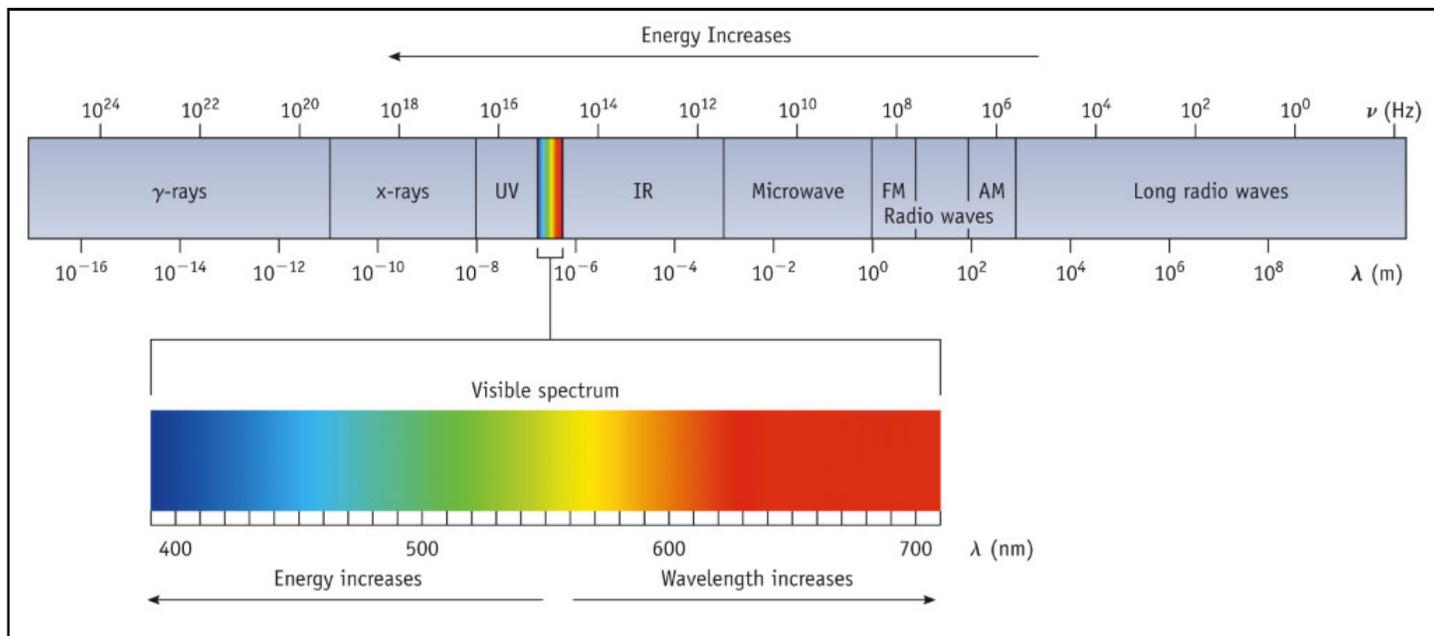


These Notes are to SUPPLEMENT the Text, They do NOT Replace reading the Text Material. Additional material that is in the Text will be on your tests! To get the most information, READ THE CHAPTER prior to the Lecture, bring in these lecture notes and make comments on these notes. These notes alone are NOT enough to pass any test! The author is not responsible for errors in these notes

## Chapter 6, The Structure of Atoms

The nucleus is composed of neutrons, protons and electrons are in the space outside of the nucleus

**Electromagnetic Radiation:** all forms of radiation are wave-like electronic and magnetic fields



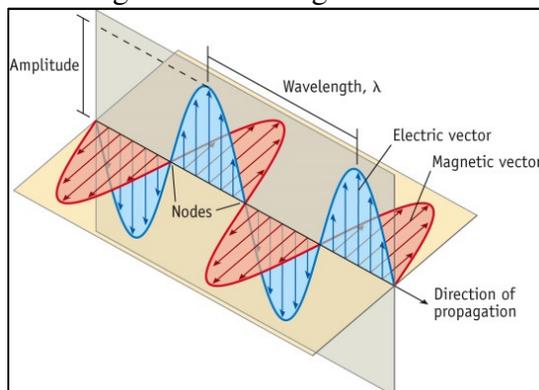
**Wavelength =  $\lambda$**  = the distance between successive high or low points on a wave. Usually expressed in meters, Nanometers or whatever!

