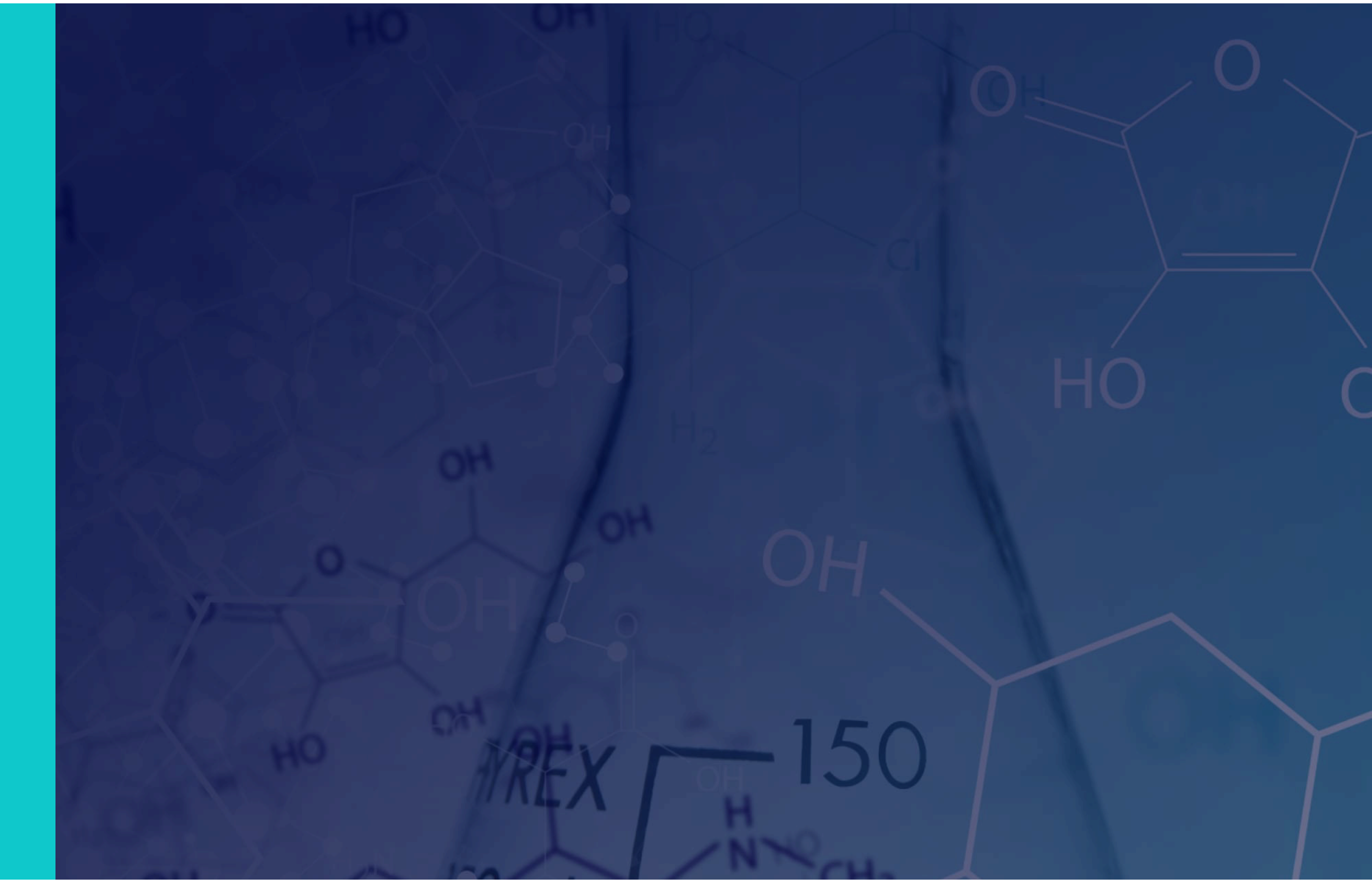

McGill

CHEM 110

Fall 2024, Chapter 1 Notes

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1. Quantum Theory and Atomic Structure

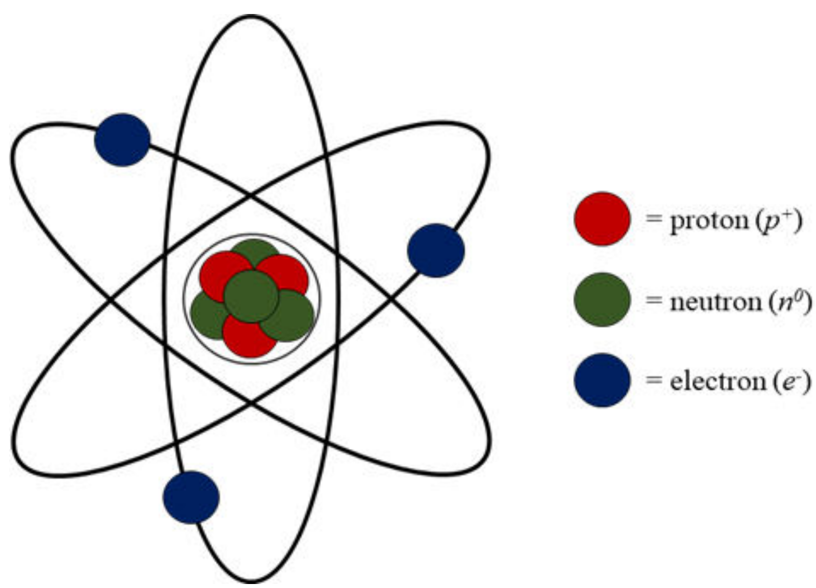
1.1 Atomic Structure

1.1.1

The Atom and its Subatomic Particles

Atoms are the building blocks of chemistry (and life!). They make up everything from the screen of your computer, to components in your eyes! They are all around us. Since atoms are such a key concept in chemistry, let's take a closer look at their structure.

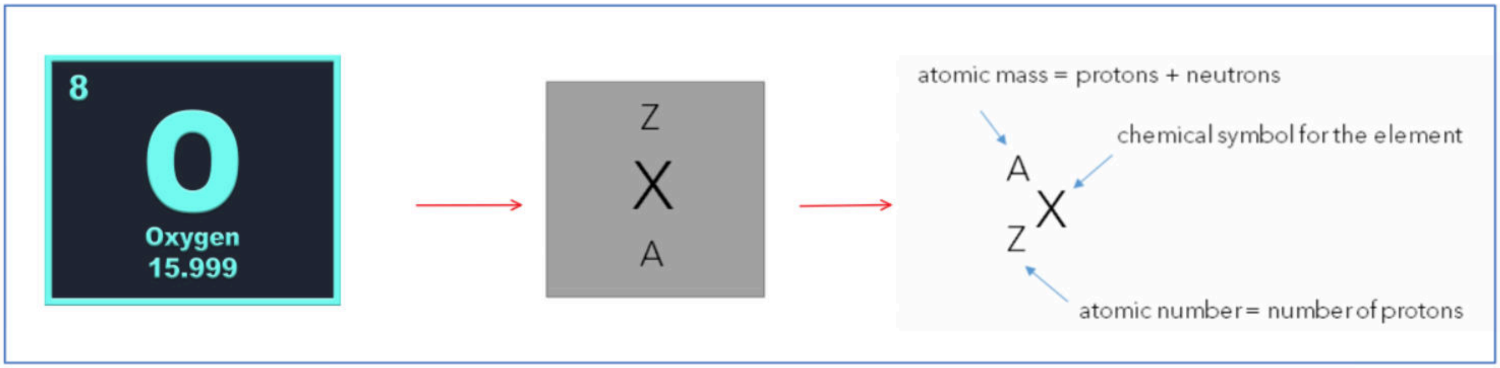
Atomic Structure



Subatomic Particles

Particle	Mass (g)	Mass (amu or $g \cdot mol^{-1}$)	Relative Charge
Proton	1.673×10^{-24}	1.007	+1
Neutron	1.675×10^{-24}	1.009	0
Electron	9.109×10^{-28}	5.485×10^{-4}	-1

Chemical Symbols and Notation



Example: Nuclear Notation

Ex1) ${}^{12}_{6}C$

# of protons: _____
# of neutrons: _____
# of electrons: _____

WIZE CONCEPT

Atomic Mass = # of protons + # of neutrons
# of neutrons = Atomic mass - # of protons

Ex2) ${}^{19}_{9}F^{-}$

# of protons: _____
# of neutrons: _____
# of electrons: _____

WIZE TIP

When **electrons are added** to an element we call it an **anion**, and it would have a **negative charge**.
When **electrons are removed** from an element we call it a **cation**, and it would have a **positive charge**

1.1.3

Practice: Nuclear Notation

How many protons, neutrons and electrons are there in $^{75}As^{3-}$?

Number of protons

Number of neutrons

Number of electrons

1.2 Early Atomic Theory

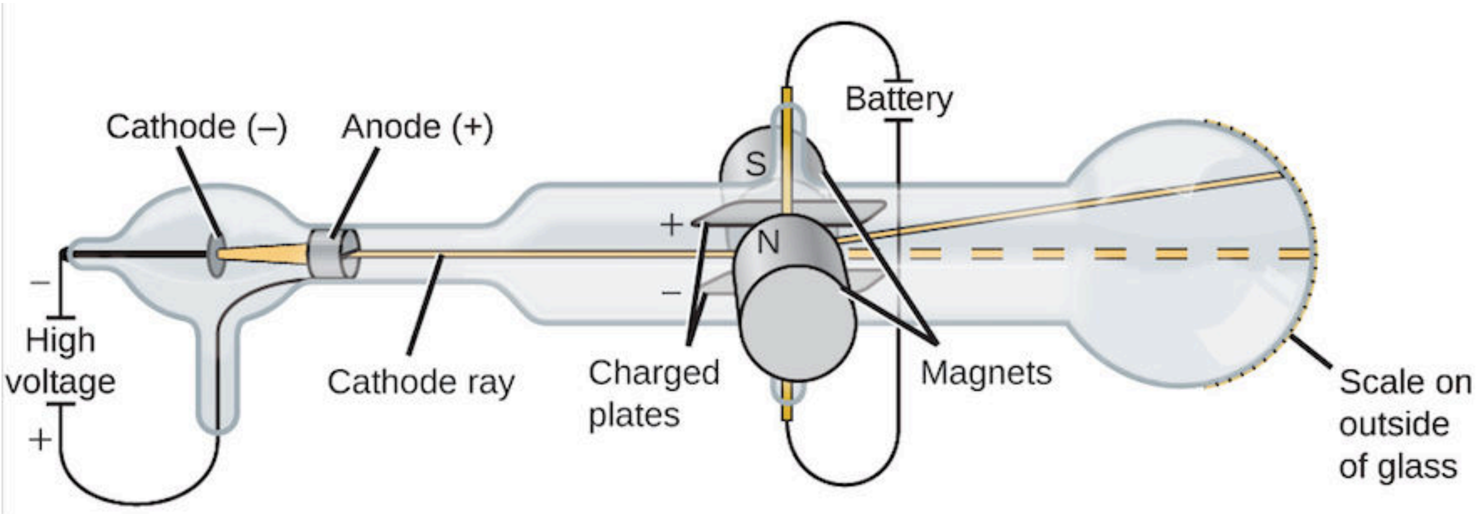
1.2.1

Review of Previous Atomic Models

Dalton's Atomic Theory

- first attempt to describe all matter in terms of atoms
  - each element is made up of tiny atoms
  - for a given element, atoms are identical and different elements have different atoms
  - chemical compounds form when different atoms combine with each other (in the same ratios)
  - said that atoms were indestructible and indivisible (but we know now that they are made up of smaller components-protons, neutrons, electrons)

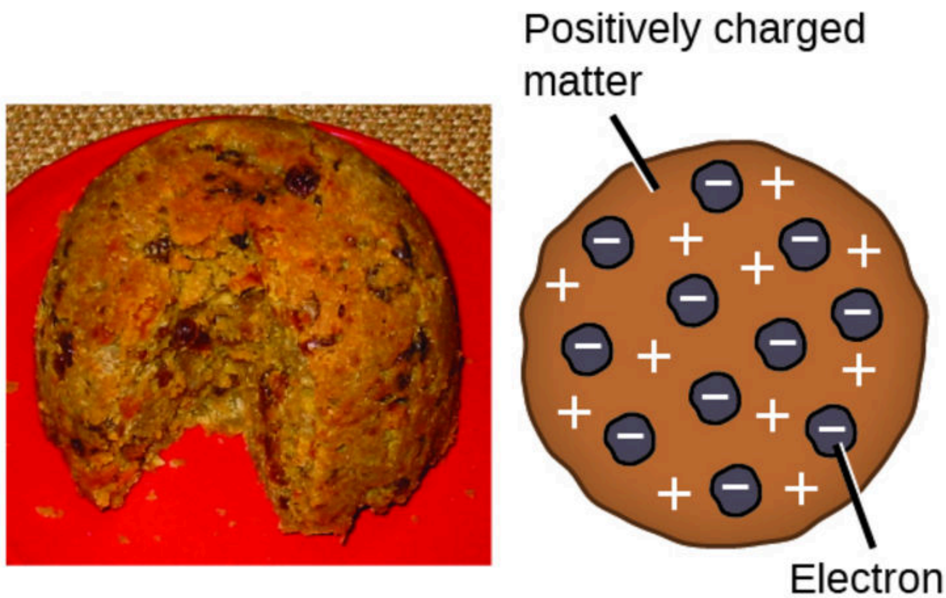
Discovery of the Electron: JJ Thomson's Experiment



- There are 2 main components here:
  - (+) and (-) charged plates
  - magnets producing a magnetic field
- The cathode ray is deflected away from the negatively-charged electric plate, and towards the positively-charged electric plate. That means the charge of the particle in the ray is

  ____

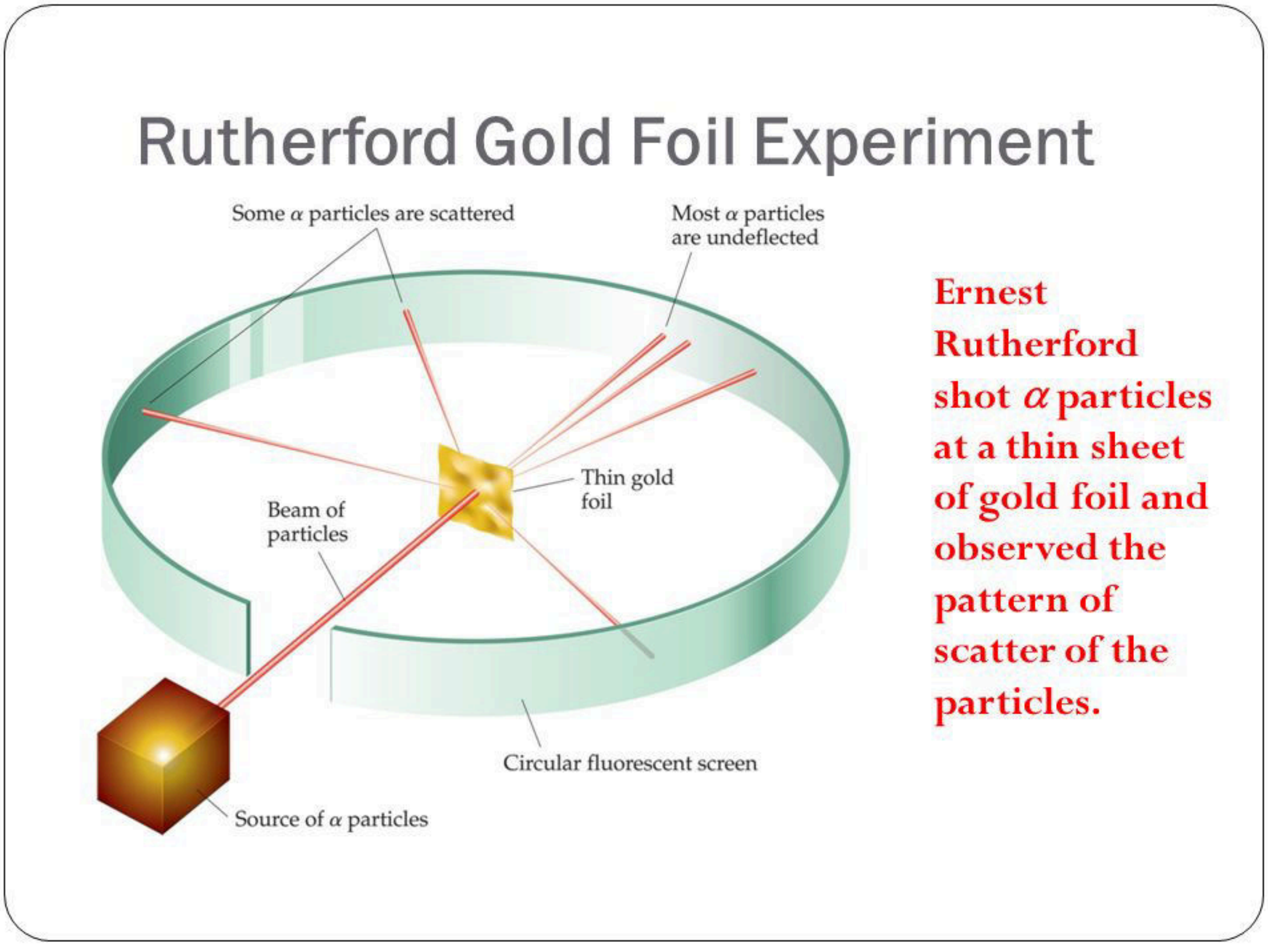
- These particles are: ____________
- Thomson also came up with the **Plum Pudding Model:**
  - Since electrons were negatively charged, and atoms were neutral he proposed that electrons were embedded in a positively charged atom



