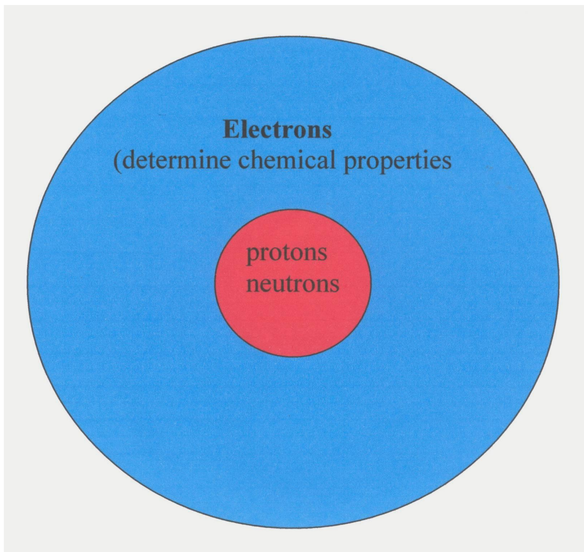
QUANTUM THEORY OF THE ATOM

- According to Rutherford's Atomic Model, an atom consists of:

    1. a very small and dense **NUCLEUS** (center)

    2. **ELECTRONS**, which surround the nucleus.

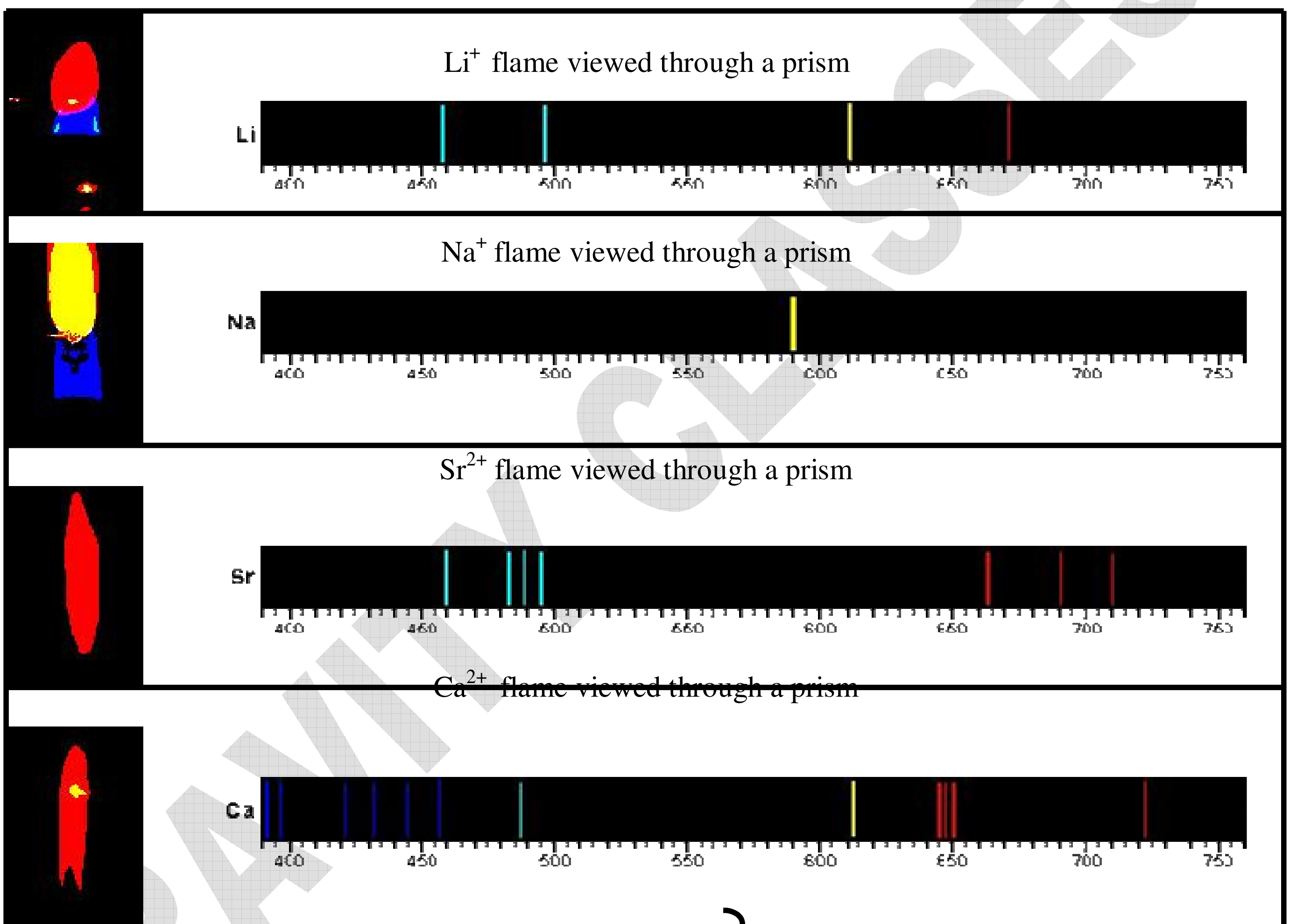


- **How are the electrons distributed around the nucleus?**

- Present knowledge of ELECTRONIC STRUCTURE (arrangement of electrons around the nucleus) is based on the study of colored flames of different metals.

ATOMIC SPECTRA

- When metal compounds burn in a flame:
  - the flame changes to a color characteristic for the element.
  - the light given off by the flame can be resolved by a prism into distinctly separated bright lines.



- The **number** of the bright lines
- The **color** of the bright lines
- The **separation** between the bright lines

} **is characteristic for every element**

- To understand the nature and origin of the light emitted by the flame tests, the nature and properties of light will be investigated.