**Frequency =  $\nu$**  = the number of waves per unit of time, usually per second. 1 wave/sec = 1/sec =  $s^{-1}$  = **hertz**

$$c = \lambda * \nu$$

$c$  ( $2.998 \times 10^8$  m/s = 186,000 miles/s) =  $\lambda$  (Wavelength in meters) \*  $\nu$  (Frequency: per second or Hertz)

**Electromagnetic Radiation** is an oscillating electric or magnetic disturbance



**Example 6.1** Cell phone frequency goes from 800 MHz to 2 GHz, what is the wavelength of a 1.12 GHz phone signal?

$$c = \lambda * \nu \quad \text{Derive: } \lambda = c / \nu$$

$$\lambda = 2.998 \times 10^8 \text{ m/s} / 1.12 \times 10^9 \text{ 1/s} = 0.268 \text{ m}$$

From the Electromagnetic Spectrum given above, note:

The Visible portion, the one that we see with our eye, is a very small portion of the spectrum

In the Visible spectrum, going from Red to Yellow to Blue, We increase in energy

We decrease in wavelength

Going from right (Radio Waves) to left (x-rays etc.)

We increase in energy

We decrease in wavelength

### Planck's Equation

As the temperature of a metal is raised, the energy of the metal and the emitted radiation increases. The max intensity (see diagram above) shifts to the left (increase in energy) to shorter wavelengths (UV). This is the cause of the change in color as the temperature is increased (Red to White hot).

Electromagnetic Radiation comes from Oscillating Atoms, each Oscillator has a Fundamental Frequency ( $\nu$ ) and the atoms can only oscillate in whole number multiples of it. Like climbing up a stairs – you can go up 1, 2, or 3 steps, but you cannot go up 1.5, 2.5 or 3.5 steps!

Atoms absorb only certain energy levels, like the flight of stairs! This is **Quantization**.

$$E = n * h * \nu$$

$$E = n \text{ (whole number freq multiplier)} * h \text{ (Planck's Const } 6.626 \times 10^{-34} \text{ Js)} * \nu \text{ (frequency in 1/s)}$$

The whole number 'n' shows how the results are a Quantized Energy, it must exist only as a whole number multiplier.

Going from a high to low energy state, energy is emitted as electromagnetic radiation

$$\Delta E = E_{\text{high}} - E_{\text{low}} = \Delta n h \nu$$

If we go from one energy level to the next lower one,  $\Delta n = 1$  and

### Plank's Equation

$$\Delta E = h \nu$$

### Einstein and the PhotoElectric Effect

Electrons are ejected when light strikes the surface of a metal, but only if the freq of light is high enough. Light has particle like properties. Light is said to consist of Photons or packets of energy. Each photon's energy is proportional to the radiation frequency defined by Plank's equation.

**CD Players** use red laser at 685 nm, what is the energy of 1 mole of photons?

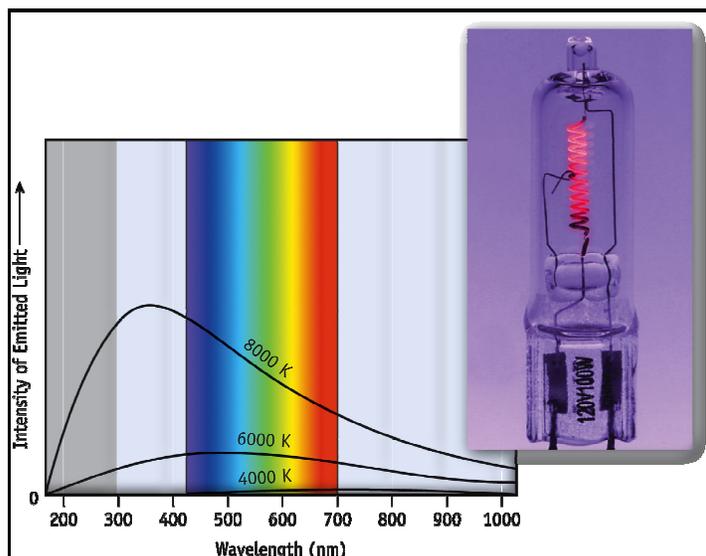
$$\text{From: } c = \lambda * \nu \quad \text{Derive: Frequency} = \nu = c / \lambda$$

$$\text{Frequency} = \nu = c / \lambda = 2.998 \times 10^8 \text{ m/s} / 685 \times 10^{-9} \text{ m} = 0.00438 \times 10^{17} / \text{s} = \mathbf{4.38 \times 10^{14} / \text{s}}$$

$$\text{Energy} = E = h \nu = 6.626 \times 10^{-34} \text{ Js/photon} * 4.38 \times 10^{14} / \text{s} = \mathbf{2.90 \times 10^{-19} \text{ J/photon}}$$

$$E_{\text{mole}} = 2.90 \times 10^{-19} \text{ J/photon} * 6.022 \times 10^{23} \text{ photons / mole} = \mathbf{175 \text{ kJ/mole}}$$

