Bohr Model for Hydrogen

Subatomic Particles:

Particle	Symbol	Mass (u)*	Charge	Location
proton	p^+	1.007276	1+	nucleus
neutron	n	1.008665	0	nucleus
electron	e^-	0.000548	1−	orbits nucleus

* 1 u (atomic mass unit) is equal to 1.6606×10^{-27} kg

Questions:

1. Where are the electrons and how do they interact with the nucleus and each other?

2. How can the atomic line spectra be explained?

3. What is the basic for the octet rule and the bonding principles that follow?

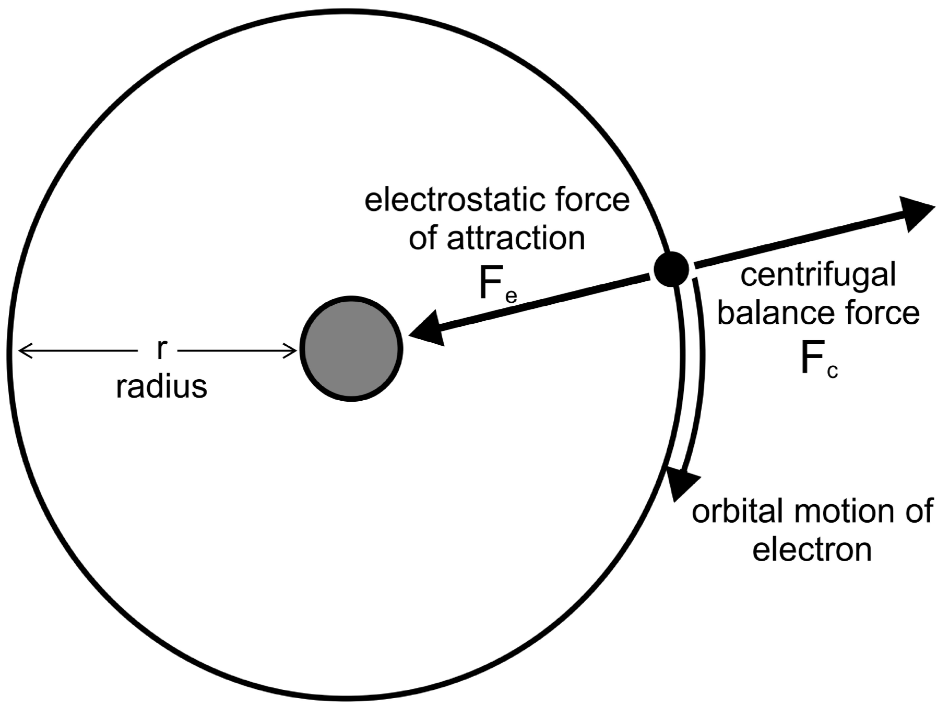
The Bohr Model of the Atom

This complex model draws on several different aspects of physics and more or less fully explains all observation about the hydrogen atom. Extrapolation to other atoms has lead to a basis from which to understand bonding principles. The components of the Bohr Model as explained here are:

I Balance of Centrifugal Force and Electrostatic Force on an Orbiting Electron
II Law of Conservation of Energy
III Properties of Light
IV Law of Conservation of Mass Energy
V Debroglie Matter Waves
VI Standing Wave Patterns
VII Bohr's Postulate
VIII Lots of Neat Math!!
IX Emission and Absorption Line Spectra for Hydrogen and the Rydberg Equation

I – Balance of Centrifugal and Electrostatic Forces

For an electron to maintain a stable orbit (does not fall into the nucleus or fly away) the forces acting on an orbiting electron must be in balance. Imagine an electron to have a circular orbit path:



In order for the electrons orbit to be stable, these two forces must exactly balance.

