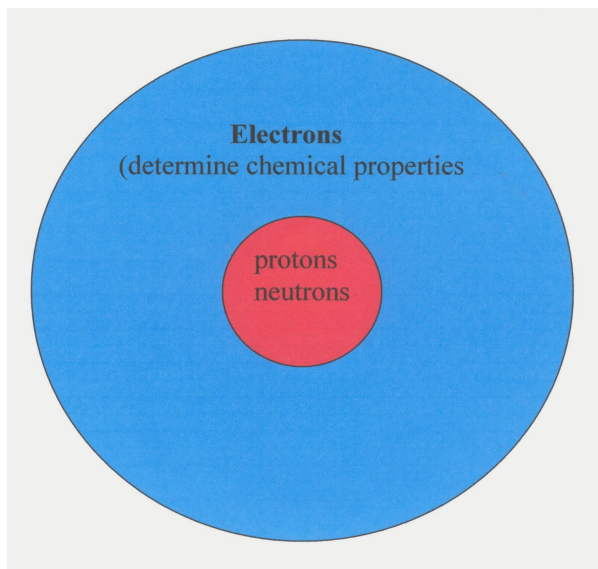


## QUANTUM THEORY OF THE ATOM

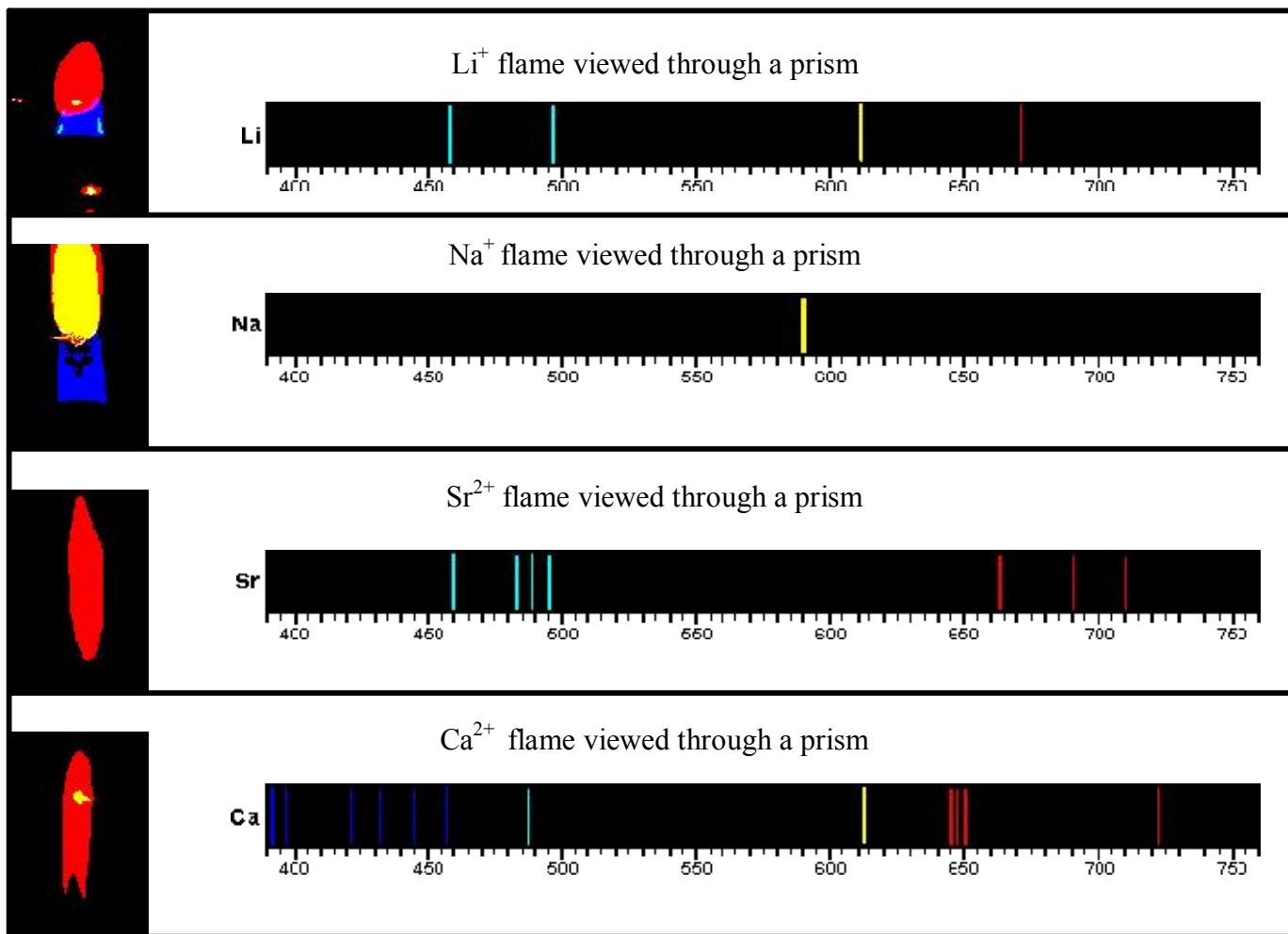
- According to Rutherford's Atomic Model, an atom consists of:
  1. a very small and dense **NUCLEUS** (center)
  2. **ELECTRONS**, which surround the nucleus.