Blue Light ( $\lambda = 400 \text{ nm}$ )  $E_{\text{mole}}$  is 300 kJ/mole



**Ultraviolet catastrophe:** As you heat a metal to a high temperature, electromagnetic radiation is emitted with a wavelength dependent on temperature. As  $T$  increases, color goes from red to white. The maximum intensity shifts to a shorter wavelength (higher energy). In the past it was assumed that as  $T$  increased, the color would continue to shift to a lower wavelength. This did not happen, it reached a peak and then started to go towards a longer wavelength. Planck proposed that the energy is Quantized – only certain energies are valid:  $\Delta E = \Delta n h \nu$ . As the temperature is increased, the intensity of the lower wavelength increases – see graph above.

**Photoelectric Effect:** electrons are ejected when light of a certain frequency strikes a metal

(a) A photocell operates by the photoelectric effect. The main part of the cell is a light-sensitive cathode. This is a material, usually a metal, that ejects electrons if struck by photons of light of sufficient energy. No current is observed until the critical frequency is reached.

(b) When light of higher frequency than the minimum is used, the excess energy of the photon allows the electron to escape the atom with greater velocity. The ejected electrons move to the anode, and a current flows in the cell. Such a device can be used as a switch in electric circuits.

(c) If higher intensity light is used, the only effect is to cause more electrons to be released from the surface. The onset of current is observed at the same frequency as with lower intensity light, but more current flows with more intense light.

Infrared light photons at 2000 nm = ? kJ/mole. Causes molecular vibrations = heat

Red light photons at 685 nm = 175 kJ/mole

Blue light photons at 400 nm = 300 kJ/mole – can break bonds in proteins (human skin)

Ultraviolet light photons at 250 nm = (U figure this one out) – can really break bonds in proteins and causes severe skin damage.

## Atomic Line Spectra / Niels Bohr

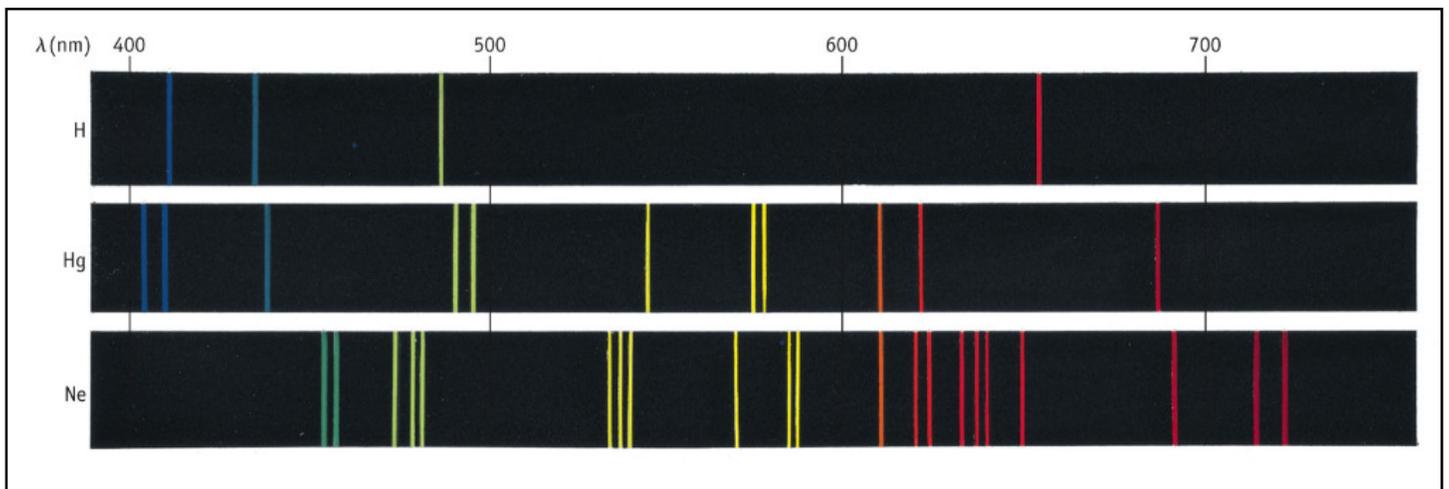
Exciting a gas with high voltage and it generates colored light

Pass this light through a prism and get colored lines of the Line Emission Spectrum

Every element has a unique Emission Spectrum

**Balmer Equation**  $1/\lambda = R(1/2^2 - 1/n^2)$   $n > 2$   $R = \text{Rydberg Const} = 1.0974 \times 10^7 \text{ m}^{-1}$

The 4 visible lines of **Hydrogen** are the Balmer Series



**Niels Bohr** postulated certain orbits correspond to particular energy levels. Levels are **quantized**  
Bohr postulated that Hydrogen had an electron moving about the center as the earth moves about the sun but in 3D.