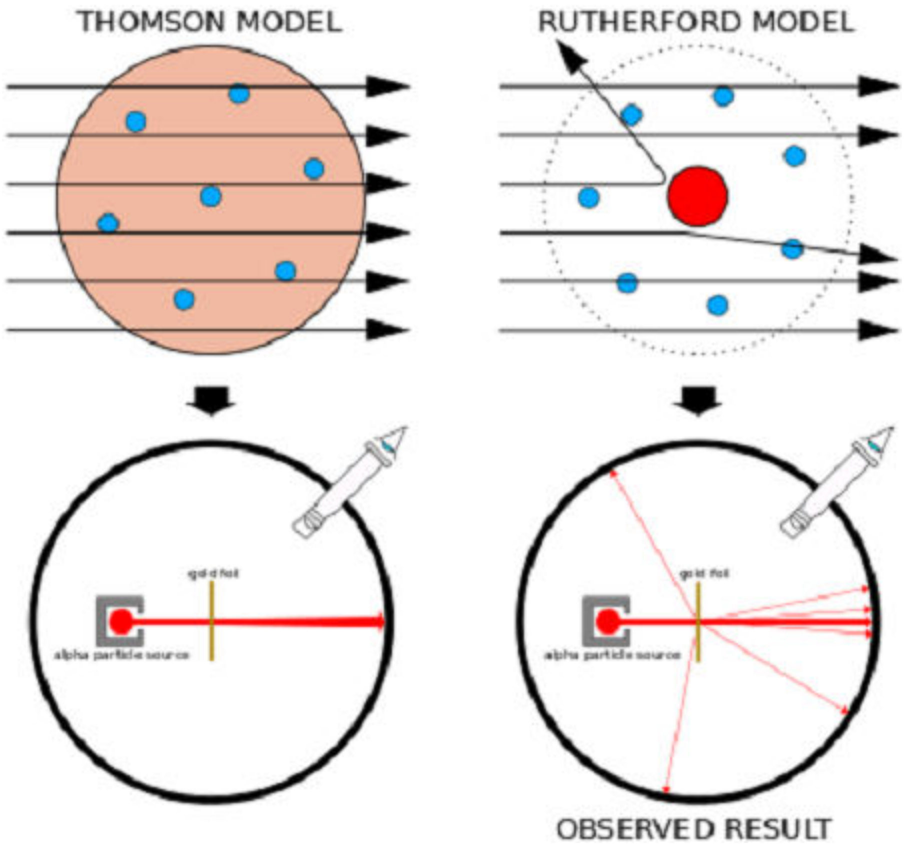
(a)

Discovery of the Nucleus

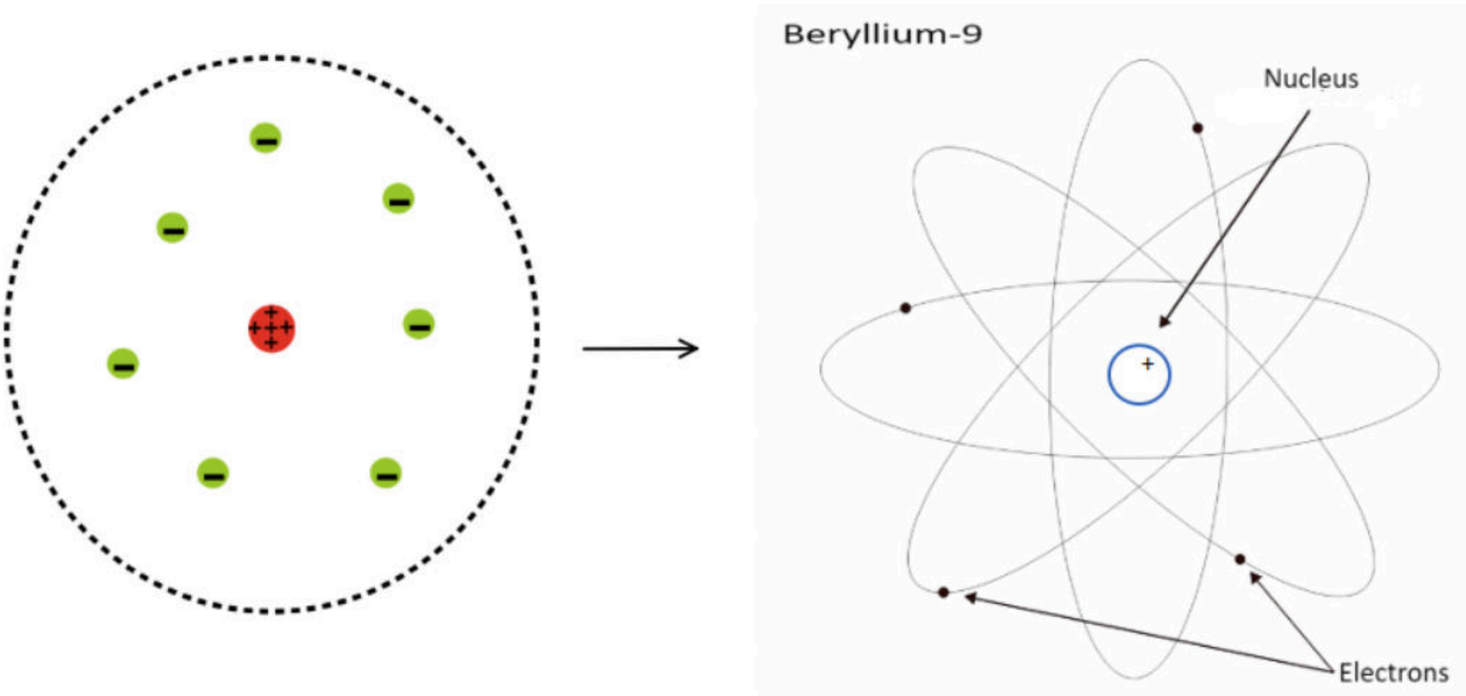
- Rutherford wanted to learn more about the contents of an atom so he conducted the following experiment:



Why was this so shocking?!



- According to the thomson/plum pudding model, since electrons were thought to be floating around in a positive space, the positive alpha particles were just expected to go right through because the positive space was thought to be too weak to affect the path of the fast moving alpha particles
- But that did not happen!
- **Conclusions from the Rutherford gold experiment:**
  - The positive charge must be localized over a very small volume of the atom, which also contains most of the atom's mass. This was the nucleus!
  - This explained how a very small fraction of the alpha particles were deflected drastically (due to the rare collision with a heavy and dense gold nucleus.)
  - Since most of the alpha particles passed straight through the gold foil, the atom must be made up of mostly empty space!
- when trying to figure out the mass of the nucleus, Rutherford was finding that the mass was too high compared to the mass of protons, which later led to the discovery of neutrons in the nucleus
- The discovery of the nucleus led to Rutherford creating a new atomic model which is referred to as the "**planetary model" of the atom** since it resembles plantets orbiting the sun (with electrons being the planets, and the central body being the nucleus)



- Another problem with this theory was that electrons in motion around a central body (the nucleus) were thought to continuously give off radiation and lose energy
- If this was the case, the radius of the electron's orbit should get smaller and smaller until the electrons spiral into the nucleus and destroys it-this does not happen!

1.3 Electromagnetic Radiation

1.3.1

Electromagnetic Spectrum

Up until this point in history, scientists were unsure if light shared the properties of waves or particles...there was some evidence for both!

The discovery of the electromagnetic spectrum showed the different wavelengths and frequencies that electromagnetic radiation could exist at. Since the different **types of radiation in this spectrum behave as waves**, and visible light is a part of this spectrum, it became clear to scientists that **light acts as waves!**

Types of Electromagnetic Radiation

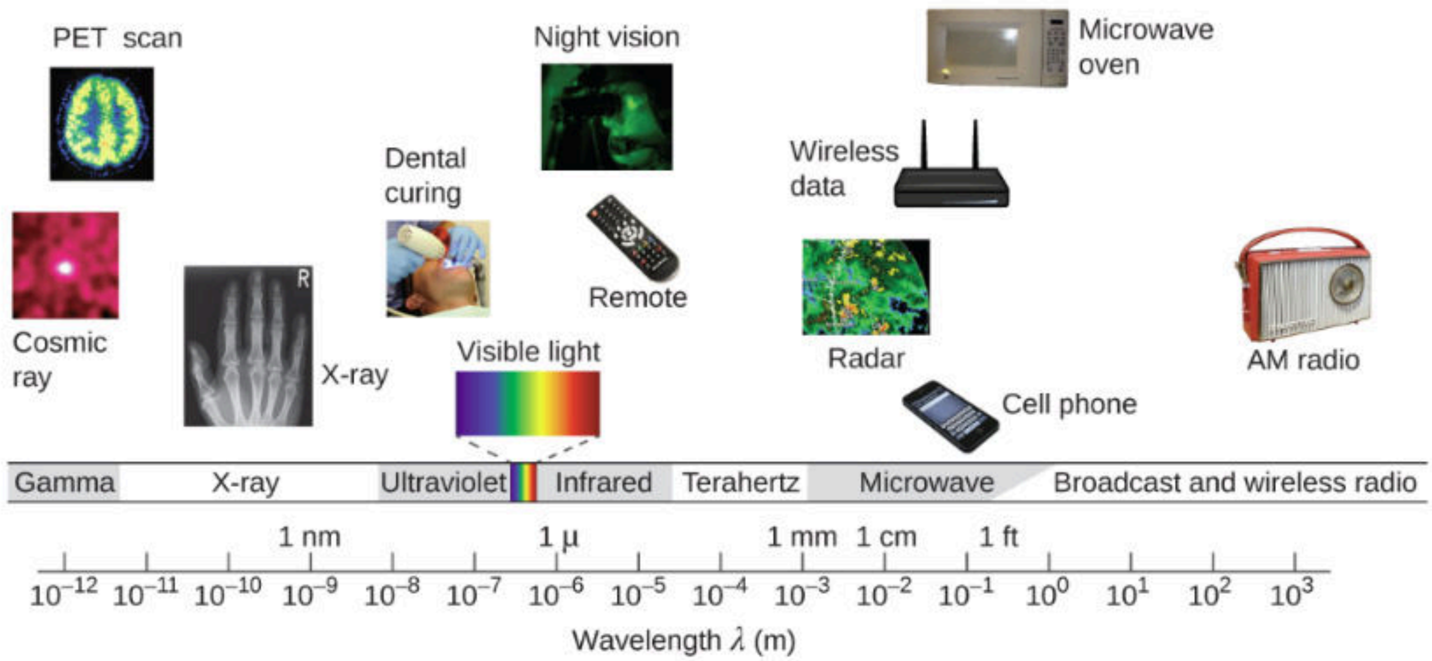


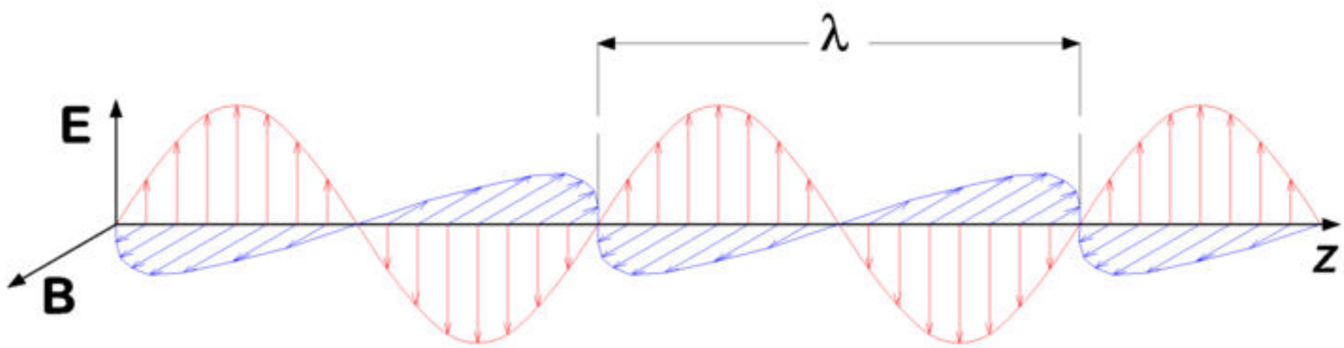
Photo by Rice University/ CC BY

- In the diagram above, the electromagnetic radiation is organized from the types of radiation that are **highest in energy (gamma rays)** to the types of radiation that are **lowest in energy (radiowaves)**
- You might recognize a lot of common household objects on the side of the spectrum with lower amounts of energy!

Photon Equations

Electromagnetic Radiation Waves

- Light (or electromagnetic radiation) behaves as a wave
- A wave is a self-propagating transverse oscillation of electric and magnetic fields



where E is the electric field and B is the magnetic field

- **To describe waves, we can use the following terms:**
  - **Amplitude (A):** the height of a wave crest or depth of a trough
  - **Wavelength (λ):** The distance a wave travels in one cycle **(m)**
  - **Frequency (*v*):** cycles per second (s^{-1} or units Hz)
  - **Energy (E):** units are Joules (J)

Energy of a Photon Equations

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

where ***h is Planck's constant: 6.626x10^{-34} Js***

and ***c is the speed of light: 3.0 x10^{8} m/s***

WIZE TIP

You should **memorize the value for the speed of light (c) = 3.0x10^{8}m/s** as that value is not always provided on exams.

Photon Equations (Cntd.)