- **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.

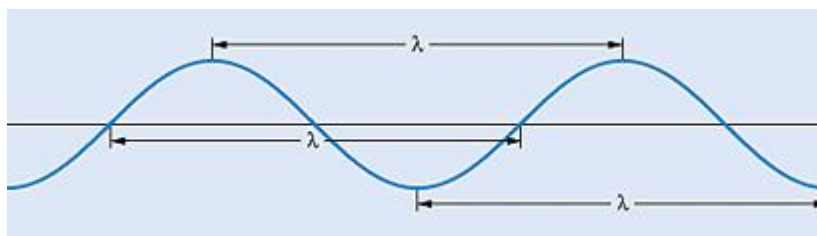
## THE WAVE NATURE OF LIGHT

### 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  $3.00 \times 10^8$  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.

### PROPERTIES OF WAVES



#### **λ (lambda) = Wavelength**

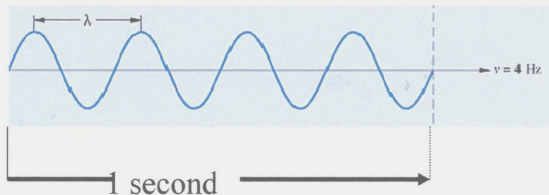
- is the distance between any two adjacent identical points of a wave
- is measured in units of length (m, cm, nm, Angstroms)

#### **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

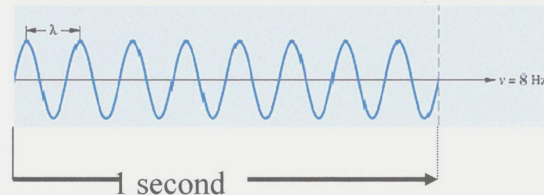
$$\frac{1}{\text{s}} = \text{s}^{-1} = 1 \text{ Hertz} = 1 \text{ Hz}$$

## Relationship between Wavelength ( $\lambda$ ), Frequency ( $\nu$ ), and Energy (E)

**WAVE 1**

$\lambda_1, \nu_1, E_1$   
speed of light (c)

**Long wavelength** ( $\lambda_1 = 2 \lambda_2$ )  
**Low frequency** ( $\nu_1 = 4 \text{ Hz}$ )  
**Same speed** (c)

**WAVE 2**

$\lambda_2, \nu_2, E_2$   
speed of light (c)

**Short wavelength** ( $\lambda_2 = \frac{1}{2} \lambda_1$ )  
**High frequency** ( $\nu_2 = 8 \text{ Hz}$ )  
**Same speed** (c)