Electrostatic Force Equation for Point Charges:

$$F_e = \frac{q_1 q_2}{4\pi\varepsilon_o d^2}$$	F_e = electrostatic force of attraction (N) q_1 and q_2 are point charges (C) $4\pi\varepsilon_o$ = the dielectric factor ($C^2N^{-1}m^{-2}$) d = distance between the point charges (m)

For the hydrogen atom:

q_1 = e (q_1 is a proton)

q_2 = –e (q_2 is an electron)

e is a fundamental unit of charge = 1.6022×10^{-19} C

d = r (distance between nucleus and electron)

Making the above substitutions the electrostatic force equation becomes:

$F_e = \dfrac{-e^2}{4\pi\varepsilon_o r^2}$	this equation will be used again in the Law of Conservation of Energy Section

Centrifugal Force Equation:

$F_c = \dfrac{mv^2}{r}$	m = mass of electron (kg) v = velocity of electron in orbit (m/s) r = radius of electron orbit (m)

If forces are balanced to create a stable electron orbit:

$F_e + F_c = 0$	requirement for stable orbit (vector aspect of forces has been ignored)
$\dfrac{-e^2}{4\pi\varepsilon_o r^2} + \dfrac{mv^2}{r} = 0$	substitutions for F_e and F_c from above
$\dfrac{mv^2}{r} = \dfrac{e^2}{4\pi\varepsilon_o r^2}$	rearrangements
$\boxed{mv^2 = \dfrac{e^2}{4\pi\varepsilon_o r}}$	**EQUATION #1** - useful later

II - Law of Conservation of Energy:

The total energy of an electron is the sum of its kinetic energy (energy of motion) and its potential energy (energy of position):

$E_T = E_K + E_P$	law of conservation of energy

$E_T = E_{e^-}$	total energy is for an electron
$E_K = \frac{1}{2}mv^2$	standard kinetic energy equation
$E_P = F_e d$	arrived at from $W = Fd$ where $W = E_P$ for small systems
$E_P = \left(\frac{-e^2}{4\pi\varepsilon_o r^2}\right) r$	substitution from above
$E_P = \frac{-e^2}{4\pi\varepsilon_o r}$	rearrangement

Performing substitutions:

$E_{e^-} = \frac{1}{2}mv^2 - \frac{e^2}{4\pi\varepsilon_o r}$	substitution form above
$E_{e^-} = \frac{1}{2}\left(\frac{e^2}{4\pi\varepsilon_o r}\right) - \frac{e^2}{4\pi\varepsilon_o r}$	substitution using **EQUATION #1**
$\boxed{E_{e^-} = \frac{-e^2}{8\pi\varepsilon_o r}}$	total energy of an electron depending on radius only **EQUATION #2**

III - Properties of Light:

Light has a wave particle duality:

As a particle, light has single photons with a mass that can be detected by the momentum of the photon when it strikes a sensitive detector (piezoelectric effect). Each photon has a specific energy that can be expressed by Planck's equation:

$\boxed{E = h\nu}$	E = energy of a single photon (J) h = Planck's constant (6.626 x 10^{-34} Js) ν = frequency of photon (Hz = s^{-1}) **EQUATION #3**

As a wave, light can be refracted and diffracted and under the right circumstances will interfere with itself in the same manner as any other wave. The general wave equation:

$v = f\lambda$	v = velocity of traveling wave (m/s) f = frequency of wave (Hz or s^{-1}) λ = wavelength (m)
$\boxed{c = \nu\lambda}$	This equation when modified for light using: c = the speed of light (3 x 10^{8} m/s) ν = frequency of light (Hz or s^{-1}) λ = wavelength of light (m) **EQUATION #4**

IV - Law of Conservation of Mass Energy:

This famous equation was developed by Albert Einstein and implies that mass and energy of expressions of the same fundamental thing. It also suggests that mass can be converted into energy and visa vera. This equation laid the basis for discovery of the atomic bomb, the hydrogen bomb and nucleus power generation (not to mention the transporter on the "Space Ship Enterprize" .

$\boxed{E = mc^2}$	E = energy (J) m = mass (kg) c = speed of light (3 x 10^{8} m/s) **EQUATION #5**

One consequence of this equation is that light photons (which have a specific energy per photon) have a mass. This was later proven to be true experimentally.