Key Relationships Between Variables in Photon Equations

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

- **Are the E and λ of a photon directly or inversely proportional?** ___________ proportional

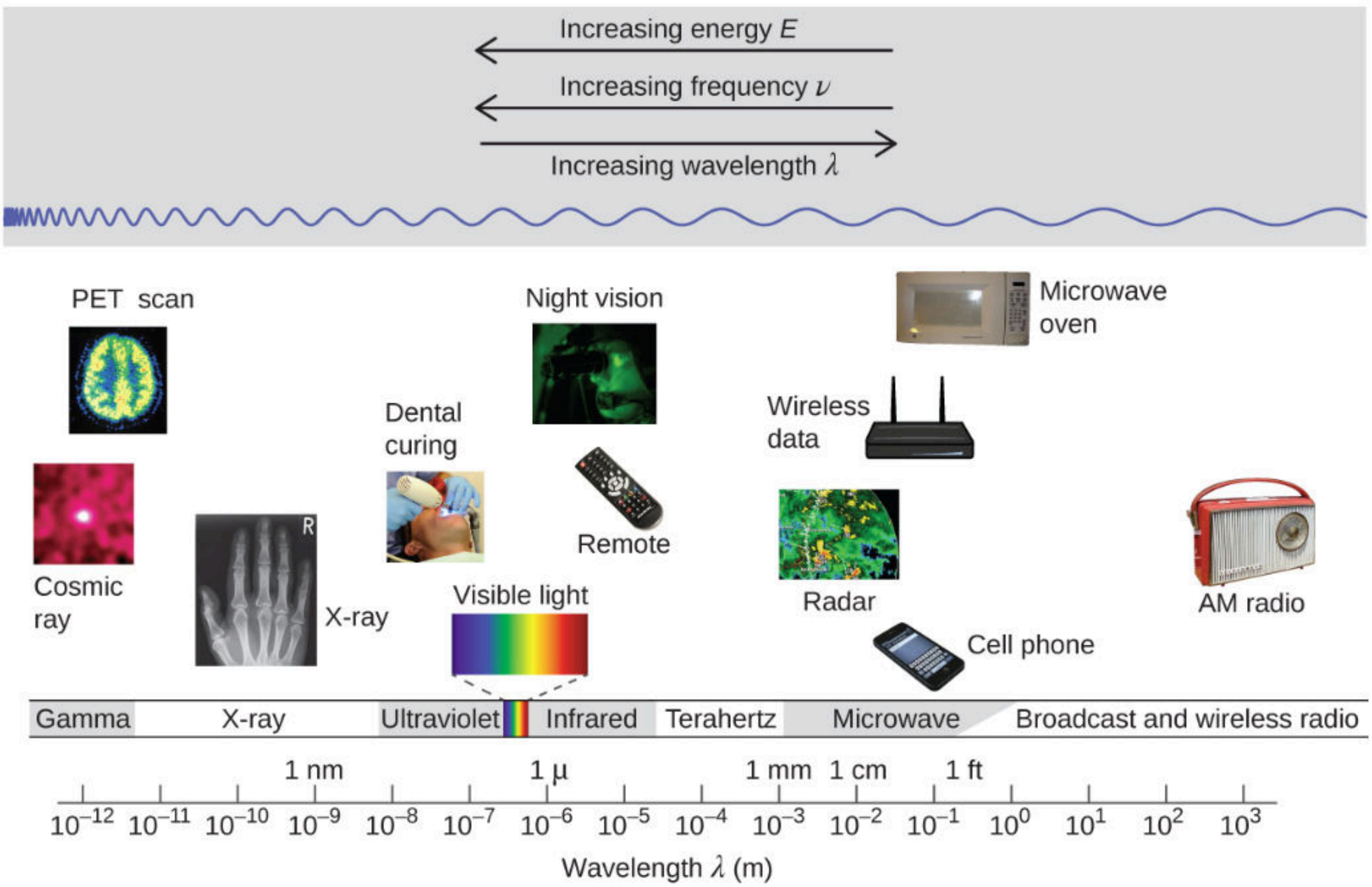
$$E = hv$$

- **Are the E and *v* of a photon directly or inversely proportional?** __________ proportional

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

- **Are the wavelength and frequency of a photon directly or inversely proportional?** ___________ proportional

Summary



Increasing energy E
Increasing frequency ν
Increasing wavelength λ
PET scan
Night vision
Microwave oven
Dental curing
Wireless data
Remote
Cosmic ray
X-ray
Visible light
Radar
AM radio
Cell phone
Gamma
X-ray
Ultraviolet
Infrared
Terahertz
Microwave
Broadcast and wireless radio
1 nm
1 μ
1 mm
1 cm
1 ft
10⁻¹² 10⁻¹¹ 10⁻¹⁰ 10⁻⁹ 10⁻⁸ 10⁻⁷ 10⁻⁶ 10⁻⁵ 10⁻⁴ 10⁻³ 10⁻² 10⁻¹ 10⁰ 10¹ 10² 10³
Wavelength λ (m)

1.3.4 Example

Example: Calculating Energy of a Photon Given Wavelength

A photon of light was found to emit light at 723 nm. How much energy is associated with this light? $h=6.626x10^{-34}$ Js

WATCH OUT!

Don't forget that for the photon equations **E must in joules (J)** and **λ (wavelength) must be in m (meters) not nm (nanometers)!**

- If you are given a wavelength value in nm, you would have to convert it to m before plugging it into an equation.

Remember: 1nm=1x10^{-9}m

Example: Calculating Frequency of a Photon Given Energy

Calculate the frequency of a photon with an energy of 236 kJ.
$h=6.626 \times 10^{-34}$ Js

1.3.6

Practice: Different Types of Electromagnetic Radiation

Rank the following types of electromagnetic radiation from lowest to highest energy.

Radio Waves, Infrared Radiation, X-rays, Microwaves, Visible Light, UV Radiation

- X-rays < Infrared Radiation < Microwaves < UV Radiation < Visible Light < Radio Waves
- Radio Waves < Microwaves < Infrared Radiation < Visible Light <UV Radiation < X-rays
- Radio Waves < Infrared Radiation < Microwaves < Visible Light < UV Radiation < X-rays
- Radio Waves < Infrared Radiation < Visible Light < Microwaves < UV Radiation < X-rays

1.3.7

Practice: Calculating Frequency of a Photon Given Wavelength

A photon of light has a wavelength of 700 nm. What is its frequency?

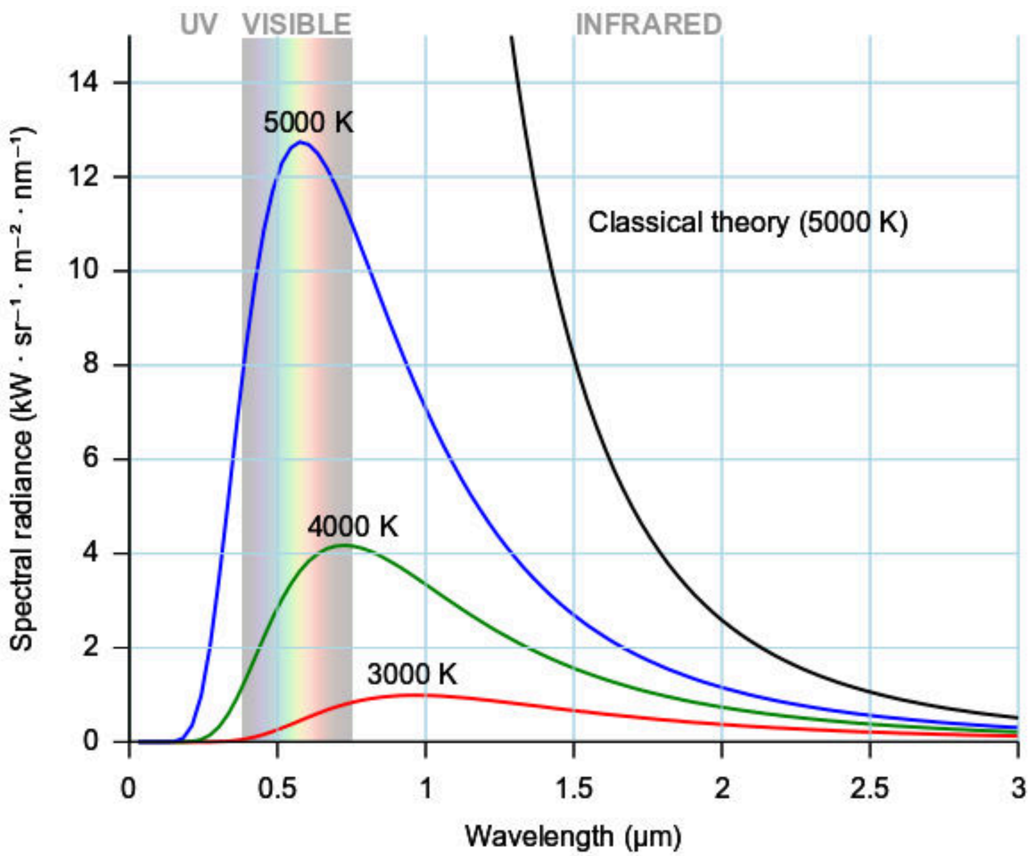
- $4.29 \times 10^{-11}\ s^{-1}$
- $6.72 \times 10^{12}\ s^{-1}$
- $4.29 \times 10^{14}\ s^{-1}$
- $7.23 \times 10^{16}\ s^{-1}$

1.4 Blackbody Radiation

1.4.1

Blackbody radiation

Classical Problem:



Issues:

1. Classical Theory does not do a good job predict the emission of bodies in the infrared region, especially for cooler bodies.
2. Near the UV-range classical theory predicts an infinite increase in radiance which means an infinite amount of light being emitted. This is a clear contradiction of energy conservation, a BIG ISSUE! Known as the UV-Catastrophe

Solution:

1. Max Plank discovered that if he the restricted energy that can be released or absorbed by atoms into discrete energy packets he could successfully predict the experimental observations.

Results:

1. The smallest quantity of energy that can be emitted or absorbed as electromagnetic radiation, is called a quanta

The energy of a single quantum is:

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

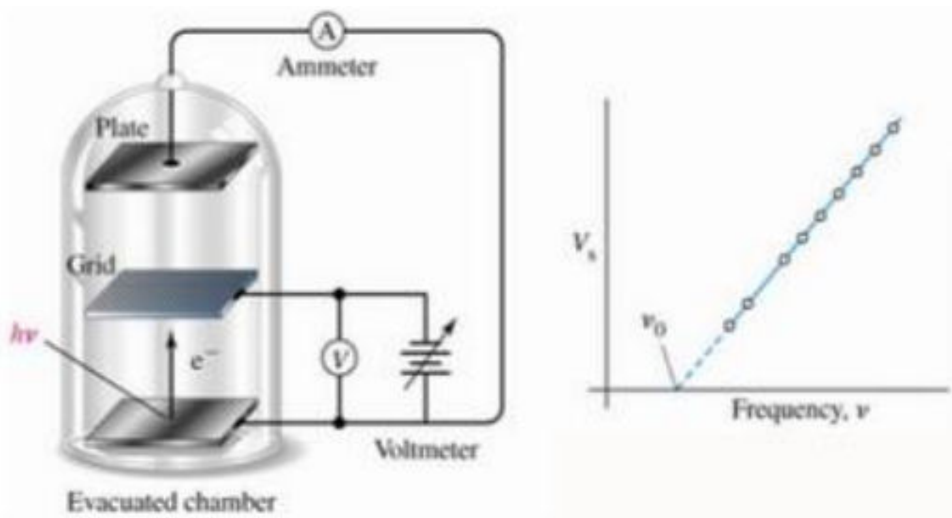
$$\begin{aligned}
&\mathrm{E} = \text{energy of the photon in J} \\
&h = 6.626 \text{ x } 10^{-34}\text{Js (Planck's Constant)} \\
&\nu = \text{frequency in } \mathrm{s}^{-1}
\end{aligned}$$

1.5 The Photoelectric Effect

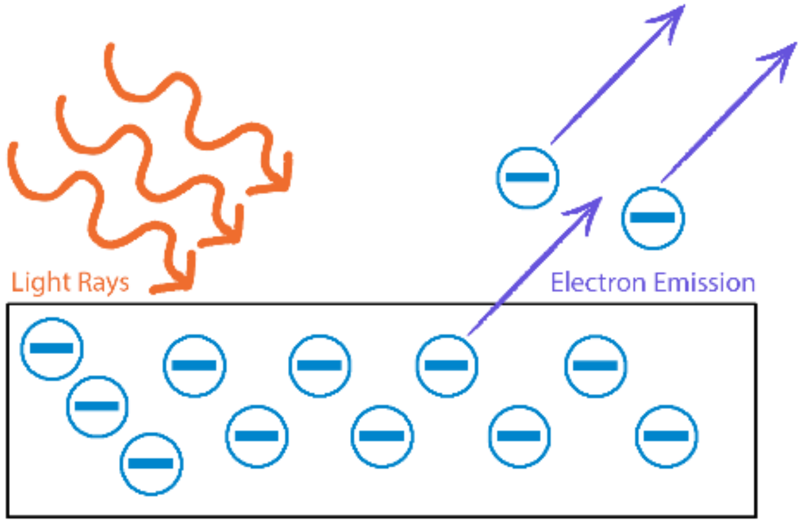
1.5.1

The Photoelectric Effect

In 1905, Einstein conducted his **photoelectric effect experiment.**

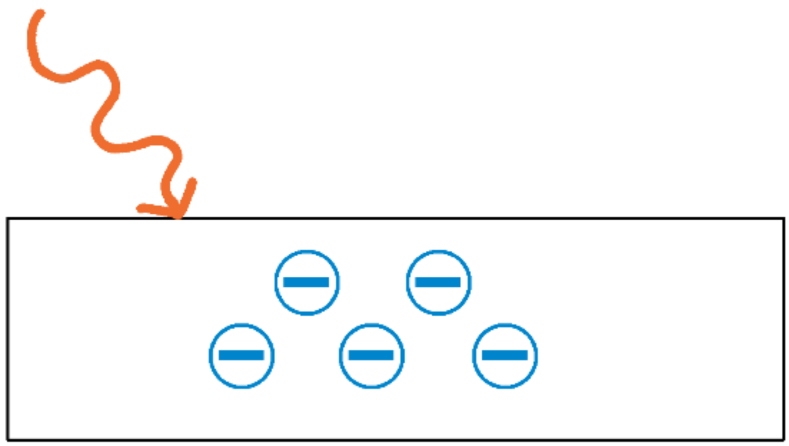


- The apparatus is made of a metal grid in which light of different intensities and frequencies was shown onto it.
- The ammeter (A) measures current (the **number of electrons emitted**).
- The voltmeter (V) measures the stopping potential (the **energy of the electrons emitted**).