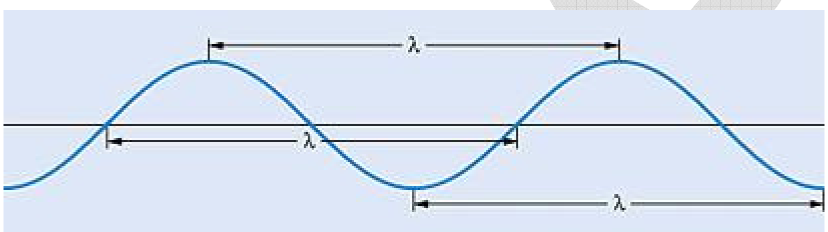
THE WAVE NATURE OF LIGHT

LIGHT:

- is a form of energy
- is considered sometimes to travel as waves
- consists of oscillations in electric and magnetic fields that can travel through space at a speed of 3.00×10^8 m/s (in vacuum)
- is referred to as a form of **ELECTROMAGNETIC RADIATION**

NOTE: Visible light, X rays, gamma rays, radio waves are all forms of electromagnetic radiation.

PROPERTIESOFWAVES



λ (lambda) = Wavelength

- is the distance between any two adjacent identical points of a wave
- is measured in units of length (m, cm, nm, Angstroms)

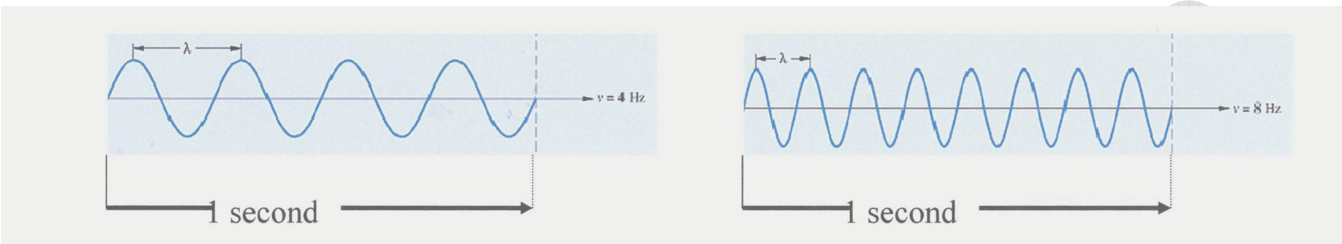
ν (nu, new) = Frequency

- is the number of waves that pass through a point in one unit of time (1 s)
- is measured in waves/second, or simply 1/second

$$\frac{1}{s} = s^{-1} = 1 \text{ Hertz} = 1 \text{ Hz}$$

Relationship between Wavelength(λ),Frequency(ν), and Energy(E)

