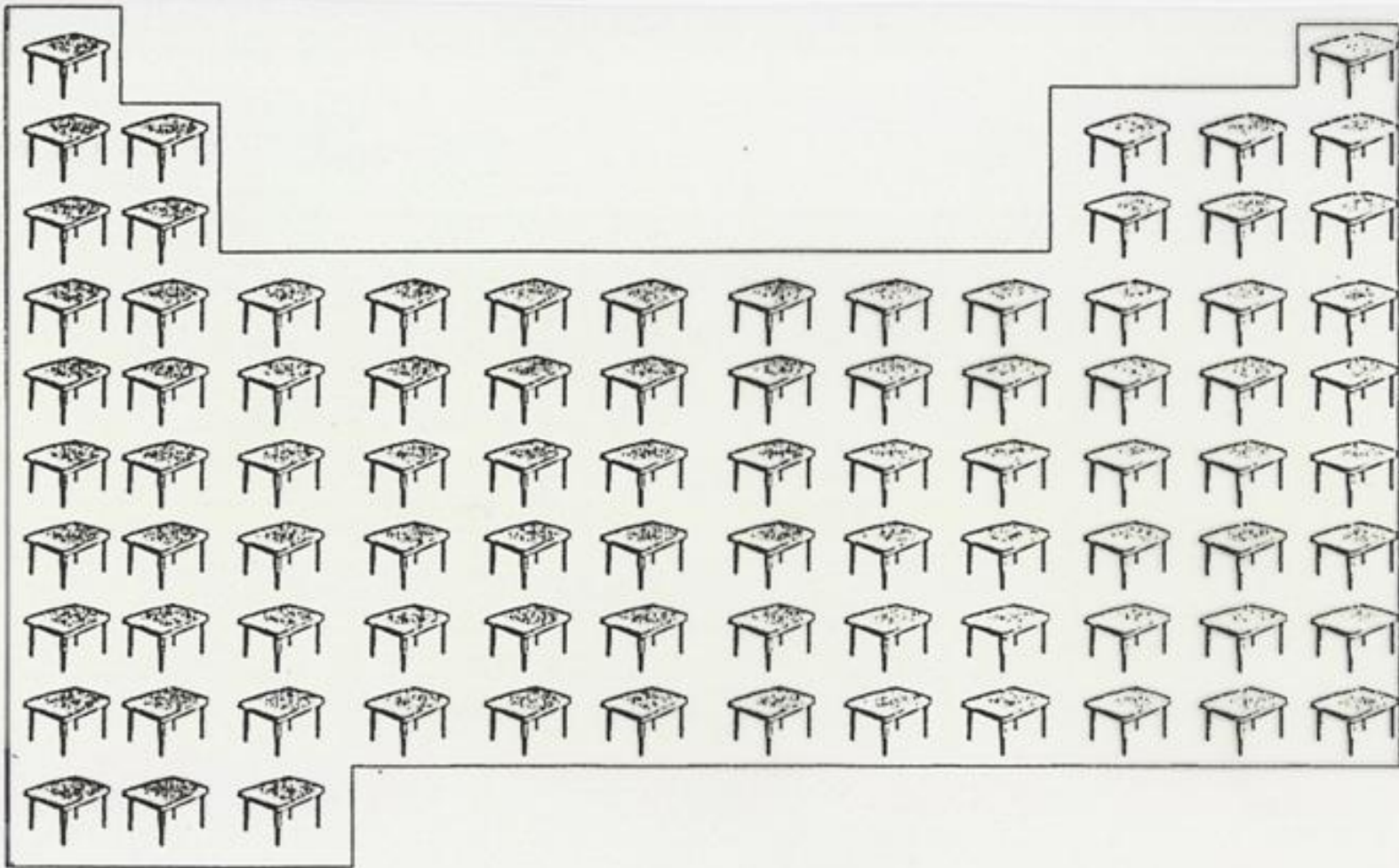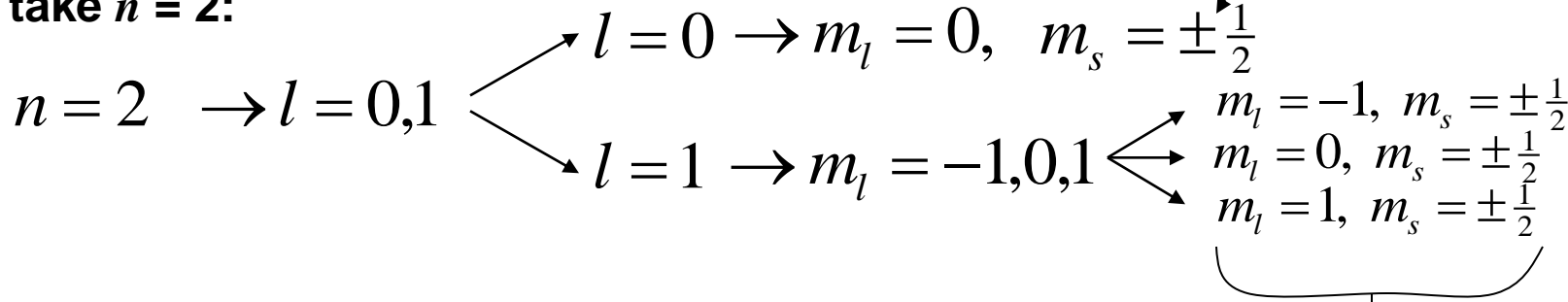
The Periodic Table