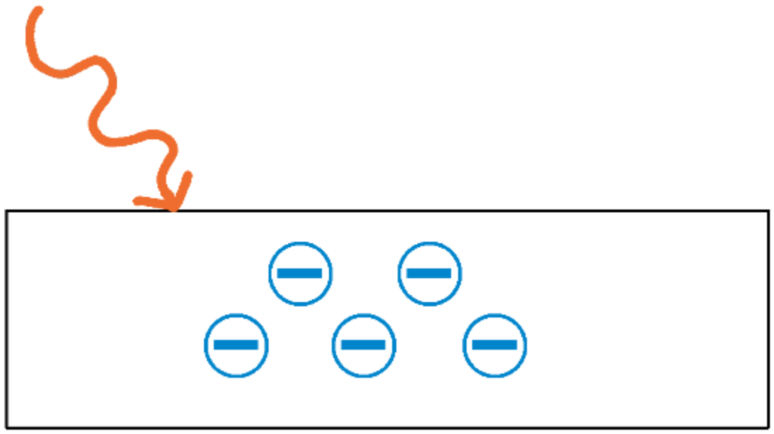


Experimental Findings

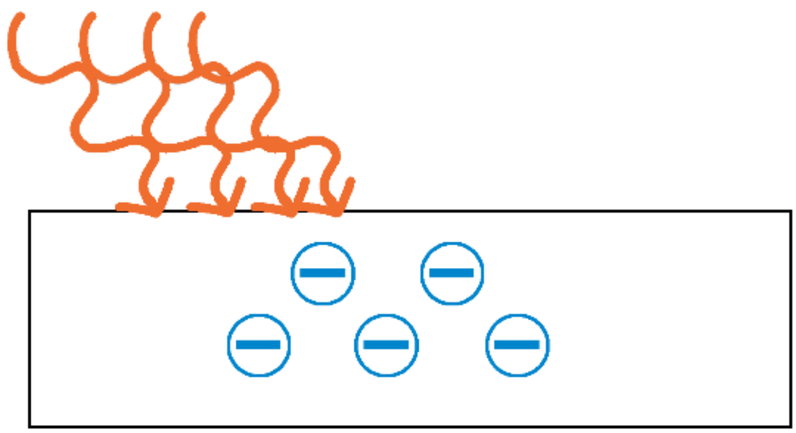
1) 1 photon with sufficient energy to eject an electron:



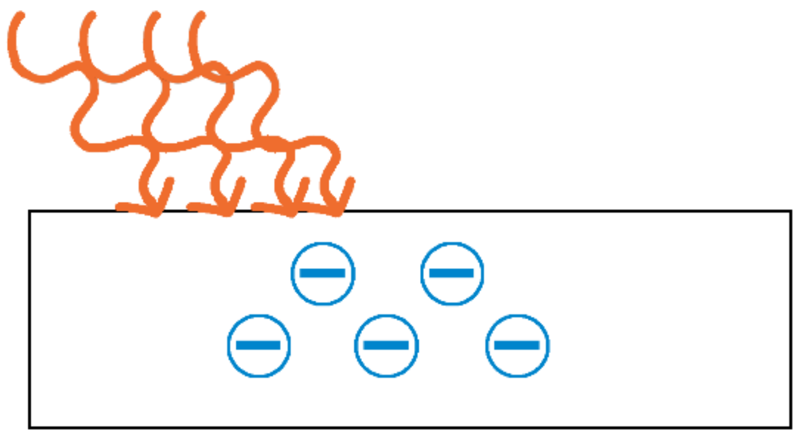
2) 1 photon with insufficient energy to eject an electron



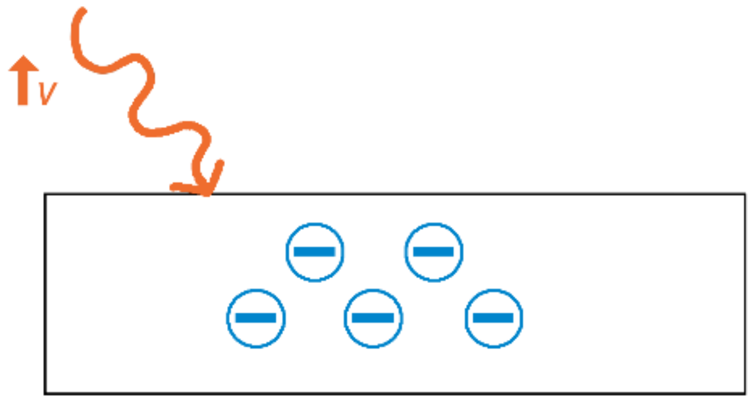
3) Multiple photons hitting the metal, individually they have insufficient energy to eject an electron but if you add up the their energy they have more energy than required to eject an electron



4) Multiple photons, each with sufficient energy needed to eject an electron hitting the metal



5) A photon with an increased frequency than the photons with minimum sufficient energy to eject an electron



Summary of the Findings:

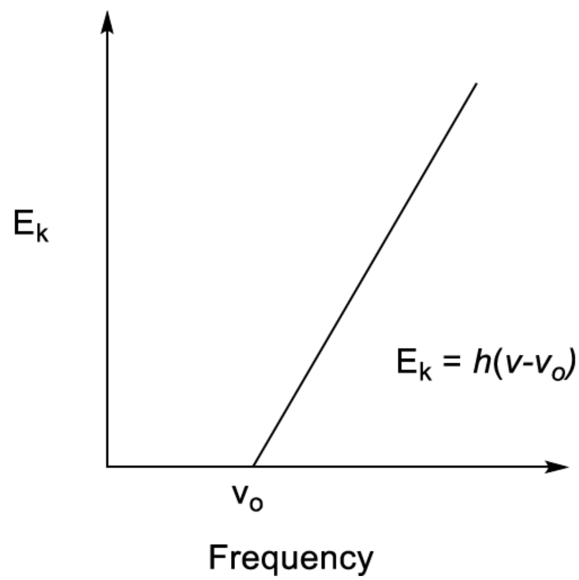
- **Electrons must be ejected by 1:1, photon : electron collisions**
- **Increased intensity** of the light (**more photons** for a given part of the light beam), **increased the number of electrons emitted** (if **each of the photons had sufficient energy** to eject electrons)
- **Increased frequency** of the light, **increased the energy of the electrons emitted**

Before this experiment, people thought of light only as WAVES, but **Einstein showed that light could also be thought of as particles (photons).**

  - When particle A hits particle B, particle A transfers its momentum to particle B. This is not the case for waves!
  - The photoelectric effect showed that light can behave like particles since photons of light can hit a solid substance and cause electrons to be emitted

Photoelectric Effect Equation

This experiment shows that light can behave like a particle "knocking" electrons out of a material.



- The **y-axis** shows the **kinetic energy (Ek) of the emitted electron**
- The **x-axis** shows the **frequency of the photon** that is hitting the metal's surface
  - When the **frequency is too low**, the energy of the photon is too low and an **electron is not emitted**
  - When the **frequency reaches the threshold frequency**, there is **enough energy to emit an electron**
  - At even **higher frequencies**, the **kinetic energy (Ek) of the electron is increased further!**

The energy corresponding to v_o is called the '**binding energy**' and represents the amount of **energy required to remove the electron, $E_{Binding}$**

$$\boxed{Ek_{\ electron\ being\ ejected} = E_{photon} - E_{binding}}$$

$$where\ E_{photon} = hv = \frac{hc}{\lambda}$$

$$and\ Ek_{electron} = \frac{1}{2}mv^2$$

and $E_{binding}$=minimum amount of energy needed to eject an electron

WIZE TIP

The **binding energy for each metal is unique.**
Example: The binding energy of iron and gold are different.

The **binding energy for a specific metal is constant** so if you are given the binding energy for iron in a question, you can use that for part a) b) c) for example.

Does an electron get displaced when E_{photon} > or < than $E_{binding}$?

Example: Ejecting an Electron

When lithium metal is irradiated by a laser with a wavelength of 400 nm no electrons are ejected from the surface. If you want to ionize lithium which of the following types of radiation should you use?

a) UV-Laser
b) IR-Radiation
c) Red Light Laser
d) Green Light Laser
e) Radio Wave

WIZE TIP

When you see a question that mentions **electrons being ejected** from the surface of a metal, you know the question is going to have something to do with the **photoelectric effect**!

1.5.4

Practice: No Electrons are Ejected

A metal surface is irradiated by light from a laser with a wavelength of 492 nm. No electrons are measured leaving the surface. What is the most likely explanation?

- All of the electrons which are easy to remove have already been removed
- The frequency of the photons is less than the threshold frequency of the metal
- The energy of the photons is greater than the threshold value
- The light is not irradiating the surface at the correct angle
- None of the above

1.5.5

Practice: Calculate the Binding Energy

An element is bombarded with a beam of X-rays of wavelength 0.75664nm. Upon irradiation, electrons are ejected with a velocity of 2.35×10^{7} m/s. The mass of an electron is 9.11×10^{-31}kg.

What is the binding energy for the element?
$h = 6.626 \times 10^{-34}$ Js

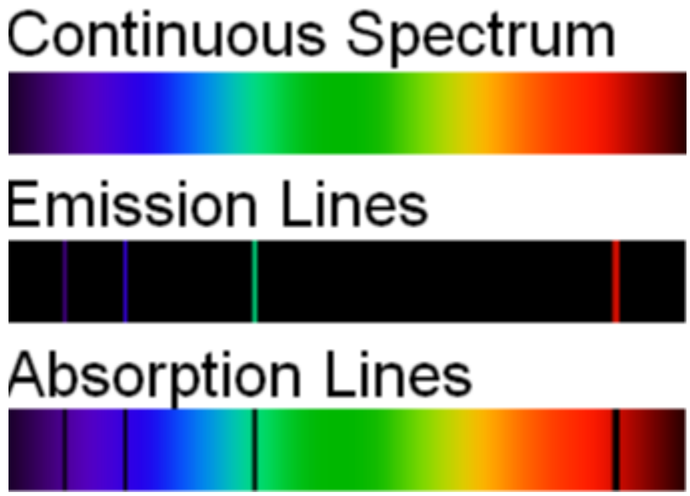
- $1.12 \times 10^{-14} J$
- $2.46 \times 10^{-17} J$
- $1.12 \times 10^{-17} J$
- $0\ J$

1.6 Understanding the Bohr Model

1.6.1

The Basics of Absorption and Emission Spectra

Each atom has a **unique** absorption and emission spectrum.

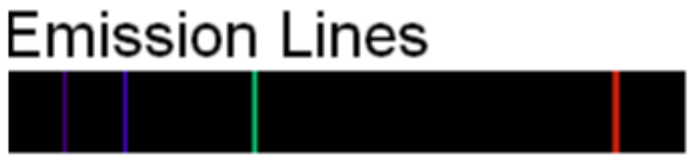


Absorption Spectra

- We get an absorption spectrum by transmitting electromagnetic radiation (light) through a substance.
- The **dark bands** in the spectra represent all of the **specific wavelengths of photons absorbed** by the atom's electrons

Emission Spectra

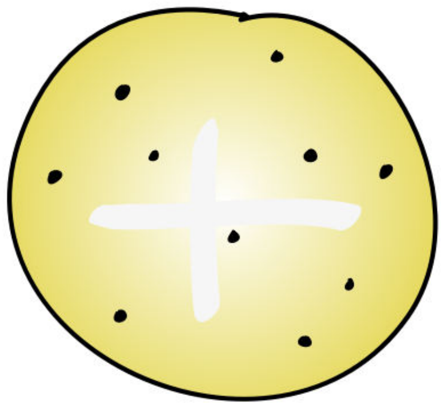
- We get an emission spectrum by measuring the electromagnetic radiation (light) that is emitted from a substance
- The background is black and the **coloured bands** represent the **wavelengths of photons that were emitted** from this atom's electrons



1.6.2

Bohr's Atomic Model

Before the Bohr model, scientists thought that electrons just assumed arbitrary energies and could be found anywhere in the atom.



If the pre-Bohr model was right, what would the emission spectra look like? Would they have lines or would they be continuous spectra? ____________________

Niels Bohr realized that the existing model at the time was inconsistent with emission spectra data... if electrons could be anywhere and have any energy, why did each element have a unique emission spectra with photons of light being emitted with specific energies and wavelengths?

Bohr realized that the **electrons must have discrete energies** in order to explain the emission spectra with photons with specific amounts of energy being released.

Bohr's Atomic Model Details

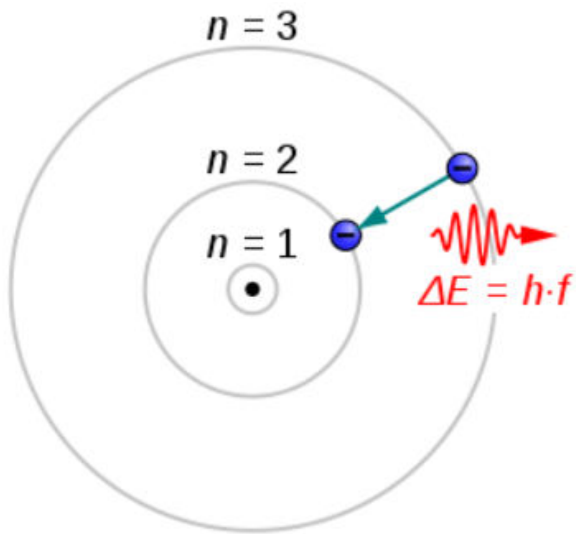


Photo by JabberWok / CC BY

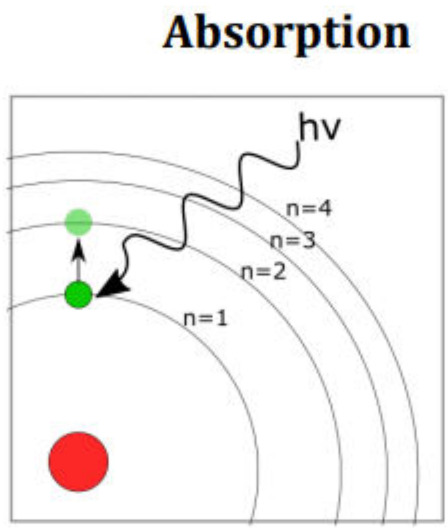
- Electrons orbit nucleus at **fixed distances** and in **circular paths** (like how planets orbit the sun!)
- Energy electrons have are **quantized** (only specific energies are allowed)
- Shell's distance from nucleus determines energy (n=1, 2, 3, etc, **higher n=higher energy shell**)
- **Gap between levels shrinks as n grows**
- Bohr model is only accurate for atoms with **1 electron** ("**Bohr atoms**")
    - The Bohr model explains why only photons with certain energies are observed in the emission spectra!

Analogy: Staircase vs Ramp

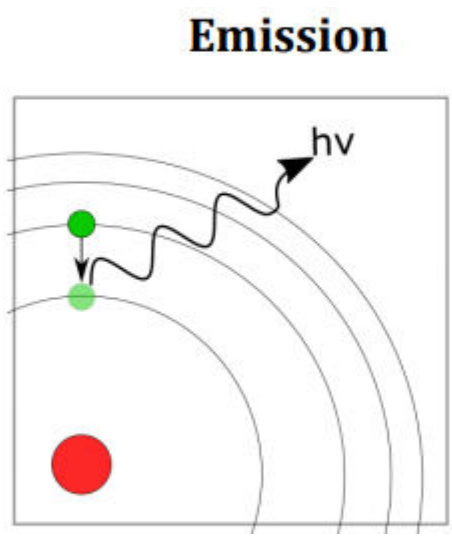
- **Ramp->**if you're walking up a ramp, you could be 12cm, 17cm, or 20cm above the ground. (Pre-Bohr Model)
- **Staircase->** if each step is 17cm high, you can never be standing 12 cm or 20cm above the ground (Bohr Model)
    - The **stairs are discrete units** just like **shells in an atom are discrete units.**
    - And just like how we can only be **certain heights above the ground when we take the stairs**, **electrons can only be in certain shells with certain energies (can't be between two shells)**

1.6.3

Absorption vs Emission of a Photon



- Atom **absorbs photon** with **energy** (E=hv) **equal to gap between levels**
- Electron is promoted to **higher energy level** (ex: n = 1 → n = 2)
- **Greater Δn = higher energy**



- Atom **emits photon** with **energy equal to gap between levels**
- Electron relaxes to **lower energy level** (ex: n = 4 → n = 2)

Example: Understanding Absorption Spectra and the Bohr Model

To collect an absorption spectra of a gaseous mixture a gas is irradiated with light from each wavelength in a given range and the amount of light which passes through the sample is recorded. Some of the light at certain wavelengths is absorbed by the sample and these wavelengths become peaks in the absorption spectra.

1) An absorption event occurs when...

a) The atom is destroyed

b) The nuclear charge increases by 1

c) An isotope ejects an electron

d) An electron is excited from one energy level to a higher energy level

e) None of the above

2) The wavelength of light which is absorbed corresponds with ...

a) The difference in energy between the energy levels which the electrons occupy

b) The energy level of the orbit the electron was initially in

c) The energy level of the orbit the electron ends up in

d) The distance between the two orbits the electron moves between

e) None of the above

1.6.5

Example: Electron Transitions

An electron in the n = 4 shell of an excited hydrogen atom relaxes to it's ground state. Which of the following is true?

a) A photon is absorbed and with energy equal to the energy of the ground state
b) A photon is absorbed with energy slightly less than the difference in energy between n = 4 and n = 1
c) A photon is absorbed with energy equal to the difference in energy between n = 4 and n = 1
d) A photon is released with energy equal to the energy of the ground state
e) A photon is released with energy slightly less than the difference in energy between n = 4 and n = 1
f) A photon is released with energy equal to the difference in energy between n = 4 and n = 1

1.7 Bohr Model Equations

1.7.1 Bohr Model Equations

Bohr Model Equations

There are a few important equations we should be familiar with that are related to the Bohr model. **These equations can only be used for one electron systems!** Recall that **Bohr's model** was only able to explain species with **1 electron.**

Calculating the Energy of a Specific *n* Level

$$\boxed{E = \frac{\left(-2.178 \times 10^{-18}\mathrm{J}\right)\left(Z^2\right)}{n^2}}$$

*where **n** is the shell # and it can be 1, 2, 3...etc*
***E** represents the **energy** of a specific n level*
***Z=atomic # (# of protons)** in an atom (ex. Hydrogen has 1 proton, Z=1, He+ has 2 protons, Z=2)*

Calculating the Energy Difference Between n Levels

$$\boxed{\Delta E = -2.178 \ \times 10^{-18} J \left(Z^2\right) \left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)}$$

*where **ΔE** represents the **difference in energy** between 2 energy levels*
***Z=atomic # (# of protons)** in an atom*
*n_f is referring to the **final energy level***
*n_i is referring to the **initial energy level***

- If **ΔE is positive**, energy was (absorbed/released) __________ and the electron should go to a (higher/lower) ________ energy level

- If **ΔE is negative,** energy was (absorbed/released) ________ and the electron should go to a (higher/lower) ________ energy level

WATCH OUT!