V - deBroglie Matter Waves:

Mathematical arguments have led to the prediction of matter waves

$E = h\nu$	**EQUATION #3**
$E = mc^2$	**EQUATION #5**
$h\nu = mc^2$	equating above two equation
$c = \nu\lambda$	**EQUATION #4**
$\nu = \frac{c}{\lambda}$	rearrange
$\frac{hc}{\lambda} = mc^2$	substitution for ν
$\frac{h}{\lambda} = mc$	rearrangement
$\boxed{\lambda = \frac{h}{mc}}$	This equation indicates that light has a mass, the shorter the wavelength, the higher the energy, the faster the mass **EQUATION #6**

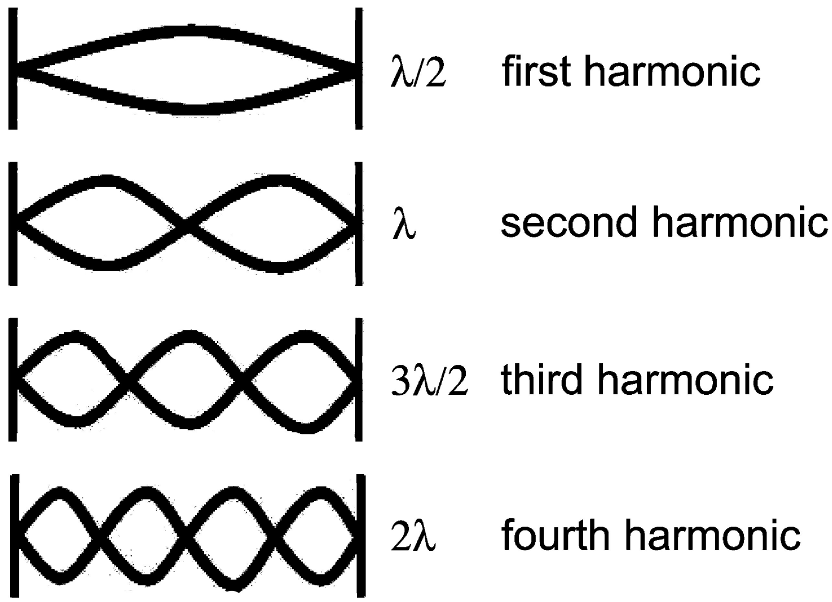
It has been shown that light has a mass as long as it is moving (light has no "rest mass"). Experimentation using electrons, neutrons, α-particles (helium nuclei) and other larger particles have demonstrated that these particles have wavelike properties. deBroglie suggested the idea of matter waves that have similar properties to light. Since these particles have rest mass, they are not capable of traveling at the speed of light and hence c must be replaced by v:

$\boxed{\lambda = \frac{h}{mv}}$	The "c" has been replaced by a "v" for velocity since the speed of small particles cannot be as fast as the speed of light. **EQUATION #7**

This establishes a relationship for the electron's mass, velocity and wavelength.

VI – Standing Wave Patterns:

A natural amplification of a wave pattern occurs when the length traveled by the wave is equal to one half wavelength ($\lambda/2$) or some multiple of $\lambda/2$. This amplification is referred to as a standing wave pattern. There are many natural examples of this (basis for all pitch on musical instruments).



VII – Bohr's Postulate:

Bohr postulated that the circular path that an electron takes while orbiting the nucleus of an atom has a length that exactly matches a deBroglie wave pattern for the electron. This allows the electron to set up a standing wave pattern as it orbits the nucleus, creating an extremely stable electron orbit. This constraint means that electrons must orbit in specific patterns. Assuming a circular orbit for the electron:

$2\pi r = n\left(\dfrac{h}{mv}\right)$	$2\pi r$ is the circumference of the orbit h/mv from **EQ #7** for deBroglie matter waves and represents one wavelength n is an integer multiple for the number of wavelenghts in the standing wave patterns

THE INTRODUCTION OF THE INTEGER N IS THE SINGLE MOST SIGNIFICANT DEVELOPMENT IN BOHR'S MODEL AND IS THE FIRST OF FOUR QUANTUM NUMBERS!!!!