Because of the PEP, there is a maximum # of electrons that can fit into each energy level and subshell:

Example: **Take n = 1:   then l = 0, m_l = 0, and m_s = $\pm$1/2.**

Thus, each l = 0 subshell can hold a maximum of 2 electrons, one with spin-up and one with spin-down.

Now take n = 2:

Again I get two states for l = 0.

$$n = 2 \;\rightarrow l = 0,1 \begin{cases} l = 0 \rightarrow m_l = 0, \;\; m_s = \pm\frac{1}{2} \\ l = 1 \rightarrow m_l = -1,0,1 \end{cases} \begin{cases} m_l = -1, \; m_s = \pm\frac{1}{2} \\ m_l = 0, \; m_s = \pm\frac{1}{2} \\ m_l = 1, \; m_s = \pm\frac{1}{2} \end{cases}$$

Thus, we get 8 total states for n = 2.

We get 6 states for the l = 1 subshell.

In general the # of possible states for any given subshell l, is: $2(2l+1)$

**Representation of the *l*-subshell is customarily done by letter:**

l	Letter Designation	Max. # of e⁻s: 2(2l+1)
0	s	2
1	p	6
2	d	10
3	f	14
4	g	18
5	h	22

In general, the maximum # of electrons in any shell (*n*) is $2n^2$:

K-shell, n = 1	→	2 electrons
L-shell, n = 2	→	8 electrons
M-shell, n =3	→	18 electrons

etc....

So here is an example of the spectroscopic notation used to specify the electronic states in multi-electron atoms:

# of e⁻s in
the subshell

$$3p^4$$

$n = 3$

$l = 1$
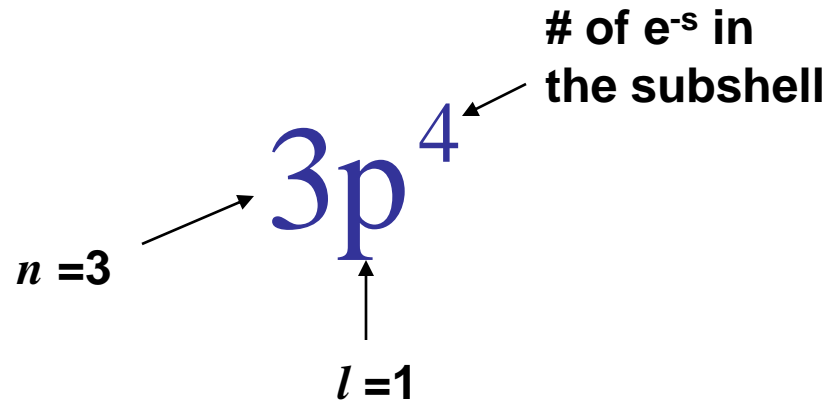
Specifying the n and l value for __each__ electron in an atom in this way is called the electronic configuration.
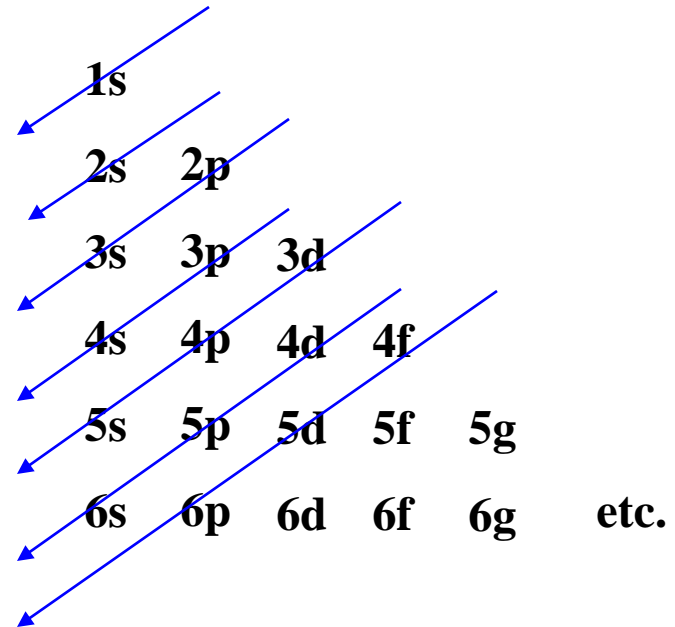