Be very careful when entering n_f and n_i values into this equation!

Example: If we are told energy is **absorbed** and an electron goes from **n=1 to n=2**

- **n=1 is the initial energy level, n=2 is the final energy level.**

Example: If we are told energy is **released** as an electron goes from **n=3 to n=2**

- **n=3 is the initial energy level, n=2 is the final energy level.**

Calculating the Wavelength of the Photon Absorbed or Emitted

Method 1:

- Use the above equation to solve for ΔE.
- Then use $E = \frac{hc}{\lambda}$ to solve for the wavelength of the photon
  - Even if ΔE is negative, use the positive value to solve for the wavelength so you **get a positive answer for wavelength** (negative wavelength doesn't make sense)

Method 2:

- Use the following equation and then take the inverse to solve for λ

$$\boxed{\frac{1}{\lambda} = R_H \left(\frac{1}{n_i^2} - \frac{1}{n_f^2} \right)}$$

*λ=wavelength of the photon (m) -always **enter answer as a positive value!***

R_H=Rydberg constant=1.097x$10^7 m^{-1}$

n_i=initial energy level, n_f=final energy level

1.7.2

Example: Releasing or Absorbing Energy and How That Differs For Different Atoms

An electron in a one-electron species transitions from the n = 4 state to the n = 2 state.

a) Is energy released or absorbed?

b) Would more energy be absorbed/released from a sample of Hydrogen atoms or Li^{2+} ions?

1.7.3

Example: Excitation and Relaxation in Atoms

Calculate the wavelength, in nm, of a photon released when an electron in a hydrogen atom relaxes from n = 3 to n = 1. What is the energy of the photon if the electron is re-absorbed from n = 1 to n = 3?

1.7.4

Practice: Using Bohr Model Equations to Determine an Energy Level

A photon of light was released by a hydrogen atom with an energy of 1.94 x 10^{-18} J. If this transition ended at n=1, from which level did this transition begin?

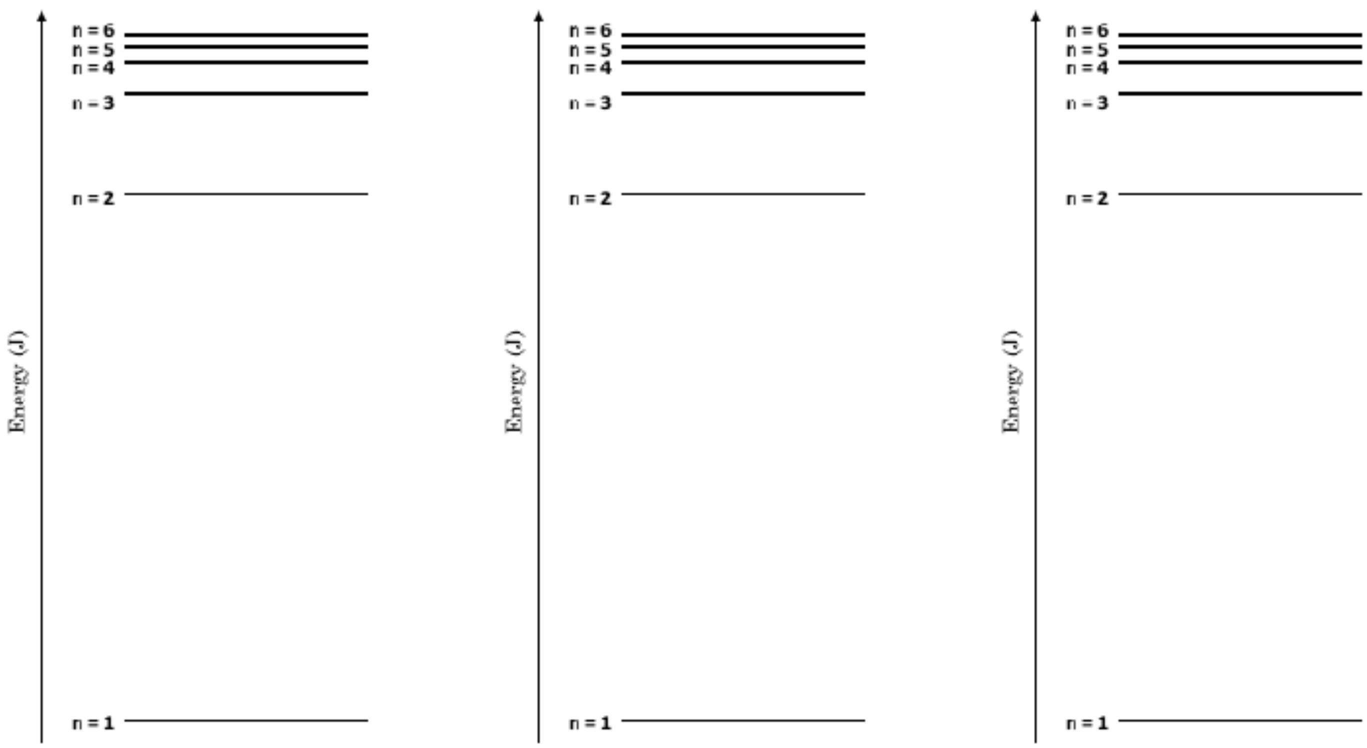
- n=1
- n=2
- n=3
- n=5
- n=6

1.8 How Atomic Spectra Relates to Electronic Transitions + Other Applications of the Bohr Model

1.8.1

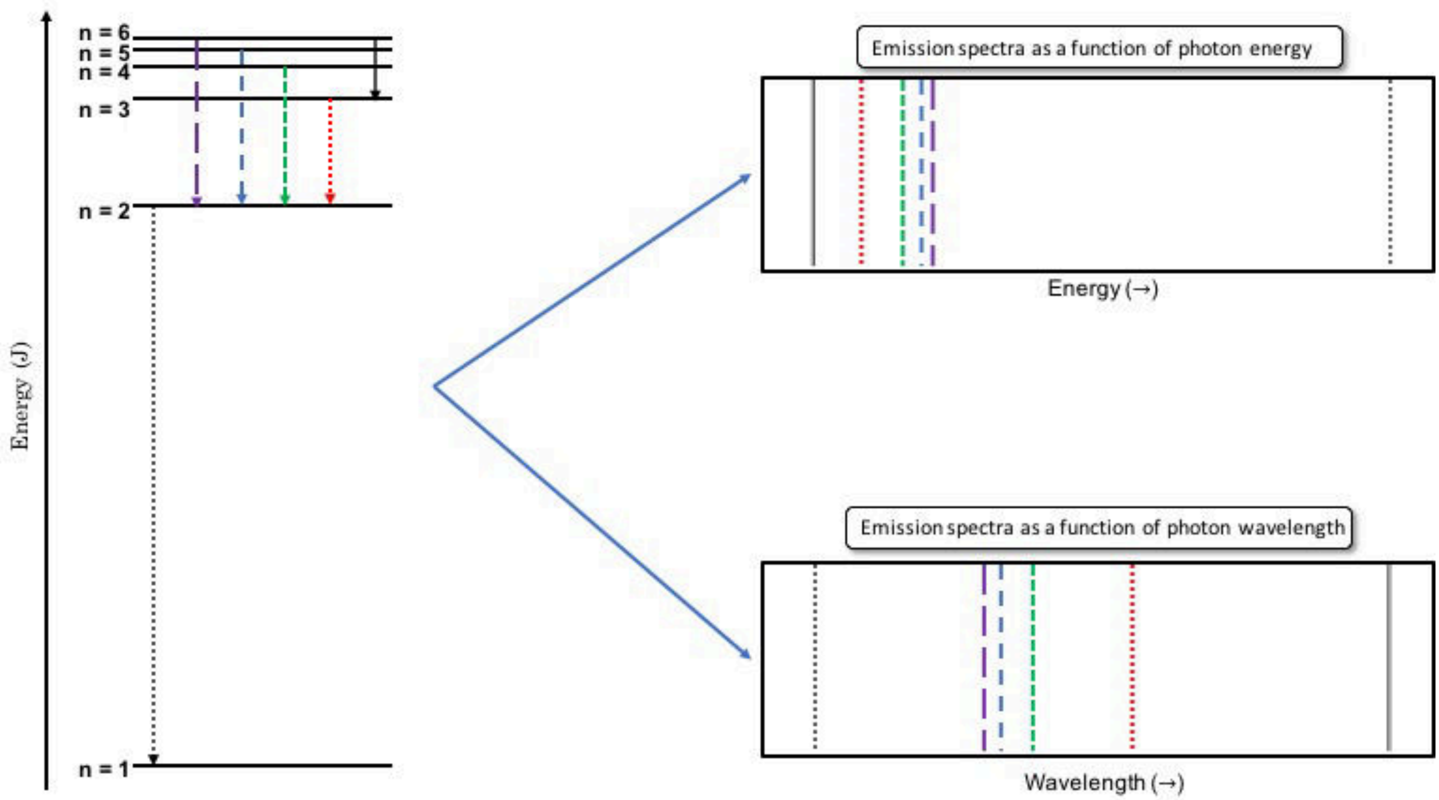
Atomic Line Spectra

Emission and Absorption



Note: **n=1 is ground state**, all other n levels are excited states

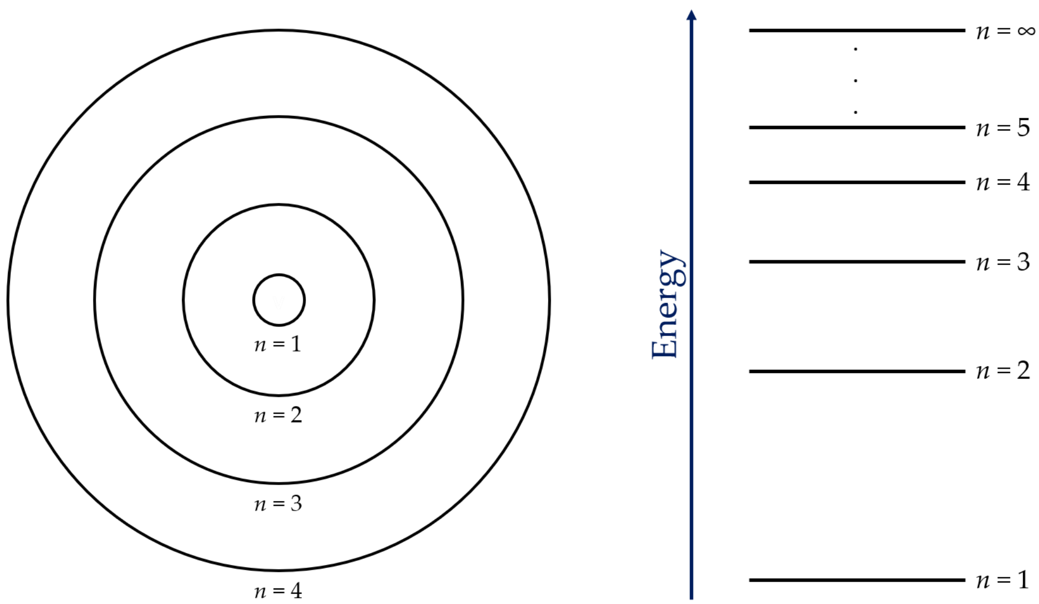
Emission Spectra

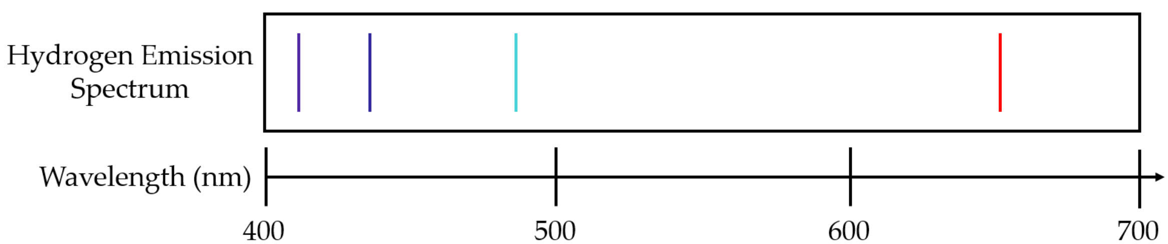


1.8.2

Relating Electronic Transitions to Emission Spectra

Bohr Model of the Hydrogen Atom





Hydrogen Emission Spectral Series:

Hydrogen Eimission Spectrum Series Name	n_f
Lyman	1
Balmer	2
Paschen	3
Brackett	4
Pfund	5

Example: Removing an Electron

What wavelength of light corresponds to the 4^{th} ionization energy of Beryllium?

Can start by solving for the energy difference for this transition:

Now you can solve for the wavelength that the energy difference corresponds to:

1.8.4

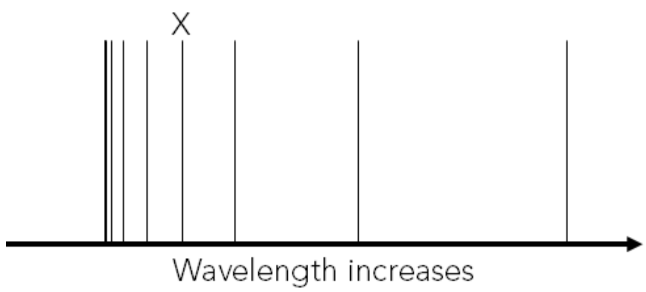
Practice: Understanding Emissions

Which of the following transitions would emit the shortest wavelength photon?

- n=2 to n=1
- n=1 to n=6
- n=5 to n=1
- n=7 to n=2
- n=1 to n=4

1.8.5

You shine light through a sample of gaseous atomized hydrogen and take an absorption spectrum as shown below. Only transitions to or from the ground state (n=1) appear in the spectrum. Which of these energy-level transitions correspond to the line labelled X in the absorption spectrum?



- n = 1 to n = 2
- n = 2 to n = 1
- n = 1 to n = 4
- n = 1 to n = 5
- n = 4 to n = 1
- n = 5 to n = 1

1.9 Wave-Particle Duality & the de Broglie Equation

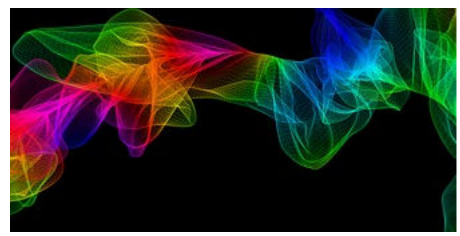
1.9.1

Wave-Particle Duality

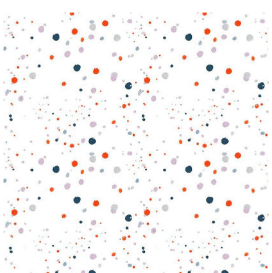
Light was originally thoughy of as only having wave-like properties, but was later shown to have particle-like properties as well.

Light as Waves

- When light was shown at a slit, interference patterns were recorded
- **Interference patterns** are a property of waves



Light as Particles



- Einstein showed that light can also be thought of as particles since they are like packages of exact amounts of energy
- The experiment was the **photoelectric effect** and it showed that there is **wave-particle duality** (light has both properties of waves and particles!).

What About Electrons?

Louis de Broglie thought that if light has both properties of waves and particles, electrons might also have properties of particles and waves.