**NOTE:** Wavelength ( $\lambda$ ) and Frequency ( $\nu$ ) are inversely proportional

$$\text{Speed} = \frac{\text{distance}}{\text{time}}$$

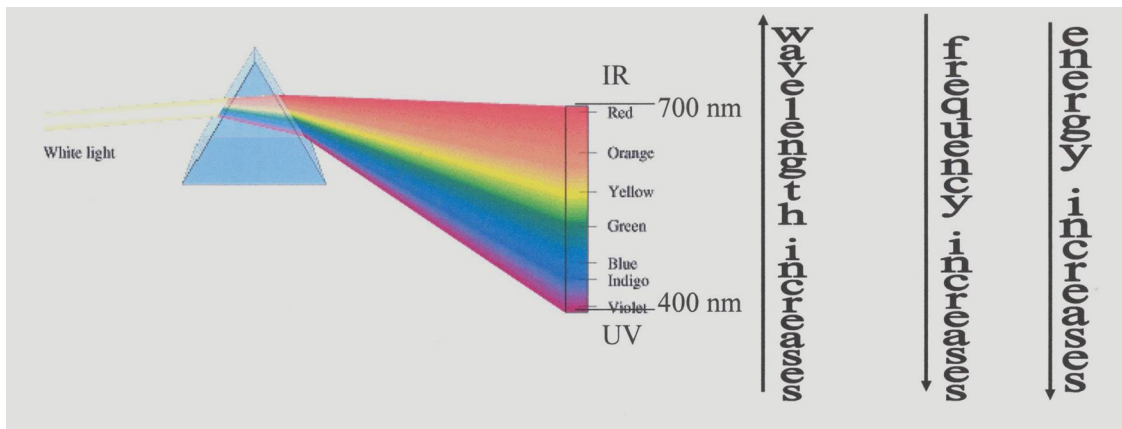
$$\begin{array}{ccccc} \text{Speed} & = & (\text{distance}) & \times & \left[ \frac{1}{\text{time}} \right] \\ \downarrow & & \downarrow & & \downarrow \end{array}$$

For Light Waves :