Bohr postulated that certain orbits correspond to a particular energy level - **Quantization**

**Energy of the nth level =  $-R * h * c / n^2$**

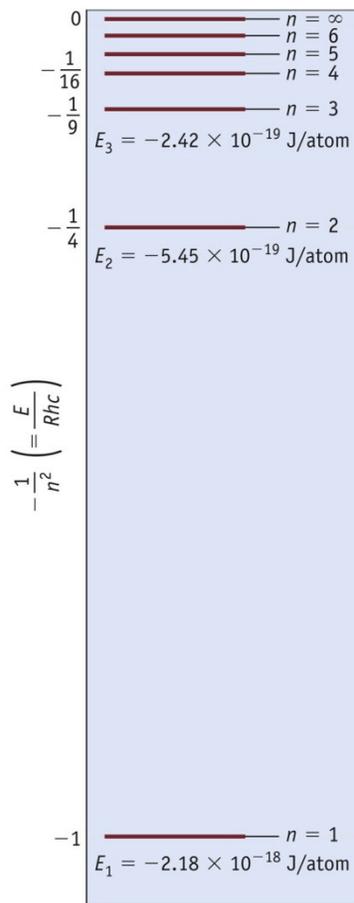
$R = \text{Rydberg const}$

$h = \text{Planck's const}$

$c = \text{speed of light}$

$n$  is the Principal Quantum Number and defines the energies of the allowed orbits

- The quantum number  $n$  defines the energies of the allowed orbits in the H atom
- The energy of an electron is negative because the electron in an orbit has lower energy than when it is free, or  $n = \infty$  the electron is separated from the nucleus
- Lowest possible energy state is the **Ground State**
- For H, when  $n > 1$ , is called the **Excited State**
- Energy is related to  $1/n^2$ , the energy levels are progressively closer together as  $n$  increases



**Bohr Theory:** An electron moves from one energy level to another, energy must be absorbed or evolved. An electron in  $n=1$  orbit is closest to the nucleus and has the lowest (most negative) energy.

**Example 6.2** Calculate the energy to move an e- from  $n=1$  to  $n=2$ , what is the difference in energy

For  $n=1$

$$-R \cdot h \cdot c / n^2 = - (1.0974 \times 10^7 \text{ m}^{-1} \cdot 6.626 \times 10^{-34} \text{ Js} \cdot 2.998 \times 10^8 \text{ m/s}) / 1^2 = -2.179 \cdot 10^{-18} \text{ J/atom}$$

For  $n=2$

$$-R \cdot h \cdot c / n^2 = - (1.0974 \times 10^7 \text{ m}^{-1} \cdot 6.626 \times 10^{-34} \text{ Js} \cdot 2.998 \times 10^8 \text{ m/s}) / 2^2 = -5.448 \cdot 10^{-19} \text{ J/atom}$$

$$\text{Difference} = (-0.5448 \cdot 10^{-18} \text{ J/atom}) - (-2.179 \cdot 10^{-18} \text{ J/atom}) = +1.634 \cdot 10^{-18} \text{ J/atom}$$

$$\text{Per mole of movement} = +1.634 \cdot 10^{-18} \text{ J/atom} \cdot 6.022 \times 10^{23} \text{ atoms/mole} = \mathbf{984 \text{ J/mole}}$$

$$\text{Line Emission Spectrum of H} \quad \Delta E = E_{\text{high}} - E_{\text{low}} = -Rhc (1/\text{Final}^2 - 1/\text{Initial}^2)$$

For H to go from  $n=1$  to  $n=2$ , what is  $\Delta E$ ? (See plot above)

$$\Delta E = -Rhc (1/\text{Final}^2 - 1/\text{Initial}^2) =$$

$$-1.0974 \times 10^7 \text{ m}^{-1} \cdot 6.626 \times 10^{-34} \text{ Js/photon} \cdot 2.998 \times 10^8 \text{ m/s} [ 1 / 2^2 - 1/1^2 ] =$$

$$16.4 \times 10^{-19} = \mathbf{1.64 \times 10^{-18} \text{ J / atom}}$$

$$1.64 \times 10^{-18} \text{ J / atom} \cdot 6.022 \times 10^{23} \text{ atoms / mole} = \mathbf{984 \text{ kJ/mole}}$$