He determined the following equation to explain the wave-nature of particles:

$$\boxed{\lambda = \frac{h}{mv} = \frac{h}{p}}$$

De Broglie Equation

λ *is the* ***de Broglie wavelength*** *of the small particle (****m****)*

h is Planck's constant*= 6.626 x10^{-34} Js (or 6.626x10^{-34} kg m^2/s)*

m *is the mass of the particle (****kg****)*

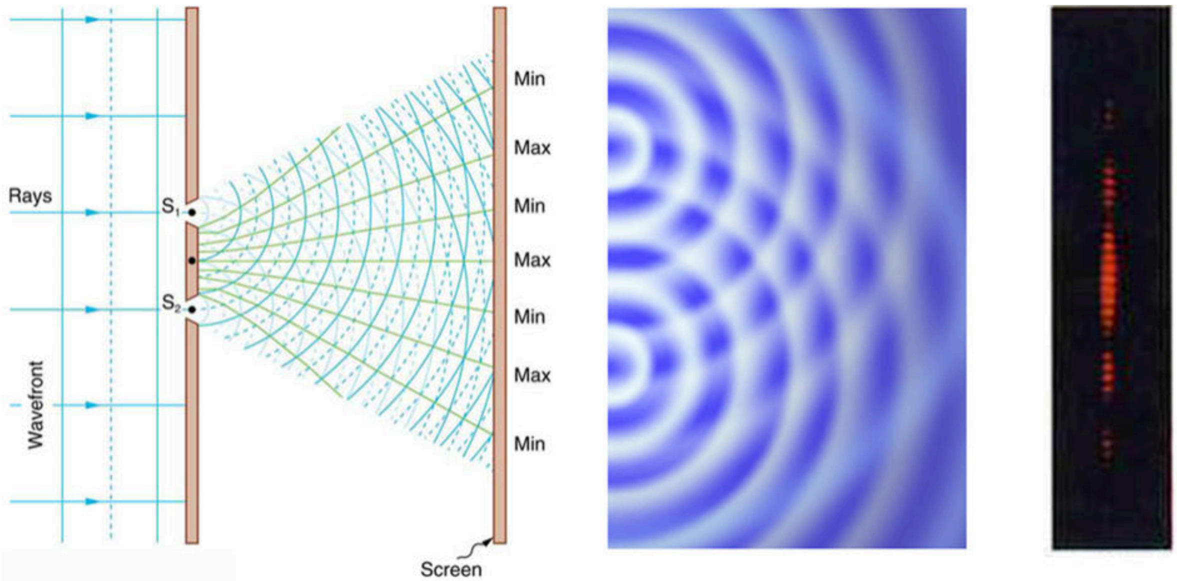
v *is the velocity of the particle (****m/s****)*

p *is the momentum of the particle (p=mv)*

WATCH OUT!

The *v* in this equation is not frequency (*ν*, Hz), it is velocity (*v*, m/s).

Light acting as a wave:



Young's double slit light experiment

Could electrons also act as waves?

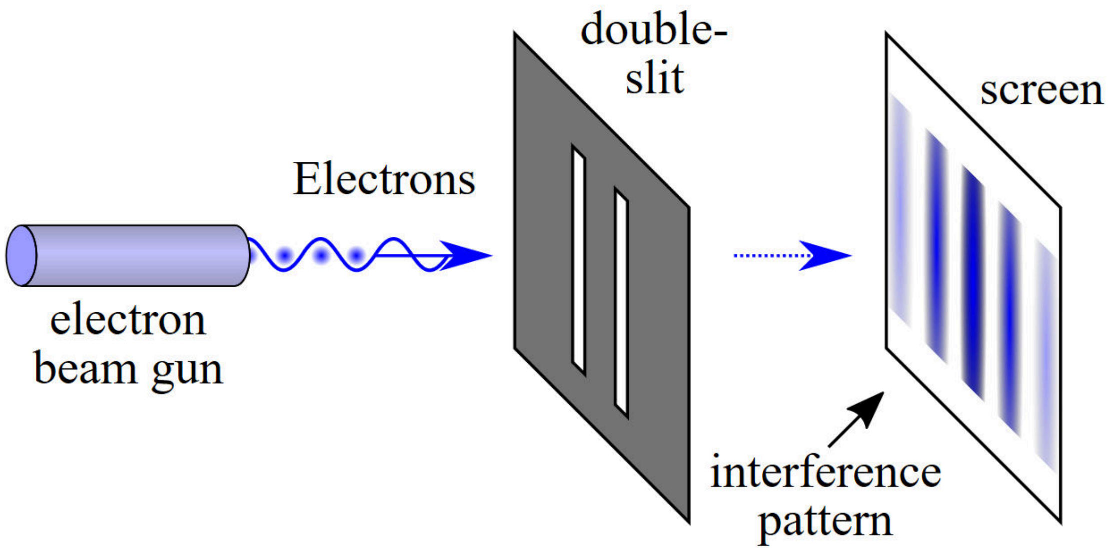


Photo by Johannes Kalliauer / CC BY

In summary

All waves can behave like particles and all particles can behave like waves! **The wave-particle duality applies to light and particles!**

1.9.2

Example: Wavelength of an Accelerated Neutron

At CERN, a neutron is accelerated to 2.4 x 10^8 m/s in a particle accelerator. The mass of the neutron is 1.675 x 10^{-27} kg, what is it's wavelength? (h is 6.626x10^{-34} kg m^2/s)

a) 1.14 x 10^{-15} m
b) 2.77 x 10^{-14} m
c) 1.65 x 10^{-15} m
d) 3.53 x 10^{-14} m

Practice: Two-Slit Experiment

If you shoot a beam of electrons at a piece of metal with two small slits in it, a diffraction pattern appears on the detector on the otherside. This is often referred to as a two slit experiment. This result shows that,

- electrons can behave as particles
- electrons are very small
- electrons can behave as waves
- electrons can behave as both particles and waves
- electrons travel very fast

1.9.4

Practice: Wave-Particle Duality

Nolan Ryan, a fastball pitcher from the 1970's, was recorded throwing a four seam fastball around 108mph (174km/h). A MLB baseball weighs approximately 145g. What is the wavelength of the baseball?

1.10 Introduction to the Quantum Model

1.10.1

Bohr Model Vs Quantum Model

What was good about the Bohr model and theory?

✔️ Could predict line spectra for hydrogen and other ions with **1 electron** (ex. Li^{2+})

❌ But it couldn't predict line spectra for species with more than 1 electron

Couldn't explain how atoms were bound together

Didn't explain why only certain orbits were allowed

❌ Tries to be too precise to describe where electrons are found

Bohr Theory was replaced by Quantum Mechanics!

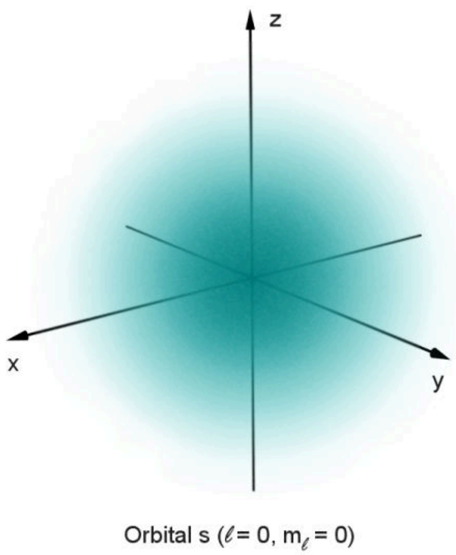
✔️ Quantum model can predict atomic spectra for **many-electron atoms**

Quantum mechanics provides us with **probabilities where electrons are most likely to be found**

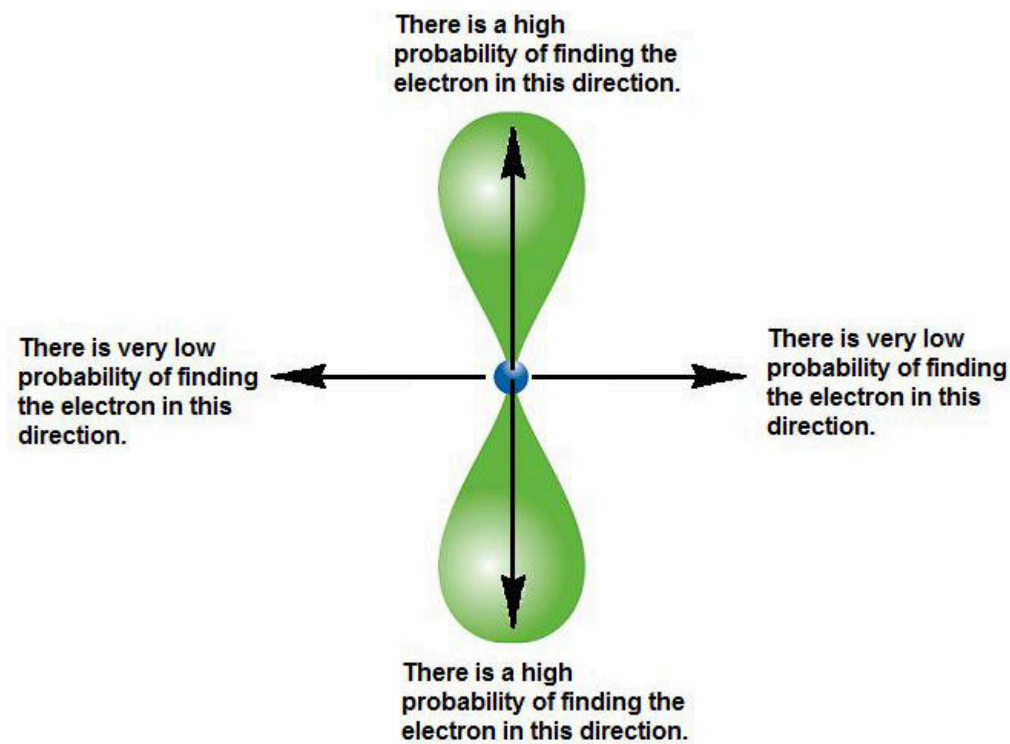
- Provides a 3D region where electrons are most likely to be found (instead of circular paths in Bohr model)

✔️ Adds on to the Bohr model:

  - Electrons are still only found at discrete energy levels with specific amounts of energy (quantized)
  - In this model, **each electron has 4 quantum #s that are unique to that electron** and describe it.



Electron Density Diagram


There is a high
probability of finding the
electron in this direction.
There is very low
probability of finding
the electron in this
direction.
There is very low
probability of finding
the electron in this
direction.
There is a high
probability of finding the
electron in this direction.

1.11 Heisenberg Uncertainty Principal

1.11.1

The Heisenberg Uncertainty Principle

As electrons were discovered to have both wave and particle properties, Heisenberg found that we **cannot determine the exact position and momentum (direction and speed) simultaneously**. This is known as the Heisenberg uncertainty principle.

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

Δx *is the* ***uncertainty in position***

Δp *is the* ***uncertainty in momentum***

Δp=mΔv *where* ***m*** *is the mass (****kg****) and* ***Δv*** *is the uncertainty in velocity (****m/s****)*

h is Planck's constant *(6.626×10^{-34} Js or 6.626×10^{-34} kg m^2/s)*

The larger the value for Δx is, the (larger/smaller) ________ the value for Δp is

- In other words, a **larger value for Δx** means we are **more uncertain about the position** of the particle and **less uncertain about the momentum** of the particle!

Max Born added to this and said that we can interpret this equation to mean that we cannot say exactly where electrons are but we can say where they are likely to be.

1.11.2

Example: Wave Particle Duality and the Heisenberg Uncertainty Principle

A beam of electrons is accelerated towards a thin metal foil and diffracts to give the exact same pattern as a blue laser with a wavelength of 480nm. The mass of an electron is 9.11×10^{-31} kg.

a) What speed were the electrons accelerated to?

b) If we measure the speed to a precision of ± 1% what is the minimum uncertainty in the position of the electron?

1.11.3

Practice: Uncertainty of Position

A circus performer is shot out of a cannon and leaves the cannon with a velocity of 6.2±0.1 m/s. If the performer weighs 82 kg, what is the minimum uncertainty in their position?

- 6.2 m
- 6.43×10^{-36} m
- 8.2 m
- 2.46×10^{-34} m

1.12 The Quantum Model & Orbitals

1.12.1

Quantum Numbers

Quantum numbers describe where electrons are positioned around atoms:

Letter	Quantum Number	Description
n	Principal	Size
l	Orbital Angular Momentum	Shape
m_l	Magnetic	Orientation
m_s	Electronic Spin	Electron Up or Down

Rules:

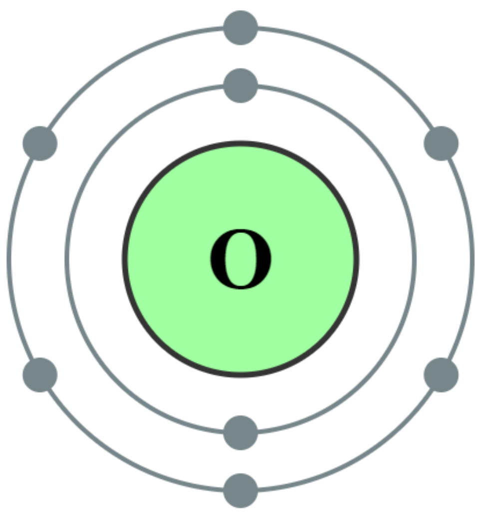
n

- Can be **any positive integer**
  Example: n = (1, 2, 3, 4...)

- As n increases, energy and size of shell ___________

WIZE TIP

n is also called the "principle quantum number"



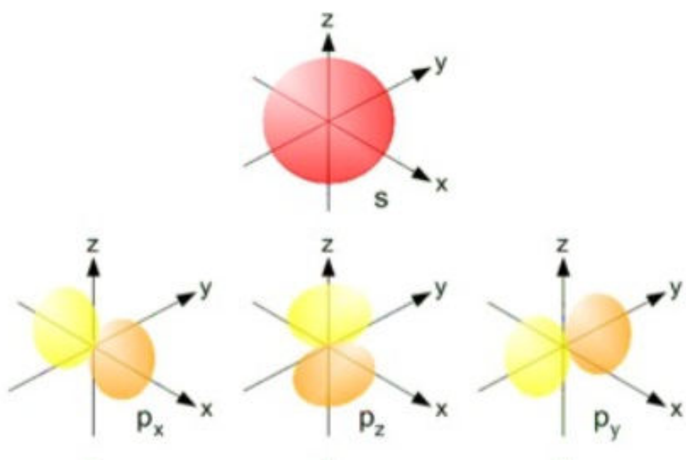
l

- Can be any **non-negative integer up to n-1**
  Example: l = (0, 1, 2, 3, ..., n-1)

- l (orbital shapes) are described as:

subshell	s	p	d	f
l	0	1	2	3

Increasing energy →



- These shapes show us where an electron is most likely to be found
- There is a 90% chance in finding an electron somewhere inside the given shape

WIZE CONCEPT

S orbitals are spheres and with increasing "n" the sphere will get larger.
There is one s orbital in a subshell.

P subshells are dumbbell shaped.
There are three p orbitals in a subshell, each orientated along an axis (px, py and pz)

m_l

- Can be any integer from **–l to +l**
  Example: m_1 = (-l, ..., 0, ..., l)

- This quantum # **designates a specific orbital within a given shell**
  Example: if n=2 and l=1, we are looking at 2p.
  - ml can be -1, 0, or +1 this designates each of the 2p orbitals: 2px, 2py, and 2pz

m_s

- **Spin** of an electron

- Can only be **+1/2 or -1/2**

1.12.2

Quantum Numbers Summary

Principle Quantum Number (n)	Angular Momentum Quantum Number (ℓ)	Magnetic Quantum Number (m_ℓ)	Electron-Spin Quantum Number (m_s)
$n = 1, 2, 3, \dots$	$\ell = 0, 1, 2, 3, \dots (n - 1)$	m_ℓ = integer values of ℓ to $-\ell$	$m_s = \pm \frac{1}{2}$
$n \uparrow \rightarrow E \uparrow$	$\ell = 0 \rightarrow s$ $\ell = 3 \rightarrow f$ $\ell = 1 \rightarrow p$ $\ell = 2 \rightarrow d$	$\mathbf{2\ell + 1}$ orbitals	Only 2 electrons per orbital, **ALWAYS**

n shell	ℓ subshell	Orbital	m_ℓ	Number of Orbitals per subshell = n^2
1	0	1s	0	1
2	0	2s	0	4
	1	2p	+1, 0, -1	
3	0	3s	0	9
	1	3p	+1, 0, -1	
	2	3d	+2, +1, 0, -1, -2	
4	0	4s	0	16
	1	4p	+1, 0, -1	
	2	4d	+2, +1, 0, -1, -2	
	3	4f	+3, +2, +1, 0, -1, -2, -3	

1.12.3

Example: Allowed Quantum Numbers

What are the allowed set of quantum numbers for the following orbitals?

a) 6s

b) 4p

c) 3d

Example: Allowed Sets of Quantum Numbers

Which of the following sets of quantum numbers (n, l, m_l, m_s) are allowed and which are not allowed? For the sets of quantum orbitals that are not allowed, state why it is not allowed.