Rearrangement of the above equation gives:

$\boxed{mvr = \dfrac{nh}{2\pi}}$	Standing Wave Pattern for an Orbiting Electron: m = mass of e^- (9.11×10^{-31} kg) v = velocity of e^- (m/s) r = radius of orbiting e^- (m) n = integer multiple of deBroglie wavelengths: n = 1,2,3,4,5 etc. h = Planck's constant(6.626×10^{-34}) **EQUATION #8**

VIII - Lots of Neat Math!!!

Combining the ideas and the equations from above it is possible to derive a clear mathematical representation for the allowed Bohr orbits of the electron around a hydrogen atom. This mathematics will allow us to calculate the radius of each allowed Bohr orbit and more importantly the potential energy of each orbit.

$mv^2 = \dfrac{e^2}{4\pi\varepsilon_o r}$	**EQUATION #1**
$m^2v^2r^2 = \dfrac{e^2 mr}{4\pi\varepsilon_o r}$	multiply both sides by mr^2
$(mvr)^2 = \dfrac{e^2 mr}{4\pi\varepsilon_o r}$	laws of exponents
$mvr = \dfrac{nh}{2\pi}$	**EQUATION #8**
$\left(\dfrac{nh}{2\pi}\right)^2 = \dfrac{e^2 mr}{4\pi\varepsilon_o r}$	substitution for mvr

$\dfrac{n^2h^2}{4\pi^2} = \dfrac{e^2mr}{4\pi\varepsilon_o r}$	laws of exponents
$r = \dfrac{n^2h^2 4\pi\varepsilon_o}{4\pi^2 e^2 m}$	rearrangement
$\boxed{r = \left(\dfrac{h^2\varepsilon_o}{\pi e^2 m}\right) n^2}$	This equation gives the radius of the electron orbit using constants (separated in the bracket) and as a function of n (the number of deBroglie wavelengths of the orbiting electron) **EQUATION #9**

Further calculations:

$E_{e^-} = \dfrac{-e^2}{8\pi\varepsilon_o r}$	**EQUATION #2**
$E_{e^-} = \dfrac{-e^2}{8\pi\varepsilon_o} \text{ x } \dfrac{\pi e^2 m}{h^2\varepsilon_o n^2}$	substitution for r using **EQUATION #9** above (note that reciprocal has been taken)
$E_{e^-} = \dfrac{-e^4 m}{8\varepsilon_o^2 h^2} \text{ x} \left(\dfrac{1}{n^2}\right)$	simplification

Performing numerical substitutions for all constants:

$e = 1.6022 \text{ x } 10^{-19}$ C (fundamental unit of charge)

$m = 9.110 \text{ x } 10^{-31}$ kg (resting mass of an electron)

$\pi = 3.141592653_{58979323846264338327950288419716939937510582097494459230781640628620899862803482534211706798214808651328230664709384460955058 2}$

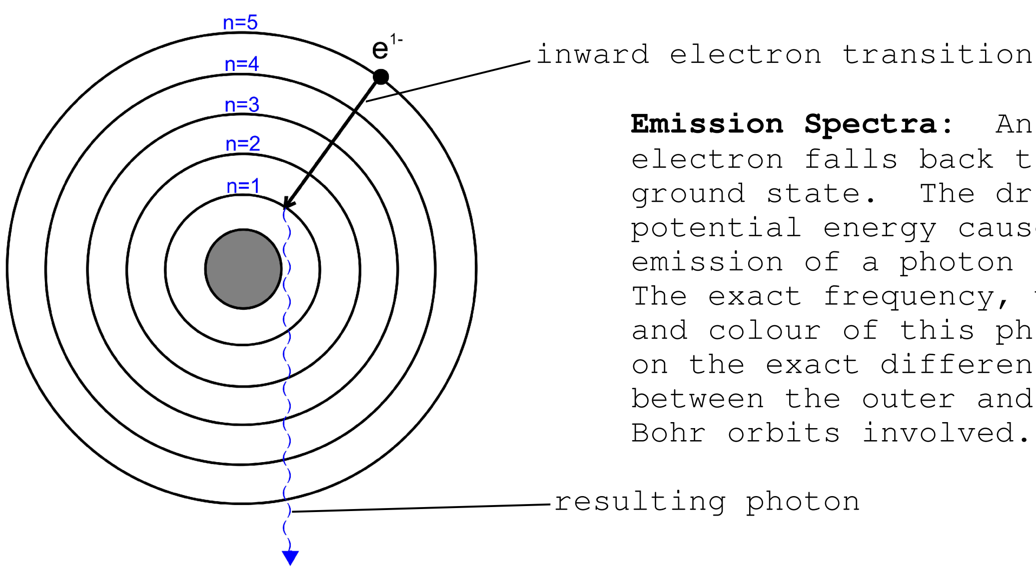
$\varepsilon_o = 8.854 \text{ x } 10^{-12}\ C^2N^{-1}m^{-2}$ (dielectric constant)