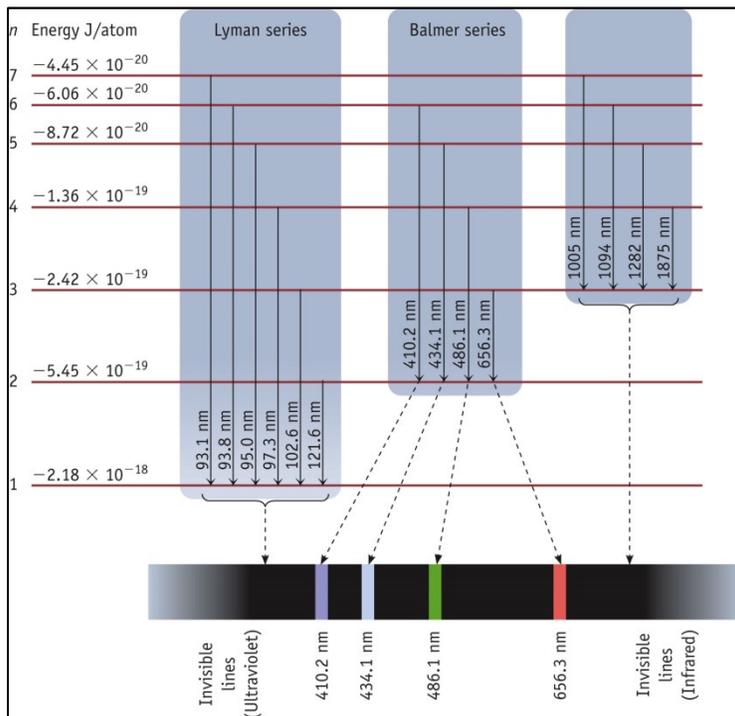
Going from a low  $n$  state to a higher  $n$  state, you must put energy into the system

Going from a high  $n$  state to a lower  $n$  state, energy is released by the system

So, the Line Emission spectrum of Hydrogen is from the various transitions

$$n = 2 \rightarrow n = 1 \quad n = 3 \rightarrow n = 2 \quad n = 3 \rightarrow n = 1 \quad \text{etc.}$$

These are exact energy transitions, thus show as a pure spectral line. This line represents the energy of  $\Delta E = -Rhc (1/\text{Final}^2 - 1/\text{Initial}^2)$ .

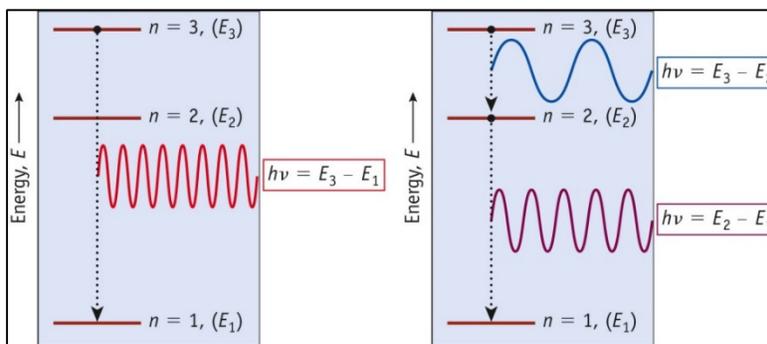


**Lyman Series:** For H, emission lines in the UV

**Balmer Series** For H, emission lines in the Visible,  $e^-$  move from  $n > 2$  to  $n = 2$

There are IR lines from transitions from  $n = 3, 4, 5 \dots$  to lower  $n$ 's.

The greater the separation of the energy levels ( $n$ ), the greater the energy, the higher the frequency



**Example 6.2** What is the wavelength of the green line in the visible spectrum of H atoms  
From the chart 2 pictures above, the green line corresponds to  $n = 4$  to  $n = 2$ .

$$\Delta E = -Rhc (1/\text{Final}^2 - 1/\text{Initial}^2) =$$

$$-1.0974 \times 10^7 \text{ m}^{-1} * 6.626 \times 10^{-34} \text{ Js/photon} * 2.998 \times 10^8 \text{ m/s} [ 1 / 2^2 - 1/4^2 ]$$

$$= 4.0874 \times 10^{-19} \text{ J/photon}$$

Taking  $E = h \cdot \nu$  and  $c = \lambda \cdot \nu$  ..or..  $\nu = c / \lambda$       **Derive:  $E = h c / \lambda$**

From:  $E = h c / \lambda$       **Derive  $\lambda = h c / E =$**

$$6.626 \times 10^{-34} \text{ Js/photon} \cdot 2.998 \times 10^8 \text{ m/s} / 4.0874 \times 10^{-19} \text{ J/photon} = 4.8599 \times 10^7 \text{ m} =$$

$$4.860 \times 10^7 \text{ m} \cdot 1 \times 10^9 \text{ nm/m} \quad \mathbf{486. \text{ Nm}}$$

#### 6.4 Particle-Wave Duality      DeBroglie $\lambda = h / mv$

An electron with a mass of m, moving with a velocity of v will have a wavelength of  $\lambda$

Wavelength properties only for particles of extremely small mass such as protons, electrons, neutrons – as h is very small ( $h = \text{Planck's Const } 6.626 \times 10^{-34}$ ), mv must be small for the wavelength to be large.