WAVE 1 | **WAVE 2**



WAVE 1	WAVE 2
λ_1 , ν_1, E_1	λ_2 , ν_2, E_2
speed of light (c)	**speed of light (c)**

Long wavelength	($\lambda_1 = 2\lambda_2$)	**Short wavelength**	($\lambda_2 = ½\lambda_1$)
Low frequency	(ν_1 = **4 Hz**)	**High frequency**	(ν_2 = **8 Hz**)
Same speed	**(c)**	**Same speed**	**(c)**

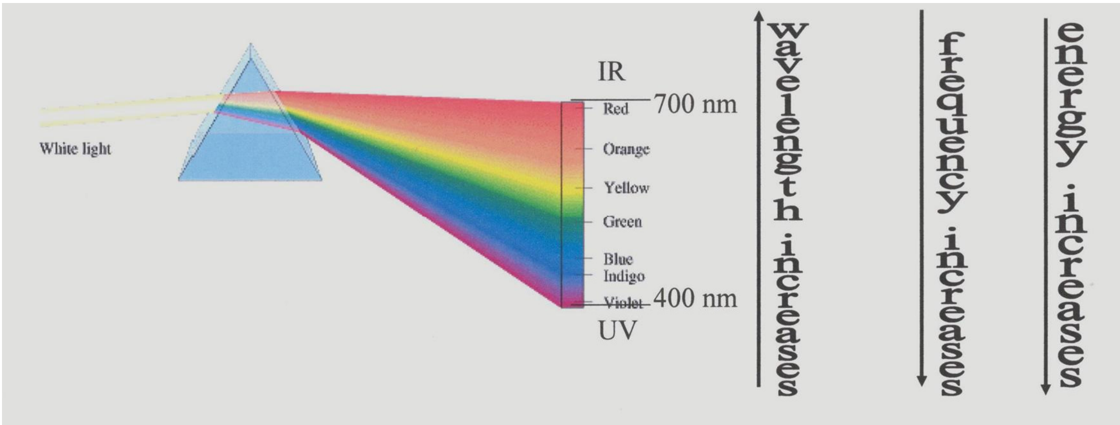
NOTE: **Wavelength(λ)andFrequency(ν)areinverselyproportional**

$$\text{Speed} = \frac{\text{distance}}{\text{time}} \qquad \text{Speed} = (\text{distance}) \times \left(\frac{1}{\text{time}}\right)$$

For Light Waves : SpeedofLight = Wavelength x Frequency

$$c = \lambda \times \nu$$

DISPERSION OF WHITE LIGHT THROUGH A PRISM



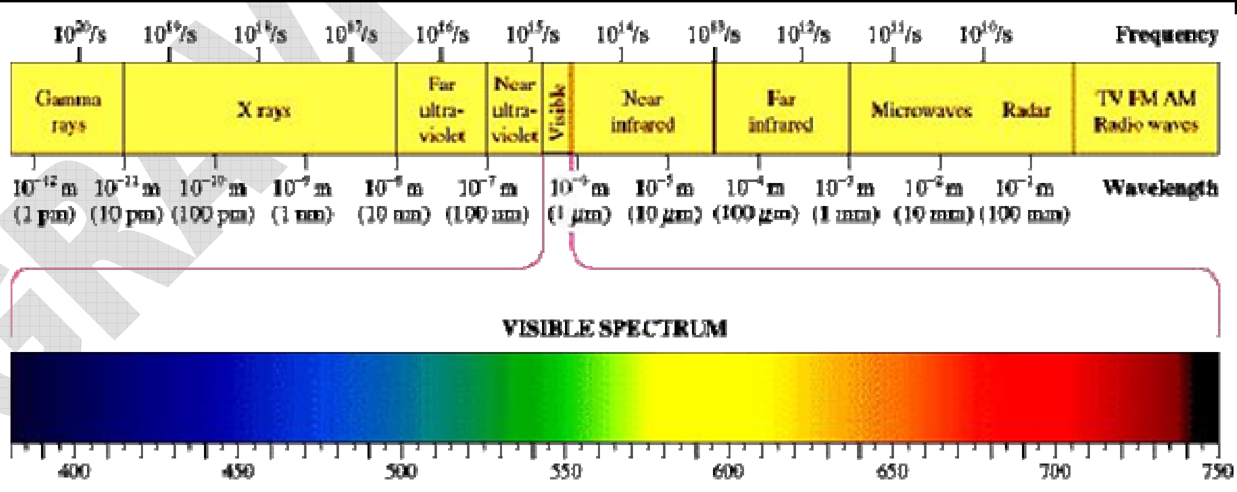
- The range of different color lights (different wavelengths) is referred to as a **SPECTRUM**
- **THE SPECTRUM OF WHITE LIGHT IS A CONTINUOUS SPECTRUM**