$h = 6.626 \text{ x } 10^{-34}$ Js (Planck's constant)

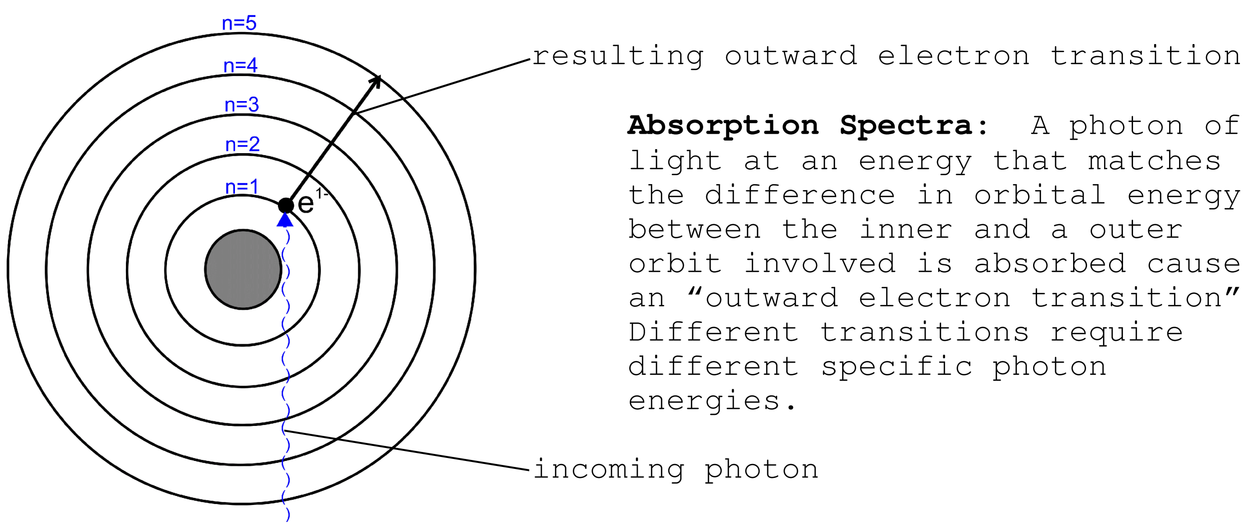
$\boxed{E_{e^-} = -2.1792 \text{ x } 10^{-18} \text{ J} \left(\dfrac{1}{n^2}\right)}$	This equation gives the energy of the electron as a function of n **EQUATION #10A**
$\boxed{E_{e^-} = -13.6 \text{ eV} \left(\dfrac{1}{n^2}\right)}$	Using 1 eV = $1.6022 \text{ x } 10^{-19}$ J, the energy is now in the unit of eV (electron volts) **EQUATION #10B**

IX – Emission and Absorption Line Spectra for Hydrogen and the Rydberg Equation

Finally one can calculate the energy and hence wavelength of light expected for any electron transition in a hydrogen atom. When the electron undergoes a transition from one Bohr orbit to another, the difference in energy will be tied to a photon of light. If the transition is the result of an exited electron falling inwards towards the nucleus, the electrons energy drops and the energy release shows up as an emission (given off) of a photon of light with a precise frequency to match the energy difference in the Bohr orbits. For the opposite process to occur, and outwards transition, energy must be added. If this energy comes from a photon of light the, again the frequency must be an exact energy match to the difference in energy between the Bohr orbits. In this case the photon is absorbed. This principle accounts for the observation of line spectra (either emission or absorption spectra).