$$\text{Speed of Light} = \text{Wavelength} \times \text{Frequency}$$

$$\boxed{c = \lambda \times \nu}$$

**DISPERSION OF WHITE LIGHT THROUGH A PRISM**

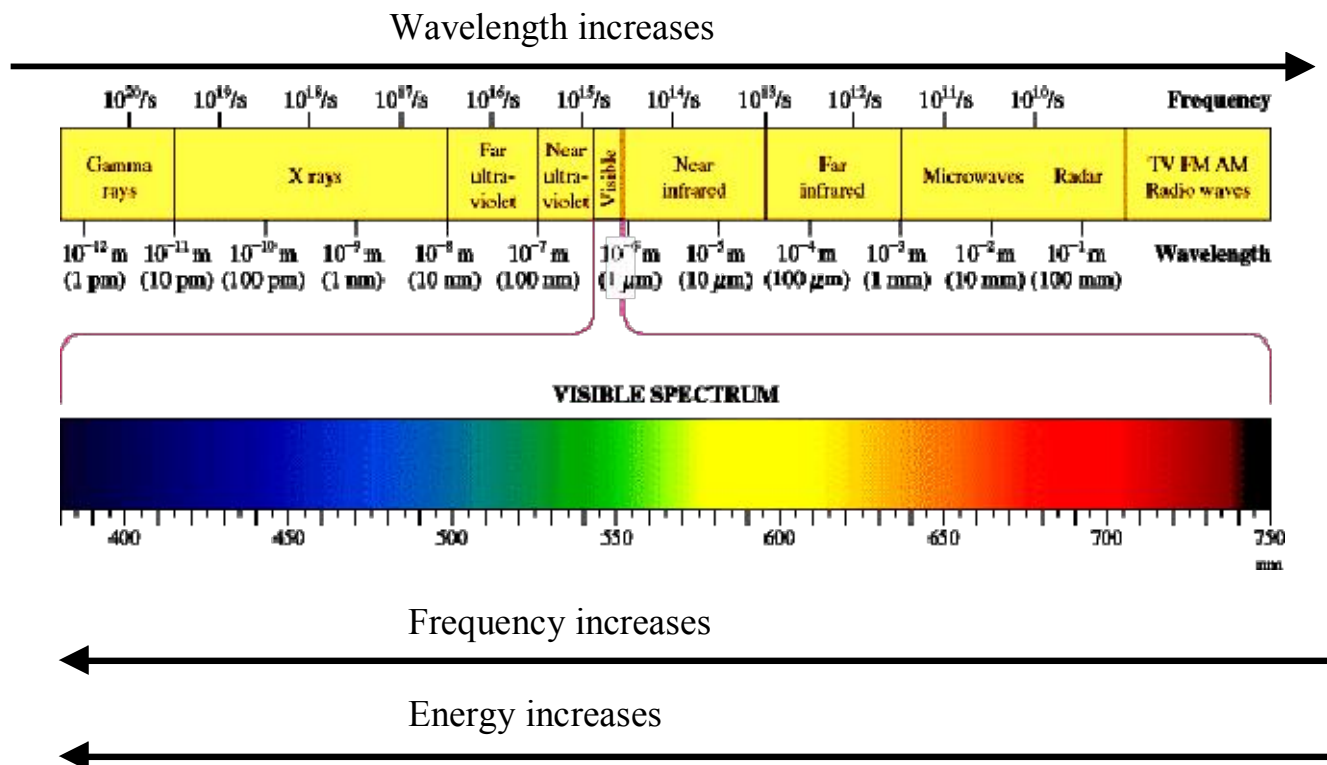


- The range of different color lights (different wavelengths) is referred to as a **SPECTRUM**
- **THE SPECTRUM OF WHITE LIGHT IS A CONTINUOUS SPECTRUM**

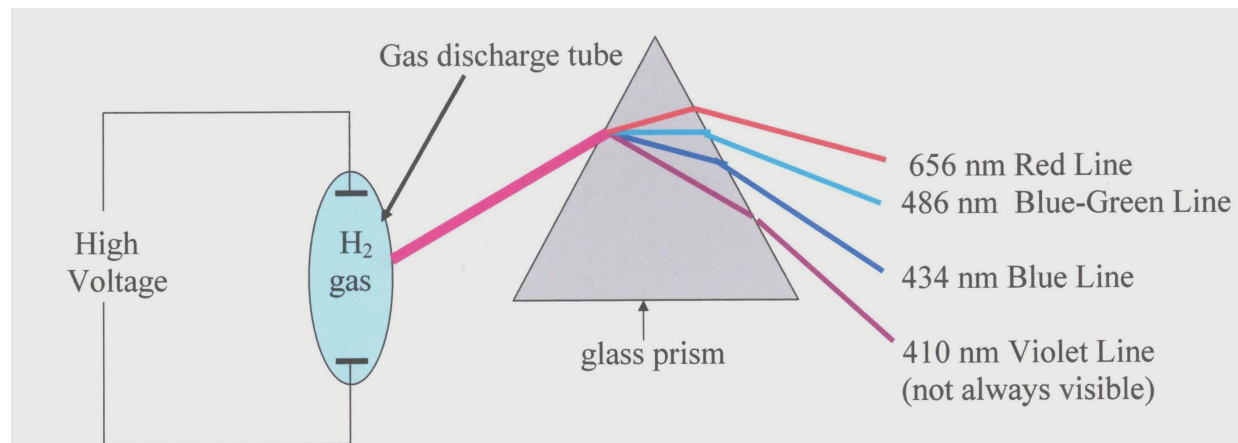
Meaning: - the colors fuse together  
 - there is **gradual transition** from

- 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.



## DISPERSION OF LIGHT EMITTED BY HYDROGEN BULB THROUGH A PRISM



**The Emission Spectrum of Hydrogen**



**NOTE:**

**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'S EQUATION**:

$$\frac{1}{\lambda} = 1.097 \times 10^7 \left( \frac{1}{2^2} - \frac{1}{n^2} \right) \text{ m}^{-1} \qquad \frac{1}{2^2} = 0.25$$

$n$  = an integer greater than 2

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

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

### GENERALIZED RYDBERG EQUATION:

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

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

**Rydberg did not provide an actual explanation of the line spectra**

**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's Explanation:

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

2. **An atom could have only certain energies of vibration:**       **$E = nh\nu$**

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

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

PLANCK'S CONCLUSION:

- **THE VIBRATIONAL ENERGIES OF THE ATOMS ARE QUANTIZED**  
(the possible energies of atoms are limited to certain values)



## THE DUAL NATURE OF LIGHT

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

### Einstein rationalized that:

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

### Einstein postulated that:

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

$$E = h\nu$$

where

$E$  = energy of photon (light particle)

$h$  = Planck's constant ( $6.63 \times 10^{-34}$  J . s)

$\nu$  = frequency of light

### CONCLUSION

**LIGHT HAS A DUAL NATURE**

**PARTICLE NATURE**

and

**WAVE NATURE**

This is illustrated by the formula:

$$E = h\nu$$

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

$\nu$  = the frequency of the  
associated **light wave**

**Examples:**

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

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

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

$$E = ?$$

$$E = h \nu$$

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

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

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

$$\lambda = 465 \text{ nm}$$

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

$$\nu = ?$$

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

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

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

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

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

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

$$\lambda = ?$$

$$c = \lambda \times \nu \quad \lambda = \frac{c}{\nu}$$

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

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.