Let's Play!!!

<u>**Example:**</u>   Write down the full electronic configuration for carbon.

Carbon's atomic # is 6, so it has 6 electrons to put into shells:

What order do the shells fill up???

It is given by the following construction:

The order is shown by diagonal arrows starting in the upper right and pointing toward the lower left:

1s

2s   2p

3s   3p   3d

4s   4p   4d   4f

5s   5p   5d   5f   5g

6s   6p   6d   6f   6g   etc.

 So we start filling in these shells with carbon's 6 electrons, keeping in mind that s's hold 2 electrons, p's hold 6, d's hold 10, etc.

So for carbon, we find the electronic configuration to be: $1s^2 \ 2s^2 \ 2p^2$
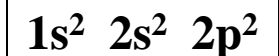
Example: Write down the full electronic configuration for calcium.

Calcium's atomic number is 20, so we have 20 electrons to put into shells:
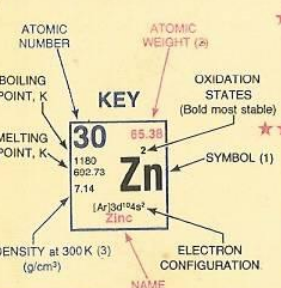
Elements in the Periodic Table are arranged by their electronic configurations:

PERIODIC TABLE OF THE ELEMENTS

Table of Selected Radioactive Isotopes

Selected Radioactive Isotopes

Naturally occurring radioactive isotopes are designated by a mass number in blue (although some are also manufactured). Letter m indicates an isomer of another isotope of the same mass number. Half-lives follow in parentheses, where s, min, h, d, and y stand respectively for seconds, minutes, hours, days, and years. The table includes mainly the longer-lived radioactive isotopes; many others have been prepared. Isotopes known to be radioactive but with half-lives exceeding 10^5 y have not been included. Symbols describing the principal mode (or modes) of decay are as follows (these processes are generally accompanied by gamma radiation):

- α alpha particle emission
- β^- beta particle (electron) emission
- β^+ positron emission
- EC   orbital electron capture
- IT   isomeric transition from upper to lower isomeric state
- SF   spontaneous fission

* Estimated Values

The A & B subgroup designations, applicable to elements in rows 4, 5, 6, and 7, are those recommended by the International Union of Pure and Applied Chemistry. It should be noted that some authors and organizations use the opposite convention in distinguishing these subgroups.

† The names and symbols of elements 104-106 are those recommended by IUPAC as systematic alternatives to those suggested by the purported discoverers. Berkeley (USA) researchers have proposed Rutherfordium, Rf, for element 104 and Hahnium, Ha, for element 105. Dubna (USSR) researchers, who also claim the discovery of these elements, have proposed different names (and symbols).

KEY
- ATOMIC NUMBER
- ATOMIC WEIGHT (2)
- OXIDATION STATES (Bold most stable)
- BOILING POINT, K
- MELTING POINT, K
- SYMBOL (1)
- DENSITY at 300 K (3) (g/cm³)
- ELECTRON CONFIGURATION
- NAME

Example:
30   65.38
1180
692.73
7.14
Zn
[Ar]3d¹⁰4s²
Zinc

NOTES:

(1) Black — solid.
Red — gas.
Blue — liquid.
Outline — synthetically prepared.