  Meaning: - the colors fuse together
  - there is **gradualtransition** from

- long wavelength light	to	short wavelength light
- low frequency light	to	high frequency light
- low energy light	to	high energy light

- Visible Light is only a very narrow portion of the Electromagnetic Spectrum which also contains other types of light radiations which are not visible to the human eye.

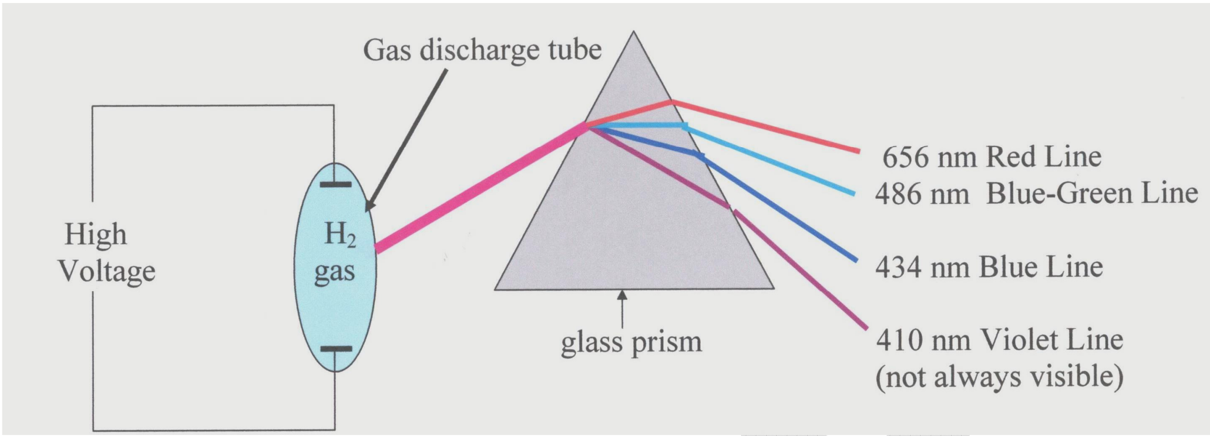
Wavelength increases



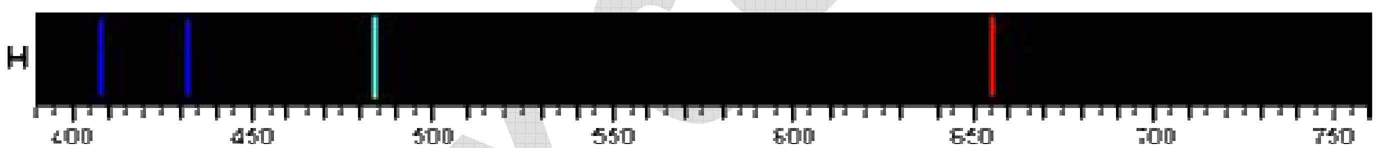
Frequency increases

Energy increases

DISPERSION OF LIGHT EMITTED BY HYDROGEN BULB THROUGH A PRISM



The Emission Spectrum of Hydrogen



<u>NOTE</u>: **The Emission Spectrum of Hydrogen is a BRIGHT LINE SPECTRUM**
The spectrum of H contains only light of specific wavelengths, frequencies and energies

Meaning:
- the light must have been emitted by H atoms that have been energized
- **the H atoms can only emit specific amounts of light energy**
- **it follows that the H atoms can only absorb specific amounts of energy**