(i) (4, 0, 0, 0)

(ii) (3, 1, 2, $-^1/_2$)

(iii) (5, 3, 0, $+^1/_2$)

(iv) (4, 4, 3, $-^1/_2$)

1.12.5

Example: Defining Orbitals from Quantum Numbers

Determine the atomic orbital described by the following sets of quantum numbers (n, l, m_l, m_s).

(i) (2, 0, 0, -$^1/_2$)

(ii) (4, 3, 0, +$^1/_2$)

(iii) (5, 1, 1, -$^1/_2$)

Practice: Valid Quantum Numbers

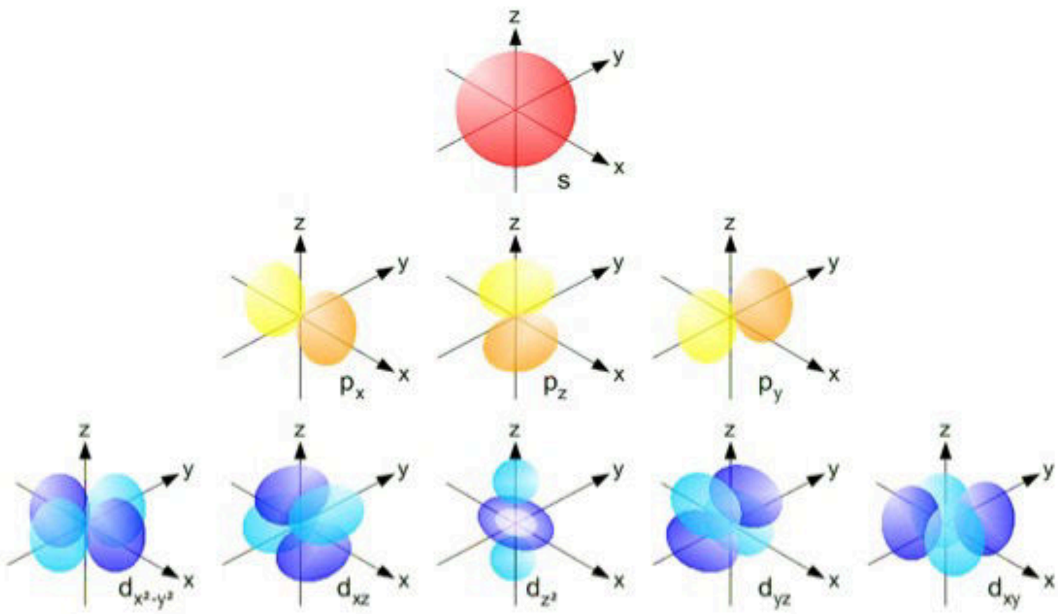
Determine which of the following sets of quantum numbers ($n,\ l,\ m_l,\ m_s$) is valid for a 3d orbital.

- a) (3, 3, 2, $+^1/_2$)
- b) (4, 2, 1, $-^1/_2$)
- c) (3, 2, -2, 0)
- d) (3, 2, -1, $-^1/_2$)
- e) (3, 2, 3, $-^1/_2$)
- f) (3, 1, 0, $+^1/_2$)

1.13 Shapes of Atomic Orbitals

1.13.1

Shapes (aka Boundary Diagrams) of Atomic Orbitals



- There is **one** s orbital in a subshell, which is a sphere
- There are **three** p orbitals in a subshell, each orientated along an axis (p_x, p_y and p_z)

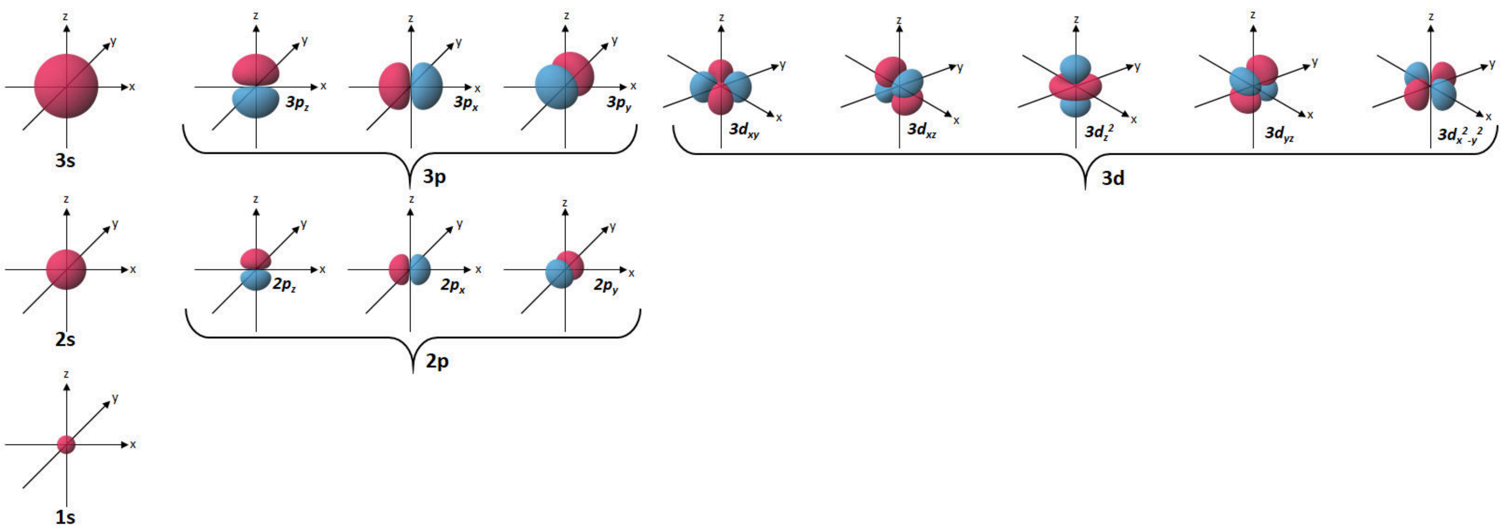
- There are **five** **d orbitals** in a subshell. The shapes of the d orbitals are more complicated than their s and p counterparts.
    - Three orbitals look like 3D cloverleaves, each lying in a plane with the lobes pointed between the axes (d_{xy}, d_{xz} and d_{yz}).
    - A fourth orbital is also a cloverleaf, but its lobes point along the axes ($d_{x^2-y^2}$).
    - The fifth orbital looks quite different with its major lobes pointing along the z- axis, but there is also a “doughnut” of electron density in the xy plane (d_{z^2})

Things to Keep in Mind:

- As the **energy level increases**, so does the **size of the orbitals**
  Example: A 2s orbital is higher in energy and larger than a 1s orbital

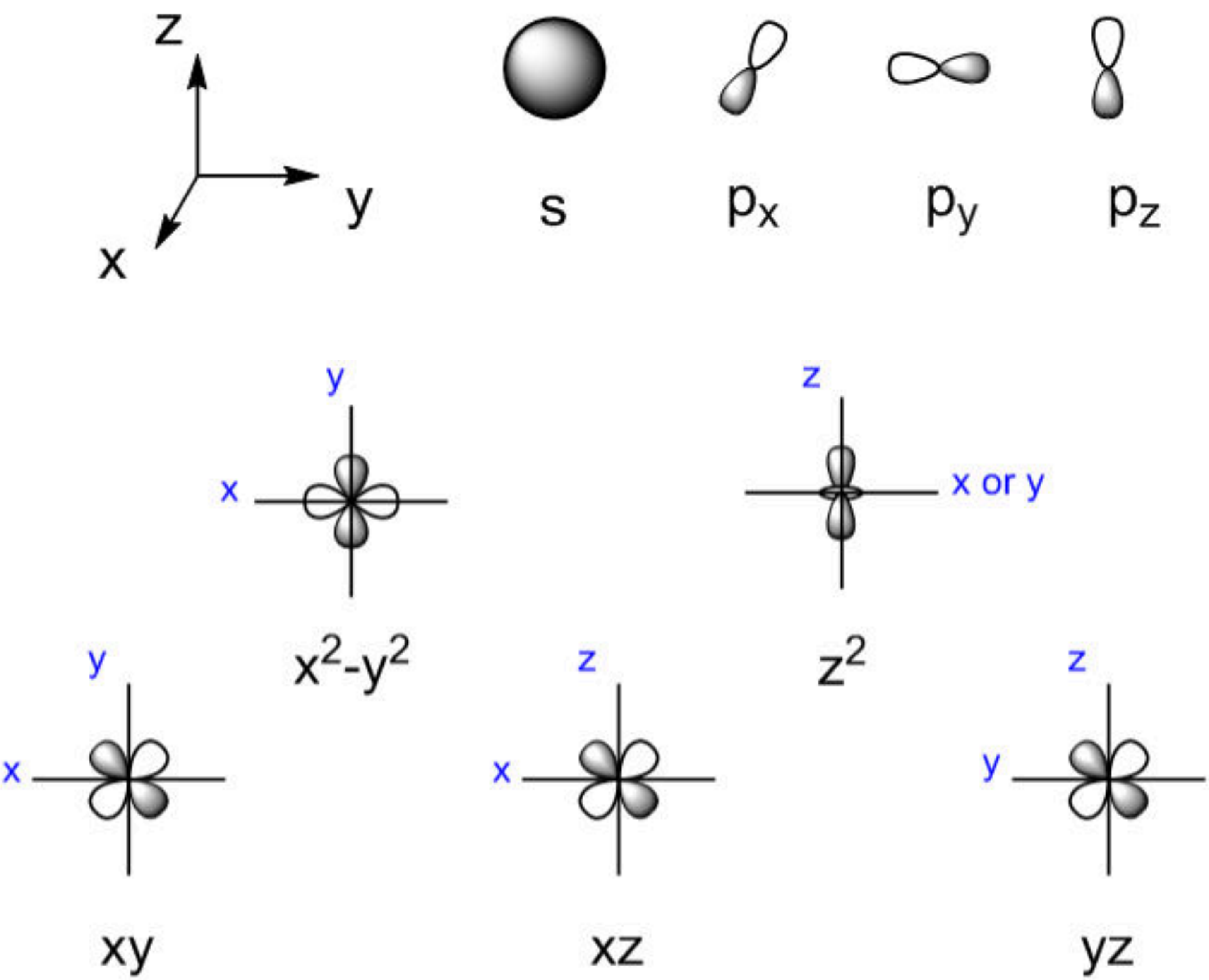
- As the **energy level increases**, so does the **number of orbitals**
  Example: when n=1 (lower energy level), we see 1 orbital, whereas when n=2 (higher energy level), there are 4 possible orbitals

- As the **number of orbitals increases**, so does their **complexity**
  Example: d orbitals are more complex than p orbitals



Drawing Atomic Orbitals

Shown below are the s, p and d orbitals:



WIZE TIP

Pay attention to whether the lobes are ON an axis or BETWEEN axes!

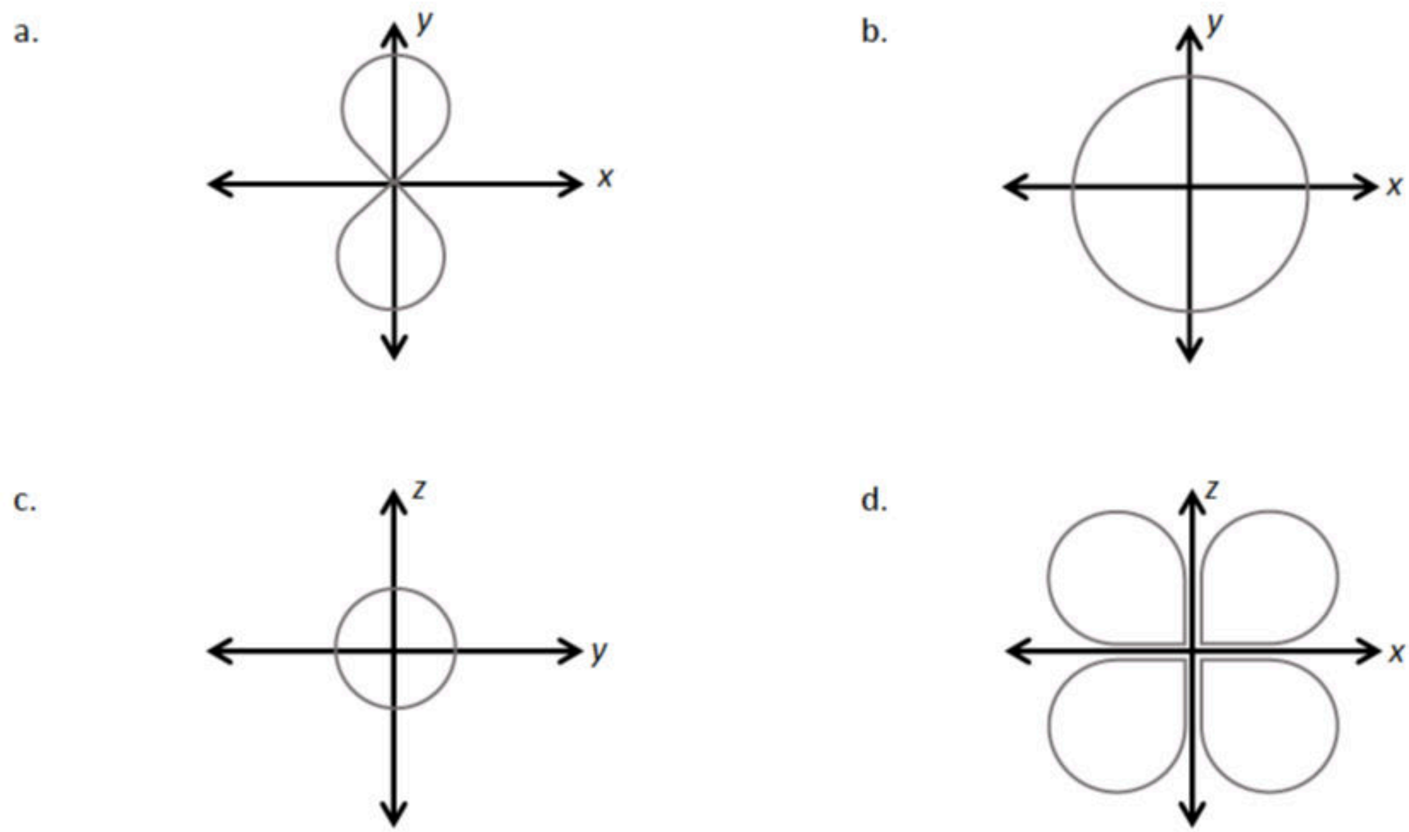
Also, notice how every other lobe is colored in gray. This gray and white coloring is indicating a "positive" lobe and a "negative" lobe. If you were asked to draw one of these orbitals on an exam, you would be expected to color in the lobes as well (or indicate which are + and which are -).