A 114 g baseball traveling at 110 mph:  $\lambda = h / mv = 6.626 \times 10^{-34} / 5.6 \text{ kg m/s} = 1.2 \times 10^{-34} \text{ m}$

**Fireworks.** Potassium salts are used instead of sodium salts because the yellow spectral line of sodium will overwhelm any other colors. Sodium salts are hydroscopic – they absorb water.

White light is from Magnesium or Aluminum

Yellow light is from Sodium

Red light from Strontium

Green light from Barium

Blue light from Copper salts

**Wave-Particle Duality:** Electrons can behave as particles and/or waves

Particle:      Electrons in a Cathode Ray Tube (Old style TV) impact a screen gives a flash of light

Wave:          Electrons possess diffraction properties (advanced physics)

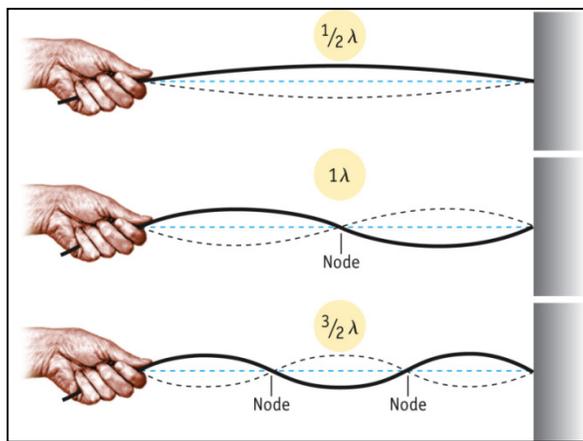
**Example 6.4** What is the wavelength ( $\lambda$ ) associated with an electron of mass  $9.109 \times 10^{-28} \text{ g}$  traveling at 40.0 % of the speed of light.

$$\lambda = h / mv = 6.626 \times 10^{-34} \text{ kg m}^2/\text{s}^2(\text{s}) / 9.109 \times 10^{-28} \text{ g} \cdot 1 \text{ kg} / 10^3 \text{ g} \cdot 0.400 \cdot 2.998 \times 10^8 \text{ m/s} =$$

$$0.6065 \times 10^{-11} = \mathbf{6.07 \times 10^{-12} \text{ m}}$$

#### 6.5 Quantum Mechanics

**Erwin Schrodinger** a German Scientist, explained the behavior of electrons in atoms and called it Quantum Mechanics or Wave Mechanics.



An electron is like a **standing wave** – see the string above

If you get it vibrating you can have one, two or three standing waves

Each of these waves are **Quantized** – they are of fixed wavelength.

An electron behaves like these waves and the quantum mechanical description of this wave function is denoted by the Greek symbol  $\Psi$ . His solution to the equations for wavefunctions is:

- Only certain wave functions are found to be acceptable – the energy of an electron is quantized
- The solutions for the equations for an electron in 3D space depend on 3 integers: **n, l and m**. These are called the **quantum numbers**

Looking at the vibrating string above, the area under the wave curve is the amplitude of the electron matter wave. This has a magnitude and sign (plus or minus) value. The probability of finding an electron in any tiny region of space is defined by the square of the wave function  $\Psi^2$  and is called the **probability density**.

Werner Heisenberg postulated the **Heisenberg uncertainty principal** which states: if we choose to know the energy of an electron in an atom with a small uncertainty, then we must accept a corresponding large uncertainty in its position.

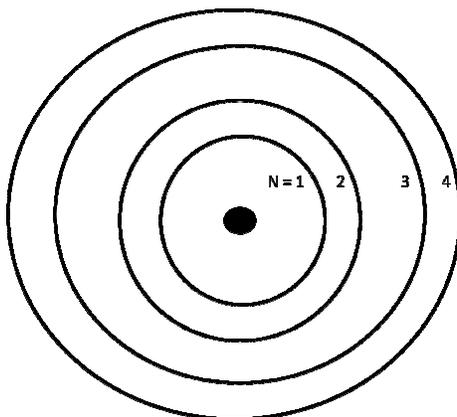
An **Atomic Orbital** is a space within which the electron is probably located.