(2) Based upon carbon-12. ( ) indicates most stable or best known isotope.

(3) Entries marked with asterisks refer to the gaseous state at 273 K and 1 atm and are given in units of g/l.

NSRDS

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Catalog Number S-18806   Side 1

Group headers

GROUP IA, IIA, IIIB, IVB, VB, VIB, VIIB, VIII, IB, IIB, IIIA, IVA, VA, VIA, VIIA, VIIIA, VIII

Elements (atomic number / symbol / name)

Z	Symbol	Name
1	H	Hydrogen
2	He	Helium
3	Li	Lithium
4	Be	Beryllium
5	B	Boron
6	C	Carbon
7	N	Nitrogen
8	O	Oxygen
9	F	Fluorine
10	Ne	Neon
11	Na	Sodium
12	Mg	Magnesium
13	Al	Aluminum
14	Si	Silicon
15	P	Phosphorus
16	S	Sulfur
17	Cl	Chlorine
18	A	Argon
19	K	Potassium
20	Ca	Calcium
21	Sc	Scandium
22	Ti	Titanium
23	V	Vanadium
24	Cr	Chromium
25	Mn	Manganese
26	Fe	Iron
27	Co	Cobalt
28	Ni	Nickel
29	Cu	Copper
30	Zn	Zinc
31	Ga	Gallium
32	Ge	Germanium
33	As	Arsenic
34	Se	Selenium
35	Br	Bromine
36	Kr	Krypton
37	Rb	Rubidium
38	Sr	Strontium
39	Y	Yttrium
40	Zr	Zirconium
41	Nb	Niobium
42	Mo	Molybdenum
43	Tc	Technetium
44	Ru	Ruthenium
45	Rh	Rhodium
46	Pd	Palladium
47	Ag	Silver
48	Cd	Cadmium
49	In	Indium
50	Sn	Tin
51	Sb	Antimony
52	Te	Tellurium
53	I	Iodine
54	Xe	Xenon
55	Cs	Cesium
56	Ba	Barium
57	La	Lanthanum
72	Hf	Hafnium
73	Ta	Tantalum
74	W	Tungsten
75	Re	Rhenium
76	Os	Osmium
77	Ir	Iridium
78	Pt	Platinum
79	Au	Gold
80	Hg	Mercury
81	Tl	Thallium
82	Pb	Lead
83	Bi	Bismuth
84	Po	Polonium
85	At	Astatine
86	Rn	Radon
87	Fr	Francium
88	Ra	Radium
89	Ac	Actinium
104	Unq	Unnilquadium
105	Unp	Unnilpentium
106	Unh	Unnilhexium

Lanthanides

Z	Symbol	Name
58	Ce	Cerium
59	Pr	Praseodymium
60	Nd	Neodymium
61	Pm	Promethium
62	Sm	Samarium
63	Eu	Europium
64	Gd	Gadolinium
65	Tb	Terbium
66	Dy	Dysprosium
67	Ho	Holmium
68	Er	Erbium
69	Tm	Thulium
70	Yb	Ytterbium
71	Lu	Lutetium

Actinides

Z	Symbol	Name
90	Th	Thorium
91	Pa	Protactinium
92	U	Uranium
93	Np	Neptunium
94	Pu	Plutonium
95	Am	Americium
96	Cm	Curium
97	Bk	Berkelium
98	Cf	Californium
99	Es	Einsteinium
100	Fm	Fermium
101	Md	Mendelevium
102	No	Nobelium
103	Lr	Lawrencium

30.7 X-Rays

Wilhelm Roentgen was a Dutch physicist working with cathode ray tubes back in the late 1800's.


The cathode ray tube looked essentially like this:

Electrons get accelerated through a large voltage and then collide with a metal target, such as Cu, Mo, or Pd.

When the electrons collided with the target, Roentgen noticed certain "rays" were produced.

Since he couldn't figure out what they were, he called them "X-Rays".

We now know that X-Rays are EM radiation – light in the non-visible part of the spectrum.