- The angular momentum quantum number, l, gives us information about the shape of the orbital.
- **Note:** There are 5 d-orbitals and 5 allowed value for m_l. Similarly for s and p the number of orbitals is determined by the # of allowed values of m_l.
- **Note:** Each ml is not associated with a particular orbital (ex. d_{xy} vs d_{xz}). Which means given a set of quantum numbers (n,l,ml) one cannot determine which direction the orbital will be pointing

1.13.3

Example: Orbitals

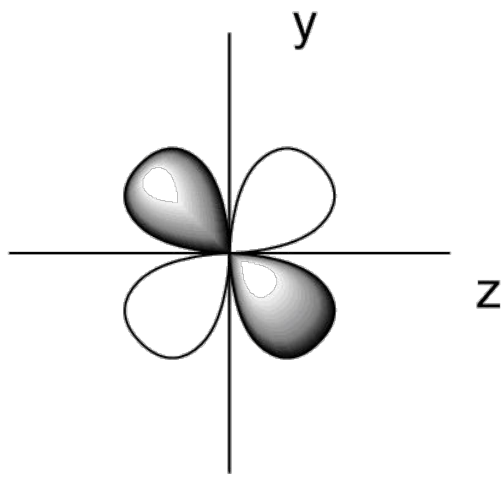
The sketches below show possible orbitals for the electron in a hydrogen atom. Which orbital would have the *lowest* energy?



1.13.4

Practice: Identify the Orbital

Identify the orbital shown below,



a) $2p_y$

b) $3d_{yz}$

c) $3p_x$

d) $3d_{xy}$

e) $3d_{x2-y2}$

1.14 Radial and Angulor Nodes

1.14.1

Angular and Radial Nodes

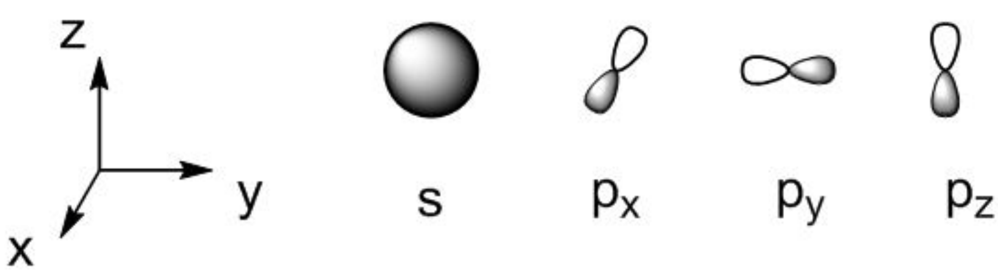
$$\boxed{Total\ number\ of\ nodes\ = n - 1}$$

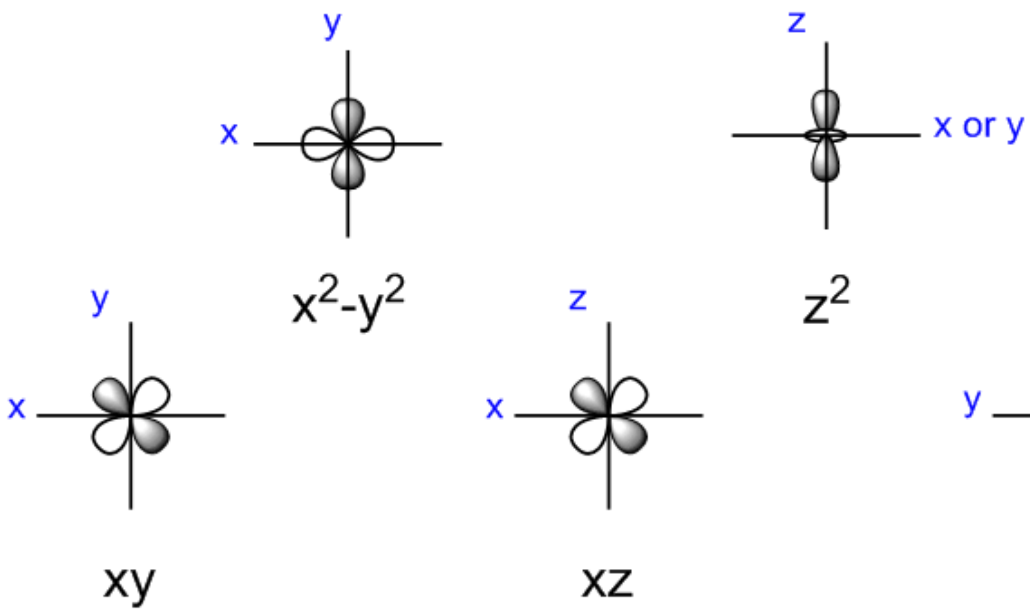
$$\boxed{Number\ of\ angular\ nodes = l}$$

$$\boxed{Number\ of\ radial\ nodes = n - 1 - l}$$

- There are two types of nodes: radial and angular.
- The number of angular nodes depends on the quantum number l.

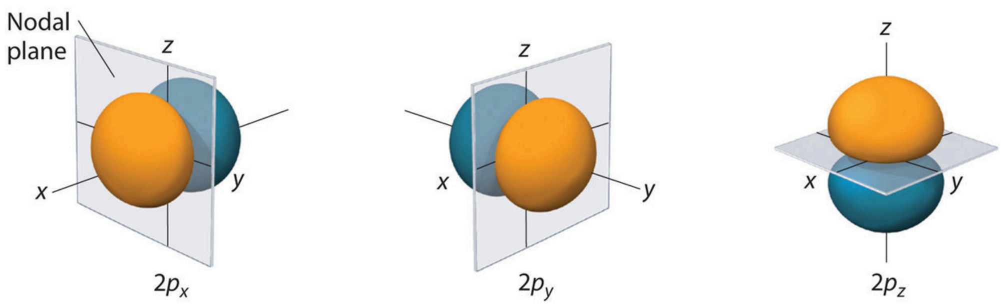
This time let's draw in the angular nodes for the 2p and 3d orbitals:

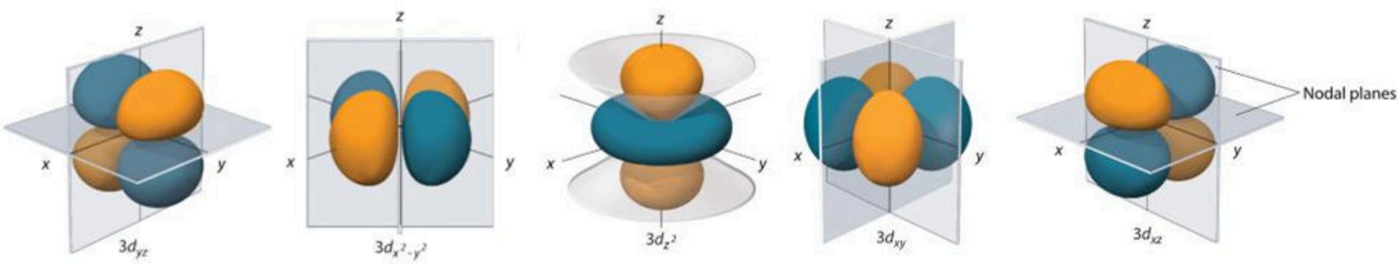



y
x
x^2-y^2
z
x or y
z^2
y
x
xy
z
x
xz
z
y
yz

Another View of the Nodes

- **Nodes** are regions in space where the probability of finding an electron is zero.
- In p orbitals and d orbitals, we have **planar nodes** between the lobes of electron densities.
- We will take a look at s orbitals and their nodes soon...

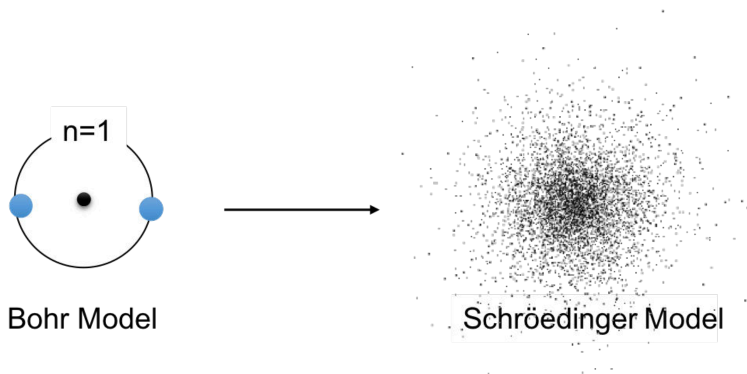




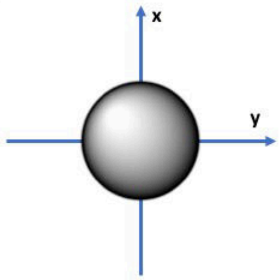
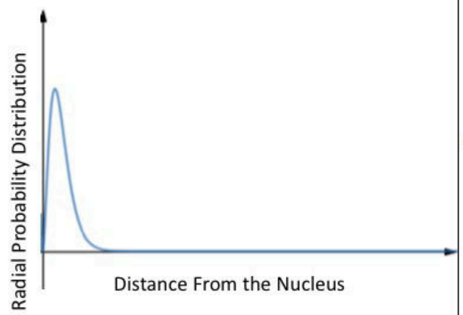
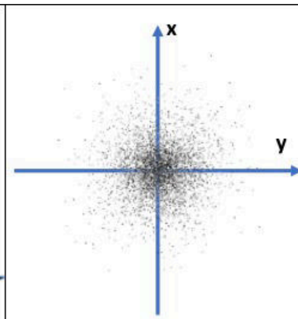
1.14.2

Wave Properties of Electrons

- Electrons have both particle and wave-like properties. Within an atom, electrons are standing waves, oscillating around the nucleus. As with all waves, there are nodes and phases.
- **Orbital:** mathematically derived region of probability in 3D space where an electron“may be” found



Representations of Atomic Orbitals

 **Boundary Diagram -** What is the shape of the area in 3D space where the electron is found?	 **Radial Probability -** What is the most probable distance the electron is from the nucleus?	 **Dot Density -** Where can the electron be within the boundary?

1.14.3

Plotting the Radial Probability

The wavefunction is a mathematical function and it can be graphed like any other function.

WIZE TIP

We will not need to know any exact values of these graphs, just their **general shape.**

The only thing you will have need to “memorize” to do these problems is how to **draw each orbital.**

Although the wavefunction has no physical meaning, the square of the wavefunction is related to the probability of finding an electron at a given point in space.

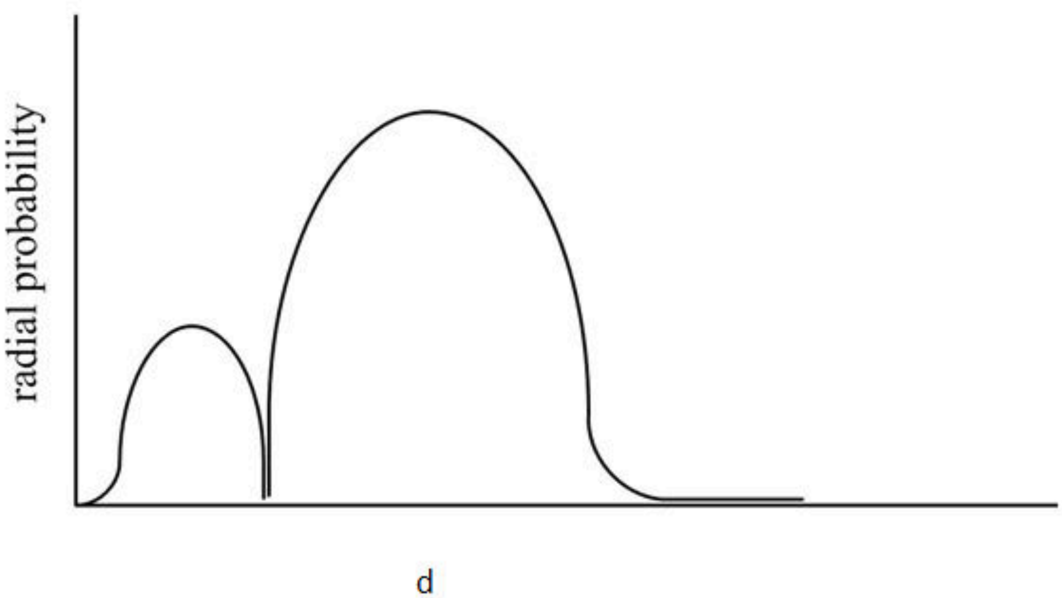
WIZE CONCEPT

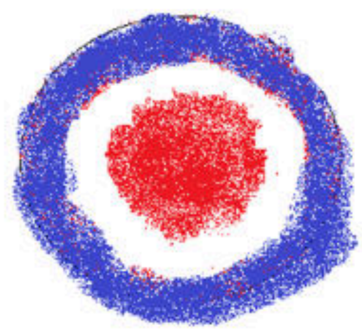
→ Each **radial node** will be indicated by a **zero point on a radial probability graph**

→ **Each graph begins at zero** (no probability of finding the electron in the nucleus)

→ **Each graph trails off to infinity** (no "edge" of an orbital")

Example: 2s Orbital





WATCH OUT!

The point where the **distance from the nucleus = 0 is NOT a radial node!**
This is a common mistake students make on exams.

Aside from that point, **every other point that touches the x axis represents a radial node!**

1.14.4

Example: Calculate the Number of Radial and Angular Nodes

How many radial and angular nodes are present in the following orbitals?

a) 7p

b) 3d

c) 4s

1.14.5

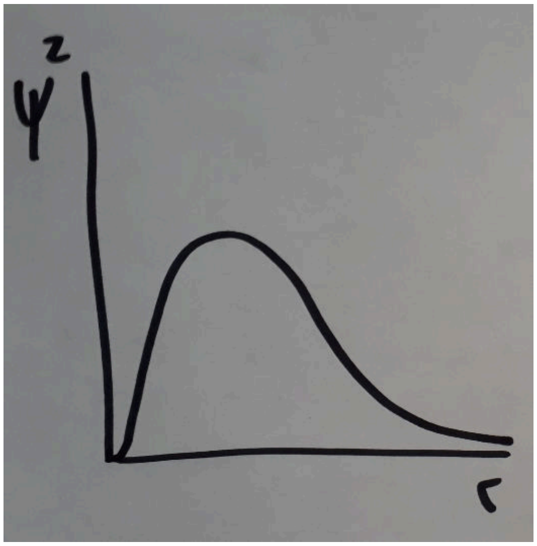
Example: Sketching Radial Probability

Sketch the radial probability of a $4d_{xy}$ orbital starting at r=0

1.14.6

Example: Identifying Orbitals from Probability Plots

Orbital X has 2 angular nodes and it's radial probability plot is shown below. Which of the following orbitals is most likely orbital X?



a) $3d_{z2}$

b)1s

c) $4p_x$

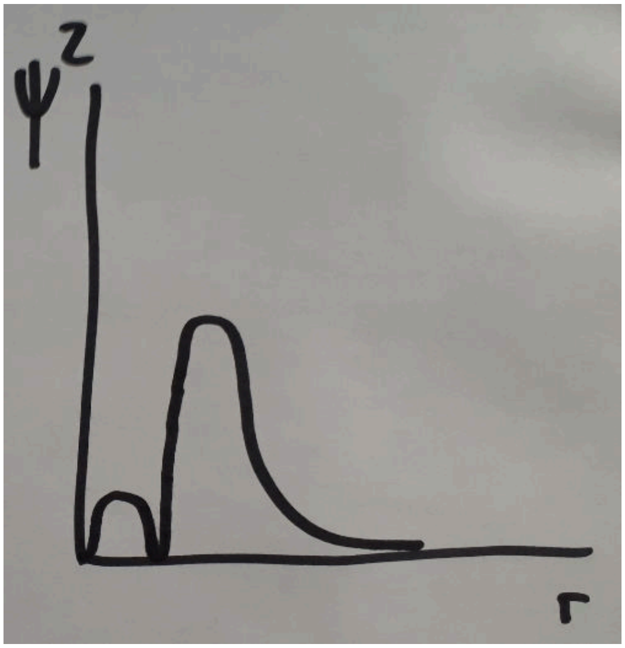
d) 3s

e) $2p_y$

1.14.7

Practice: Identifying Orbitals from Probability Plots

An orbital has only one angular node which lies along the yz plane. The radial probability plot is shown below, please identify the orbital.



- $4d_{z2}$
- $4d_{xy}$
- $3p_z$
- 2s
- $3p_x$