Emission Spectra: An excited electron falls back toward the ground state. The drop in potential energy causes the emission of a photon of light. The exact frequency, wavelength and colour of this photon depends on the exact difference in energy between the outer and the inner Bohr orbits involved.



Absorption Spectra: A photon of light at an energy that matches the difference in orbital energy between the inner and a outer orbit involved is absorbed causes an “outward electron transition” Different transitions require different specific photon energies.

The energy of the electronic transition is determine by the difference in energy between the energy of the initial and final Bohr orbit.

$E_t = E_f - E_i$	E_t = energy of transition (photon energy) E_f = potential energy of final Bohr orbit E_i = potential energy of initial Bohr orbit
substituion of **EQUATION #10A** give $E_t = \left[-2.1792 \times 10^{-18}\ \text{J}\left(\frac{1}{n_f^2}\right)\right] - \left[-2.1792 \times 10^{-18}\ \text{J}\left(\frac{1}{n_i^2}\right)\right]$	
$E_t = -2.1792 \times 10^{-19}\ \text{J}\left[\left(\frac{1}{n_f^2}\right) - \left(\frac{1}{n_i^2}\right)\right]$	rearrangement
$\boxed{E_t = 2.1792 \times 10^{-19}\ \text{J}\left[\left(\frac{1}{n_i^2}\right) - \left(\frac{1}{n_f^2}\right)\right]}$	further rearrangement **EQUATION 11A**
$\boxed{E_t = 13.6\ \text{eV}\left[\left(\frac{1}{n_i^2}\right) - \left(\frac{1}{n_f^2}\right)\right]}$	change energy units from J to eV **EQUATION 11B**

Finally by combining EQUATION #3, #4 and #11A the Rydberg equation can be achieved!

$c = \nu\lambda$	**EQUATIONS #3**
$\nu = \frac{c}{\lambda}$	rearrange
$E = h\nu$	**EQUATIONS #4**
$E = \frac{hc}{\lambda}$	substitute for ν
$\frac{1}{\lambda} = \frac{E}{hc}$	rearrange

$$\frac{1}{\lambda} = \frac{2.1792 \times 10^{-18}\ J}{hc}\left[\left(\frac{1}{n_i^2}\right) - \left(\frac{1}{n_f^2}\right)\right]$$	substitution for E using **EQUATION #11A**

$$\boxed{\frac{1}{\lambda} = 1.09737 \times 10^{7}\ m^{-1}\left[\left(\frac{1}{n_i^2}\right) - \left(\frac{1}{n_f^2}\right)\right]}$$

THE RYDBERG EQUATION - EQUATION #12

This final equation known as the **Rydburg Equation** predicts the wavelength of light related to any given electronic transition between Bohr orbits. Please note that the m^{-1} is a unit, not the mass of an electron.

If the Rydberg equation give a **negative value for λ**, it means that the energy of the electron has dropped, a photon has been emitted and the electron transition is inwards **($n_f < n_i$)**.

If the Rydberg equation give a **positive value for λ**, it means that the energy of the electron has increase because a photon has been absorbed and the electron transition is outwards **($n_f > n_i$)**.

Summary of Variables and Constants

F_e = force electrostatic (N)

F_c = force centripetal (N)

q_1, q_2 = point charges (C)

ε_o = 8.854 x 10^{-12} $C^2N^{-1}m^{-2}$
(dielectric constant)

e = 1.6022 x 10^{-19} C
(fundamental charge)

m = 9.110 x 10^{-31} kg
(rest mass of an electron)

v = velocity (m/s)

r = orbit radius (m)

E_T = total energy (J)

E_K = kinetic energy (J)

E_P = potential energy (J)

E_{e-} = electron energy (J)

c = 3 x 10^8 m/s
(speed of light)

ν = frequency (Hz or s^{-1})

λ = wavelength (m)

h = 6.626 x 10^{-34} Js
(Planck's constant)

n = # of deBroglie wavelengths
(n = 1,2,3,4, etc.)

E_t = electronic transition energy (J)

E_f = energy of final orbit (J)

E_i = energy of initial orbit (J)

n_i, n_f = initial or final orbit