### The Quantum Numbers

**N is the Principal Quantum Number** and has a value of 1, 2, 3...

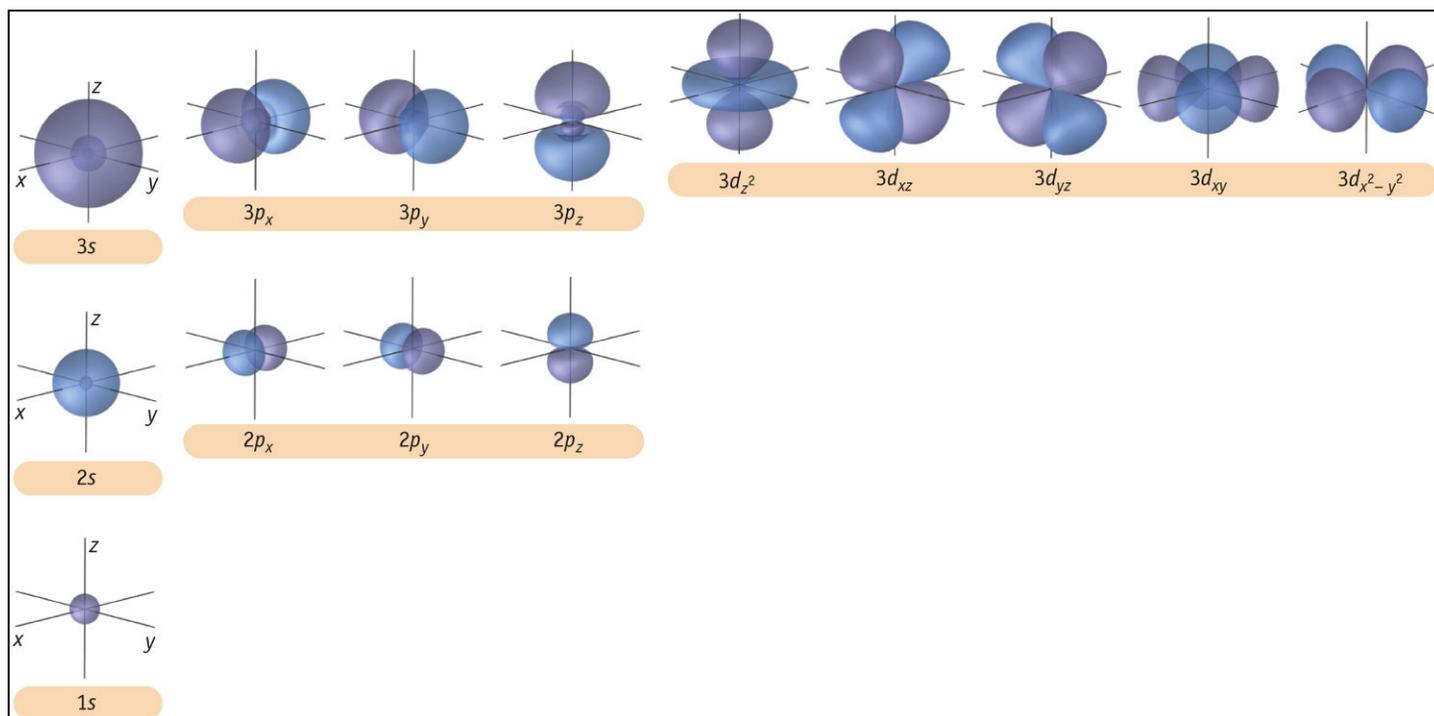
It represents the energy of an orbital – or how far from the nucleus the electron orbit is!

This area where the electron probably is located is called the **electron shell**



**l is the Orbital Angular Momentum Quantum Number** and represents the shape of the orbital

<b>l</b>	<b>Subshell Label</b>	
1	s	a sphere
2	p	3 dumbbells on x, y and z axis
3	d	4 lobes, see pic on next page
4	f	



**$m_l$  is the Magnetic Quantum Number** = 0, +1, +2, +3, ...

The range of  $m$  is  $-l$  to 0 to  $+l$

This represents the orientation or in simple terms which of the depicted shapes given above is used.

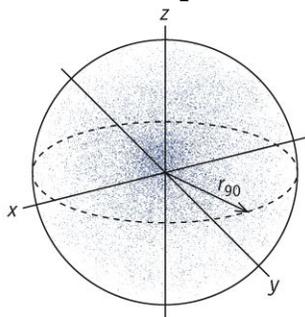
**s** had only one shape, thus only one  $m$  which is 0

**p** has 3 (look at picture above) and these represents the 3 different orientations of the dumbbell shape either in the x, y or z axis. So  $m = -1, 0$  or  $+1$

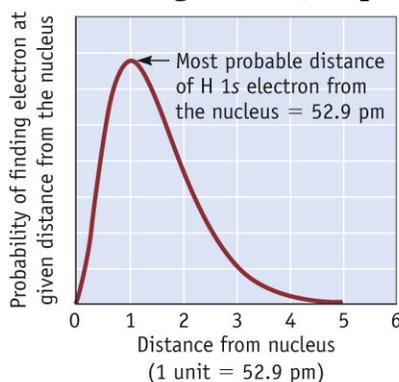
**d** has 5 shapes and these are  $m = -2, -1, 0, +1, +2$

There is also a **Spin Quantum Number,  $m_s$** , with a value of  $-1/2$  or  $+1/2$ . Each subshell can have two electrons in it, they are said to be **paired**. Each must have an opposite spin.