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

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

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

$$E = ?$$

$$E = h \times \nu \quad c = \lambda \times \nu$$

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

$$E = h \times \frac{c}{\lambda}$$

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

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

## 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's Postulates:

#### 1. **ENERGY-LEVEL POSTULATE**

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

#### 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:

$$R_H = \text{constant} = 2.179 \times 10^{-18} \text{ J}$$

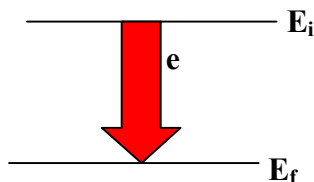
$n$  = an integer, which can have the follow values: 1, 2, 3, 4, 5... $\infty$   
(also called the principal quantum number)

#### 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,  $E_i$ ) undergoes a transition to a lower energy level (**final** energy level,  $E_f$ )



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**

$$\text{Energy of the emitted photon} = E_i - E_f = h\nu$$

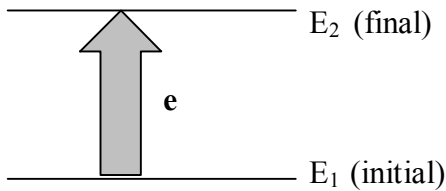
b) **Absorption of Heat or Electrical Energy**

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

- **To get into a higher energy level, the electron must gain energy or get excited.**

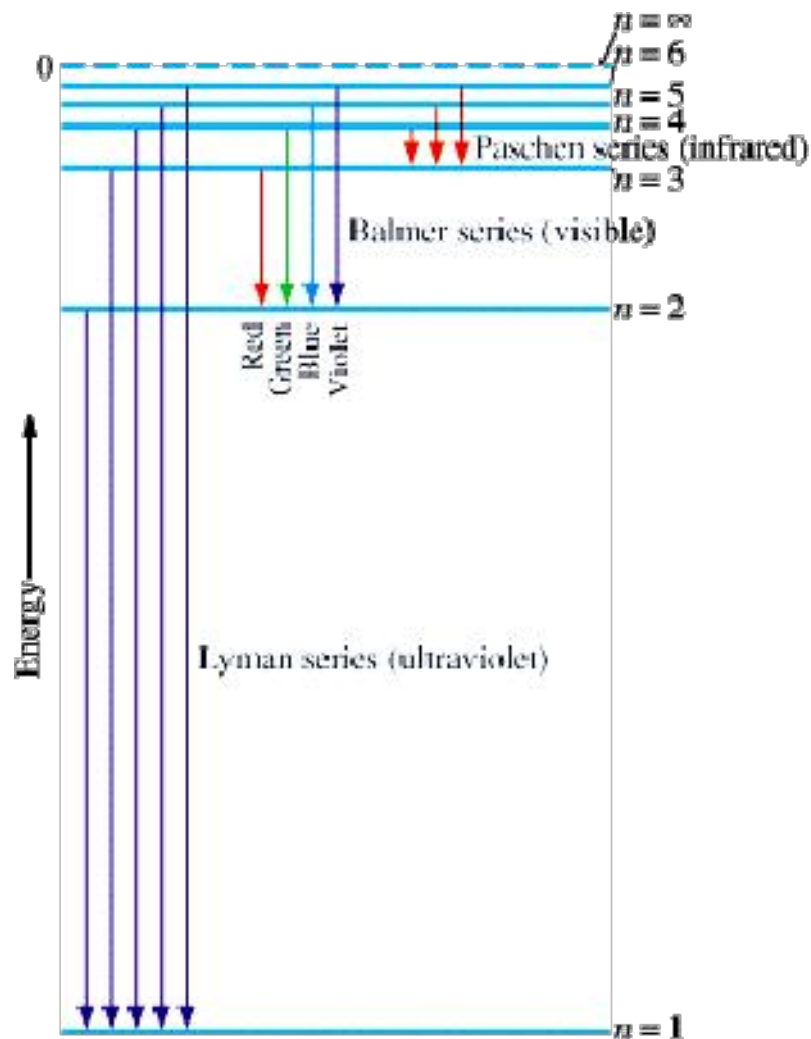
When Hydrogen gas is heated, its molecules move much faster.