THE RYDBERG EQUATION

- The source of lines in the emission spectrum of Hydrogen baffled scientists for many years.
- In 1885 Rydberg (a mathematician) and Balmer (a physicist) **empirically** discovered an equation which related mathematically the wavelengths of the 4 bright lines observed in the emission spectrum of Hydrogen.
- This equation is known as **RYDBERG'SEQUATION**:

$$\frac{1}{\lambda} = 1.097 \times 10^{7} \left(\frac{1}{2^2} - \frac{1}{n^2}\right) \text{ m}^{-1}$$

$$\frac{1}{2^2} = 0.25$$

n = an integer greater than 2

n = 3	**$\lambda = 6.56 \times 10^{-7}$ m**	**=**	**656 nm**	**Red Line**
n = 4	**$\lambda = 4.86 \times 10^{-7}$ m**	**=**	**486 nm**	**Blue-Green Line**
n = 5	**$\lambda = 4.34 \times 10^{-7}$ m**	**=**	**434 nm**	**Blue Line**
n = 6	**$\lambda = 4.10 \times 10^{-7}$ m**	**=**	**410 nm**	**Violet Line**

- Later Rydberg generalized his equation to include the wavelengths of those spectral lines whose wavelengths are not in the range of visible light.

GENERALIZEDRYDBERGEQUATION:

$$\frac{1}{\lambda} = 1.097 \times 10^{7} \left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right) \text{ m}^{-1}$$

where: n_1 and n_2 are integers
$n_2 > n_1$

Rydbergdidnotprovideanactualexplanationofthelinespectra

PLANCK'S QUANTIZATION OF ENERGY

- Planck's theory is based on experimental observations.

Background:

- **THE LIGHT GIVEN OFF BY A HOT SOLID VARIES WITH TEMPERATURE**

At lower temperatures (750 °C) - red light is emitted (a heated solid glows red)

At higher temperatures (1200 °C) - yellow and blue light is also emitted and mixes with the red light (the heated solid glows white)

Planck'sExplanation:

1. The atoms of the solid vibrate with a specific frequency which depends on the:
   - type of solid, and
   - temperature of the solid

2. Anatomcouldhaveonlycertainenergiesofvibration: $E=nh\nu$

   where: E = energy
   n = an integer, called quantum number (can be 1, 2, 3…)
   ν = frequency of vibration
   h = Planck's constant = 6.63×10^{-34} J . s

3. The only energies a vibrating atom can have are: $h\nu$, $2h\nu$, $3h\nu$, $4h\nu$…)

PLANCK'SCONCLUSION:

- **THEVIBRATIONALENERGIESOFTHEATOMSAREQUANTIZED**
  (the possible energies of atoms are limited to certain values)

THE DUAL NATURE OF LIGHT

- **Traditionally**: Light was considered to be made of **waves**

<u>Einsteinrationalizedthat</u>:

- If a vibrating atom changed energy (say **from 3hν to 2hν**):
    - the energy of the atom would **decrease by hν**,
    - a quantum of light energy equal to **hν would be emitted**,
    - (called this quantum of energy a **photon**)

<u>Einsteinpostulatedthat:</u>

- Light consists of quanta of energy, called photons, which are particles of electromagnetic energy (particles of light)

E=hν **where** E = energy of photon (light particle)
h = Planck's constant (6.63 x 10^{-34} J . s)
ν = frequency of light

<u>CONCLUSION</u>

<u>LIGHT HAS A DUAL NATURE</u>

PARTICLE NATURE **and** **WAVE NATURE**

This is illustrated by the formula: E = h ν

E = energy of a **light particle** (a photon)

ν = the frequency of the associated **light wave**

Examples:

1. What is the energy of a photon corresponding to radio waves of frequency $1.255 \times 10^6\ s^{-1}$?

$\upsilon = 1.255 \times 10^6\ s^{-1}$

$h = 6.63 \times 10^{-34}\ J.s$

E = ?

$E = h\upsilon$

$E = (6.63 \times 10^{-34}\ J.\cancel{s})(1.255 \times 10^6\ \cancel{s^{-1}})$

$\mathbf{E = 8.32 \times 10^{-28}\ J}$

2. Light with a wavelength of 465 nm lies in the blue region of the visible spectrum. Calculate the frequency of this light.