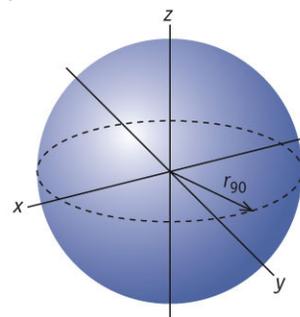
An Orbital has a probability of an electron being in that 3D space about 90% of the time.



(a) Dot picture of an electron in a 1s orbital. Each dot represents the position of the electron at a different instant in time. Note that the dots cluster closest to the nucleus.  $r_{90}$  is the radius of a sphere within which the electron is found 90% of the time.



(b) A plot of the surface density ( $4\pi r^2 \psi^2$ ) as a function of distance for a hydrogen atom 1s orbital. This gives the probability of finding the electron at a given distance from the nucleus.



(c) The surface of the sphere within which the electron is found 90% of the time for a 1s orbital. This surface is often called a "boundary surface." (A 90% surface was chosen arbitrarily. If the choice was the surface within which the electron is found 50% of the time, the sphere would be considerably smaller.)

**Table 6.1** Summary of the Quantum Numbers, Their Interrelationships, and the Orbital Information Conveyed

Principal Quantum Number	Angular Momentum Quantum Number	Magnetic Quantum Number	Number and Type of Orbitals in the Subshell
Symbol = $n$ Values = 1, 2, 3, ...	Symbol = $\ell$ Values = 0 ... $n - 1$	Symbol = $m_\ell$ Values = $+\ell$ ... 0 ... $-\ell$	$n$ = number of subshells Number of orbitals in shell = $n^2$ and number of orbitals in subshell = $2\ell + 1$
1	0	0	one 1s orbital (one orbital of one type in the $n = 1$ shell)
2	0 1	0 +1, 0, -1	one 2s orbital three 2p orbitals (four orbitals of two types in the $n = 2$ shell)
3	0 1 2	0 +1, 0, -1 +2, +1, 0, -1, -2	one 3s orbital three 3p orbitals five 3d orbitals (nine orbitals of three types in the $n = 3$ shell)
4	0 1 2 3	0 +1, 0, -1 +2, +1, 0, -1, -2 +3, +2, +1, 0, -1, -2, -3	one 4s orbital three 4p orbitals five 4d orbitals seven 4f orbitals (16 orbitals of four types in the $n = 4$ shell)

The shapes of each of the orbital's – s, p, d and f is not shown – is given above

**Paramagnetic** are elements or compounds that have unpaired electrons and are attracted by a magnet. The electrons are not aligned in the same direction

**Ferromagnetism:** the spins of the unpaired electrons are aligned in the same direction

**Diamagnetic** are elements or compounds that have all the electrons paired (two electrons with the opposite spin) and experience a slight repulsion to a magnetic field.

Discuss how and NMR and MRI work and why we do not feel pain in an MRI!

## EQUATIONS WE HAVE DISCUSSED

$$c = \lambda * \nu$$

$c$  (2.998 x 10<sup>8</sup> m/s = 186,000 miles/s) =  $\lambda$  (Wavelength in meters) \*  $\nu$  (Frequency: per second or Hertz)

### Plank's Equation

$$\Delta E = h \nu$$

$E = n * h * \nu$   $E = n$  (whole number) \*  $h$  (Planck's Const 6.626 x 10<sup>-34</sup> Js) \*  $\nu$  (frequency in 1/s)

### Balmer Equation

$$1/\lambda = R (1/2^2 - 1/n^2) \quad n > 2$$

$R = \text{Rydberg Const} = 1.0974 \times 10^7 \text{ m}^{-1}$

**Total Energy of the nth level =**  $-R * h * c / n^2$

$R = \text{Rydberg const}$

$h = \text{Planck's const}$

$c = \text{speed of light}$

Line Emission Spectrum of H

$$\Delta E = E_{\text{high}} - E_{\text{low}} = -Rhc (1/\text{Final}^2 - 1/\text{Initial}^2)$$

## 6.4 Particle-Wave Duality

**DeBroglie**  $\lambda = h / mv$