Metal target

High voltage source

+
V
−

X-rays

Electrons

Heated filament

Filament voltage
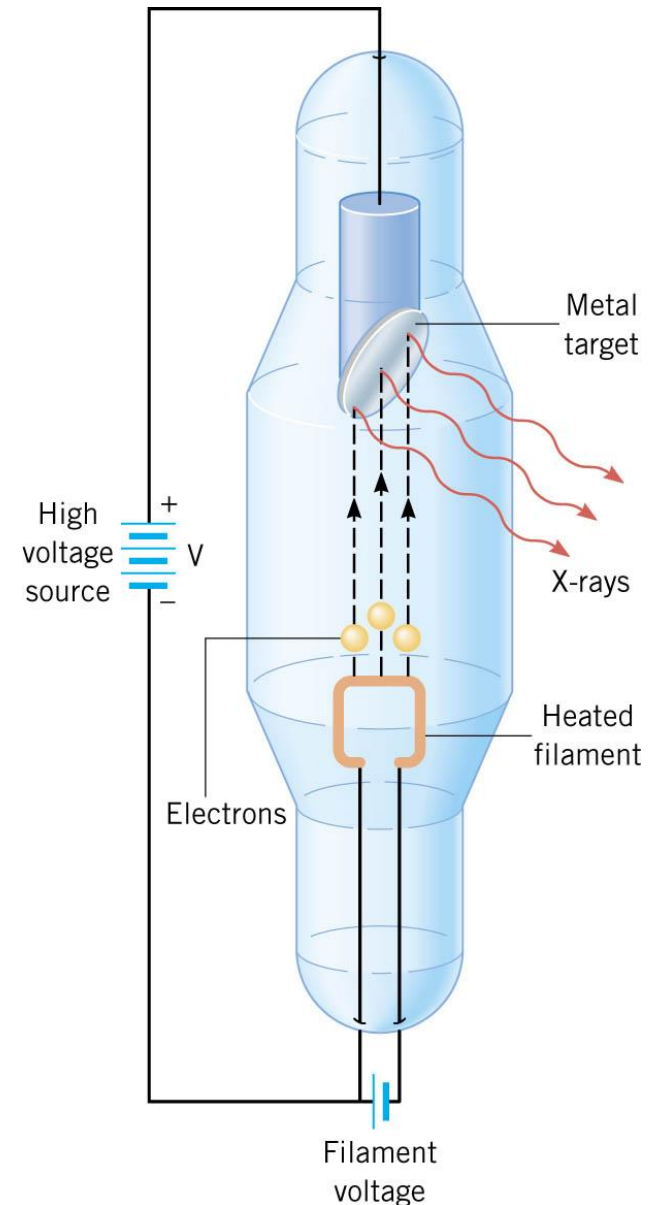
If we measure the intensity of the X-Rays as a function of wavelength, we get the following characteristic plot:
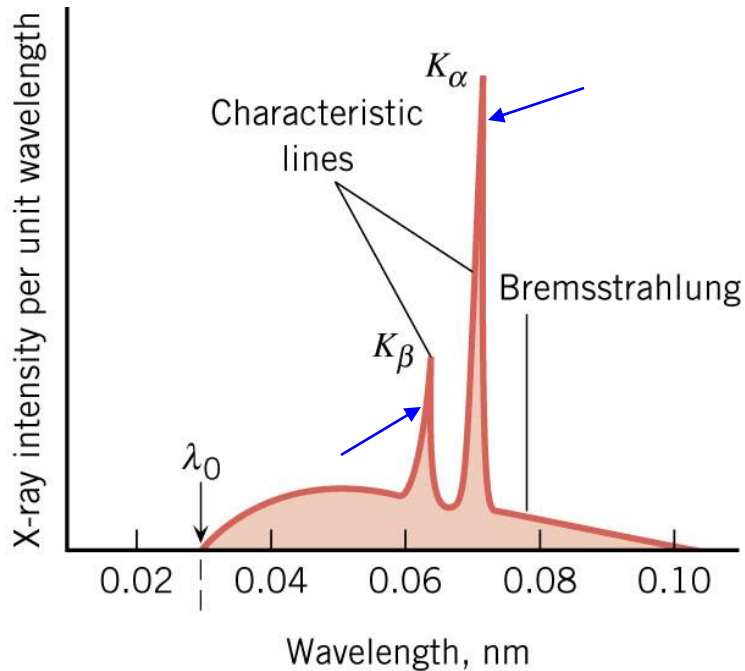
As the electrons slow down (decelerate) upon striking the metal target, the broad background part of the curve, called Bremsstrahlung radiation, is produced.