$\lambda = 465\ nm$

$c = 3.00 \times 10^8\ m/s$

$\upsilon = ?$

$c = \lambda \times \upsilon$

$\upsilon = \dfrac{c}{\lambda}$

$$\upsilon = \frac{3.00 \times 10^8\ \frac{\cancel{m}}{s}}{465\ \cancel{nm} \times \frac{1\ \cancel{m}}{10^9\ \cancel{nm}}} = 6.45 \times 10^{14}\ s^{-1}$$

3. What is the wavelength of microwave radiation whose frequency is $1.145 \times 10^{10}\ s^{-1}$?

$\upsilon = 1.145 \times 10^{10}\ s^{-1}$

$c = 3.00 \times 10^8\ m/s$

$\lambda = ?$

$c = \lambda \times \upsilon \qquad \lambda = \dfrac{c}{\upsilon}$

$$\lambda = \frac{3.00 \times 10^8\ \frac{m}{\cancel{s}}}{1.145 \times 10^{10}\ \frac{1}{\cancel{s}}} = 2.62 \times 10^{-2}\ m$$

4. The green line in the atomic spectrum of thallium has a wavelength of 535 nm. Calculate the **energy** of a photon of this light.

$$\lambda = 535\ \cancel{nm} \times \frac{1\ m}{10^9\ \cancel{nm}} = 5.35 \times 10^{-7}\ m$$

$c = 3.00 \times 10^8\ m/s$

$h = 6.63 \times 10^{-34}\ J.s$

E = ?

$E = h \times \upsilon \qquad c = \lambda \times \upsilon$

$\upsilon = \dfrac{c}{\lambda} \qquad \boxed{E = h \times \dfrac{c}{\lambda}}$

$$E = \frac{(6.634 \times 10^{-34}\ J\,s)(3.00 \times 10^8\ \cancel{m}/s)}{5.35 \times 10^{-7}\ \cancel{m}}$$

$\mathbf{E = 3.72 \times 10^{-19}\ J}$

BOHR'S POSTULATES

- Bohr tried to account for two phenomena that were unaccounted for in his time:
  1. The electron in the H atom does not spiral into the nucleus (the electron would continuously give off energy as it spirals into the nucleus)
  2. The line spectrum of the H atom.

Bohr'sPostulates:

1. **ENERGY-LEVEL POSTULATE**

   An electron can have only **specific energy values** in atom, called **energylevels**

   Consequence:
   - The atom can have only specific energy values.
   - Bohr derived a formula which can be used to calculate the energy values for the electron in the H atom

$$E = -\frac{R_H}{n^2}$$

where:

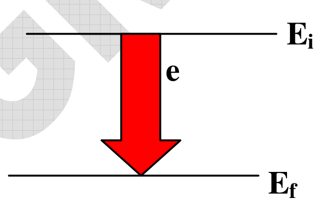
R_H = constant = 2.179 x 10^{-18} J

n = an integer, which can have the follow values: 1, 2, 3, 4, 5….∞ (also called the principal quantum number)

2. **TRANSITIONS BETWEEN ENERGY LEVELS**

   An electron in an atom can change energy only by going from one energy level to another level. The electron undergoes a transition.

   a) **Emission of Light Energy**
   - An electron in a higher energy level (**initial** energy level, $\mathbf{E_i}$) undergoes a transition to a lower energy level (**final** energy level, $\mathbf{E_f}$)



In this process, the electron loses energy, which is emitted by the atom as a photon

Result: A bright line appears in the line spectrum

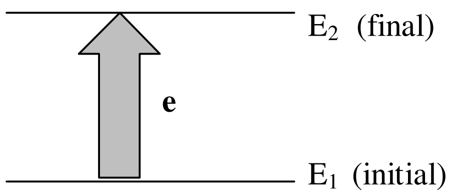
Energyoftheemittedphoton=$E_i - E_f$ =hv

b) <u>Absorbtion of Heat or Electrical Energy</u>

- Normally, the electron in the H atom exists in its lowest energy level (n = 1)