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  $E_2$ )



$$\text{Energy absorbed} = E_f - E_i = E_2 - E_1 = h\nu$$

**Transition of the electron in the H atom**



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

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

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

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

$$h \frac{c}{\lambda} = R_H \left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right) \quad \text{By rearrangement:} \quad \boxed{\frac{1}{\lambda} = \frac{R_H}{hc} \left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)}$$

By substituting:

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

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

**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?

$n_i = 5$		$\frac{1}{\lambda} = 1.097 \times 10^7 \left( \frac{1}{n_f^2} - \frac{1}{n_i^2} \right) \text{ m}^{-1}$	
$n_f = 3$			
<b><math>\lambda = ???</math></b>			
<b><math>\nu = ???</math></b>		<b><math>\frac{1}{\lambda} = 1.097 \times 10^7 \left( \frac{1}{3^2} - \frac{1}{5^2} \right) \text{ m}^{-1}</math></b>	<b><math>\lambda =</math></b>
		<b><math>\nu = \frac{c}{\lambda}</math></b>	

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?

$$\lambda = 422.7 \text{ nm} \times \text{—————} = \text{—————} \text{ m}$$

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

$$E = h \nu =$$

## QUANTUM MECHANICS

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

### DUAL NATURE OF MATTER

Einstein:

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

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

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

Louis de Broglie reasoned:

- If **Light**  
(traditionally considered a  
**Wave**)



exhibits **Particle Properties**

then

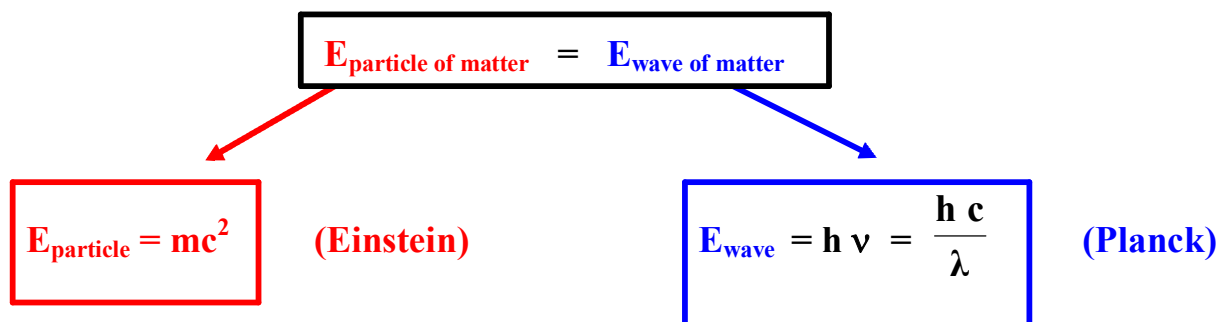
- **Matter**  
(traditionally considered  
made of **Particles**)



exhibits **Wave Properties**

- This implies, that for a particle of matter:

**ENERGY of Particle of Matter = ENERGY of Wave of Matter**



- It follows:

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

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 **short wavelengths**, which **cannot be detected**. (in the range of  $10^{-34}$  m)
2. Electrons, with a very **small mass** produce **longer wavelengths** which **can be detected** (in the range of  $10^{-9}$ )

**CONCLUSION: THE ELECTRON HAS DUAL NATURE:**

- The electron has both particle and wave properties



## WAVE FUNCTIONS

### Erwin Schrodinger (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 **continuous path**

#### **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 **path cannot be predicted.**

- **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

### **MOTION OF THE ELECTRON AS VIEWED BY QUANTUM MECHANICS**

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 **wave function**.
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. **A wave function for an electron in an atom is called an atomic orbital.**

### **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)