Bremsstrahlung comes from the German word for "braking".

But where do those large peaks in the intensity spectrum come from???

They depend on the material of the target, and are called K_α and K_β.

They are labeled "K" because they involve electrons in the $n = 1$ (K-shell).

As the electrons strike the atoms in the metal target, they slow down. But, if they have enough energy, they can knock an electron in the atom out of the K-shell.

Then another electron in the atom sitting in a higher energy state falls down to replace it. When it makes this transition, a photon is emitted with X-Ray energies.

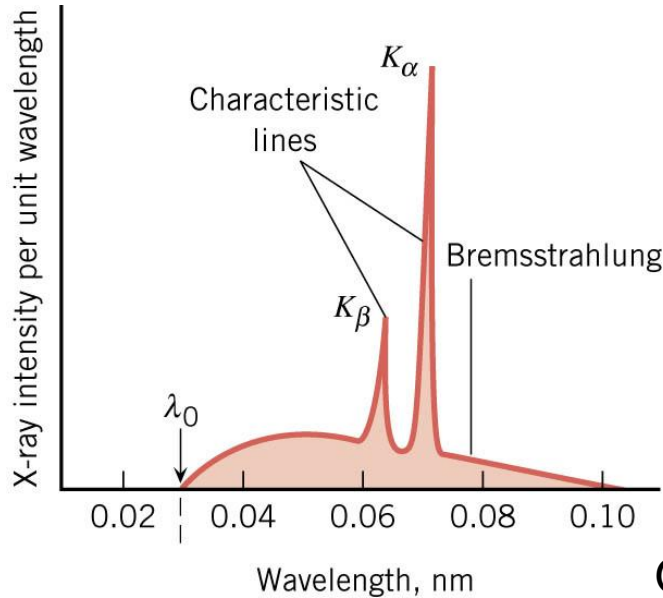Which characteristic X-Ray line, the K_α or K_β, has the larger energy?

1. K_α

✓ 2. K_β

3. They have the same energy.

0%   0%   0%

Ka   Kb   They have the same...
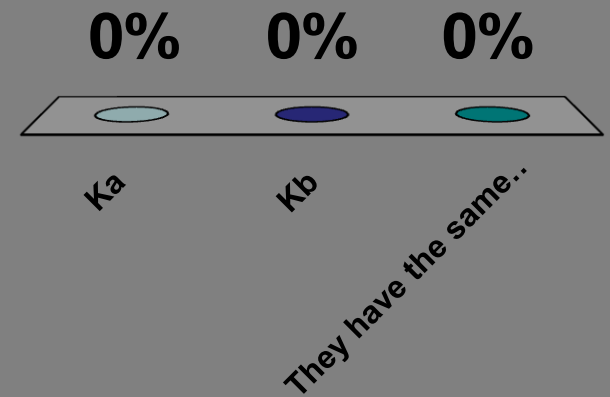
Estimate the energy/wave length of X-ray

The K_α line occurs when an n = 2 electron falls back into the K-shell.

The K_β line occurs when an n =3 electron falls back into the K-shell.

Bohr Model:

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

$$hf_{K_\alpha} = E_{n=2} - E_{n=1} = (13.6 \text{ eV}) Z^2 (1 - \frac{1}{4})$$

$$hf_{K\beta} = E_{n=3} - E_{n=1} = (13.6 \text{ eV}) Z^2 (1 - \frac{1}{9})$$

OR: $$\frac{1}{\lambda} = R \left(\frac{1}{n_f^2} - \frac{1}{n_i^2} \right), \quad n_i = \begin{cases} 2 & \text{for K}_\alpha \\ 3 & \text{for K}_\beta \end{cases} \text{ and } n_f = 1$$

where $R = 1.097 \times 10^7 \text{ m}^{-1}$

Example: Use the Bohor model to estimate the wavelength of Kα line of X-ray spectrum of aluminum (Z=12 rather than 13).

$$\frac{1}{\lambda} = 1.097 \times 10^7 \text{ m}^{-1} (13-1) \left(1 - \frac{1}{4} \right) = 9.873 \times 10^7 m^{-1}$$

$$\lambda = 1.013 \times 10^{-8} m = 10.13 nm$$