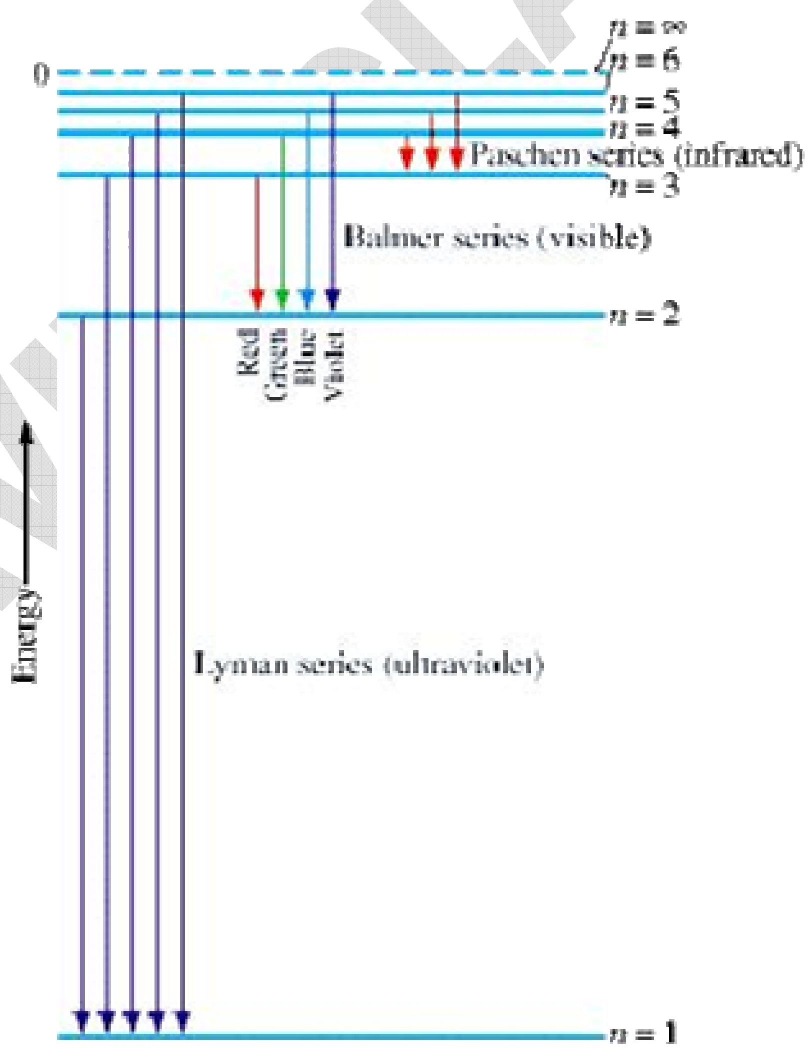
- **Togetintoahigherenergylevel,theelectronmustgainenergyorgetexcited.**

When Hydrogen gas is heated, its molecules move much faster.
High energy collision between molecules will make one atom gain energy from another, by moving the electron from the lowest energy level (E_1) to a higher level (for example E_2)



Energyabsorbed= $E_f - E_i = E_2 - E_1 = h\nu$

<u>TransitionoftheelectronintheHatom</u>



Using the concept of electron transitions, Bohr was able to reproduce Rydberg's (Balmer's) equation:

Energy of initial energy level = E_i

$$E_i = -\frac{R_H}{n_i^2}$$

n_i = principal quantum number for the initial energy level

Energy of final energy level = E_f

$$E_f = -\frac{R_H}{n_f^2}$$

n_f = principal quantum number for the final energy level

Energy of the emitted photon = $h\upsilon = E_i - E_f = \left(-\frac{R_H}{n_i^2}\right) - \left(-\frac{R_H}{n_f^2}\right)$

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

Recall: $c = \upsilon\lambda$ and therefore $\upsilon = \frac{c}{\lambda}$

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

By rearrangement:

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

By substituting:

$R_H = 2.179 \times 10^{-18}$ J $h = 6.63 \times 10^{-34}$ J.s $c = 3.00 \times 10^{8}$ m/s

$$\frac{1}{\lambda} = 1.097 \times 10^{7}\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right) m^{-1}$$

RYDBERG'S GENERALIZED EQUATION IS OBTAINED.

Examples:

1. An electron in a hydrogen atom in the level n = 5 undergoes a transition to level n = 3. What is the **frequency** of the emitted radiation?

$n_i = 5$

$n_f = 3$

$\lambda = ???$

$\upsilon = ???$

$$\frac{1}{\lambda} = 1.097 \times 10^7 \left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right) m^{-1}$$

$$\frac{1}{\lambda} = 1.097 \times 10^7 \left(\frac{1}{3^2} - \frac{1}{5^2}\right) m^{-1} \qquad \lambda =$$

$$\upsilon = \frac{c}{\lambda}$$

2. What is the difference in energy between the two levels responsible for the violet emission line of the calcium atom at 422.7 nm?

$\lambda = 422.7 \text{ nm} \times \frac{\quad}{\quad} = \qquad m$

$\upsilon = \frac{c}{\lambda} =$

$E = h\,\upsilon =$

QUANTUM MECHANICS

- Quantum mechanics is a theory that applies to extremely small particles, such as electrons.

DUALNATUREOFMATTER

Einstein: postulated that **light has a dual nature**:

Wave Properties
characterized by:
frequency and wavelength
$c = \lambda \upsilon$

Particle Properties
a particle of light, called a photon has:
Energy = E = h υ and
Momentum = mass x speed = m c

LouisdeBroglie reasoned:
- If **Light** (traditionally considered a **Wave**) → exhibits**ParticleProperties**

then
- **Matter** (traditionally considered made of **Particles**) → exhibits**WaveProperties**

- This implies, that for a particle of matter:

ENERGY of Particle of Matter = ENERGY of Wave of Matter

$$E_{\text{particle of matter}} = E_{\text{wave of matter}}$$

$$E_{\text{particle}} = mc^2$$ **(Einstein)**

$$E_{\text{wave}} = h\nu = \frac{hc}{\lambda}$$ **(Planck)**

- It follows:

$$mc^2 = \frac{hc}{\lambda} \Rightarrow mc = \frac{h}{\lambda}$$

For Light Particles

$$\lambda = \frac{h}{m\,c}$$

speed of light

For any kind of particles

$$\lambda = \frac{h}{m\,v}$$

speed of particles

NOTE:

1. Wave properties of common forms of matter are not observed because their relatively **large mass** results in a very **shortwavelengths**, which **cannotbedetected**. (in the range of 10^{-34} m)

2. Electrons, with a very **smallmass** produce **longerwavelengths** which **canbedetected** (in the range of 10^{-9})

CONCLUSION:THEELECTRONHASDUALNATURE:

- The electron has both particle and wave properties

WAVE FUNCTIONS

ErwinSchrodinger(1926)

- Based on de Broglie's work devised a theory that could be used to find the wave properties of electrons
- Established the basis of **quantum mechanics** (the branch of physics that mathematically describes the wave properties of submicroscopic particles)
- Motion is viewed differently by Classical Mechanics and by Quantum Mechanics;

Motion in Classical Mechanics:

(for example: the path of a thrown ball)

- The path of the ball is given by its position and velocity at various times
- We think of the ball as moving along a **continuouspath**

Motion in Quantum Mechanics:

For example: the motion of an electron in an atom

- The electron is moving so fast and it has such a small mass, that its **pathcannotbepredicted.**

- **Heisenberg's Uncertainty Principle** states that for particles of very small mass and moving at high speeds, it is impossible to predict:
  - the exact location of the particle at any particular time,
  - the direction in which the particle is moving

- In Bohr's theory, the electron was thought of as orbiting around the nucleus, in the way the earth orbits the sun.
- Quantum Mechanics completely invalidates this view of the motion of the electron

MOTIONOFTHEELECTRONASVIEWEDBYQUANTUMMECHANICS

1. We cannot describe the electron in an atom as moving in a definite orbit.

2. We can obtain the probability of finding the electron at a certain point in a H atom; we can say that the electron is likely (or not likely) to be at this position.

3. Information about the probability of finding the electron at a certain point is given by a mathematical expression called a **wavefunction**.

4. The wave function indicates that the probability of finding the electron at a certain position is high at some distance away from the nucleus

5. **Awavefunctionforanelectroninanatomiscalledanatomicorbital.**

CONCLUSION

- **AN ATOMIC ORBITAL IS A REGION IN SPACE WHERE THE PROBABILITY OF FINDING THE ELECTRON IS HIGH.** (A region in space where the electron is most likely to be found)