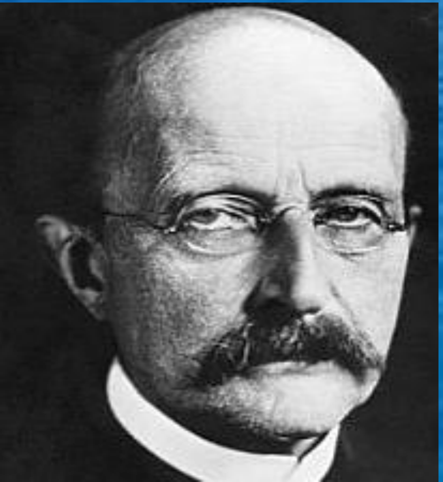
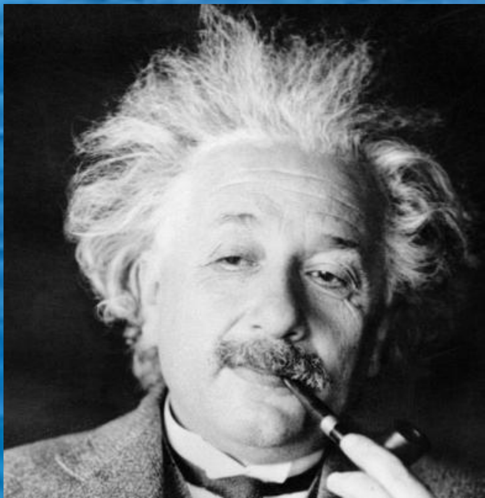
Quantum Chemistry

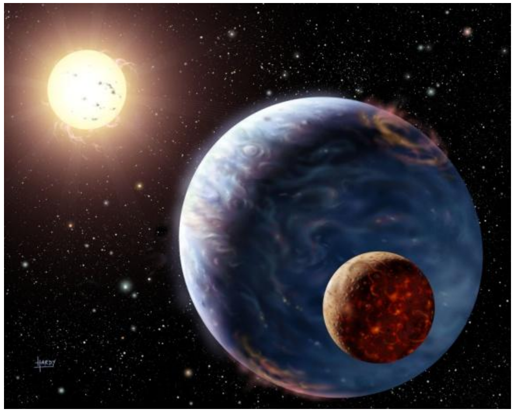




Classical mechanics and Quantum mechanics

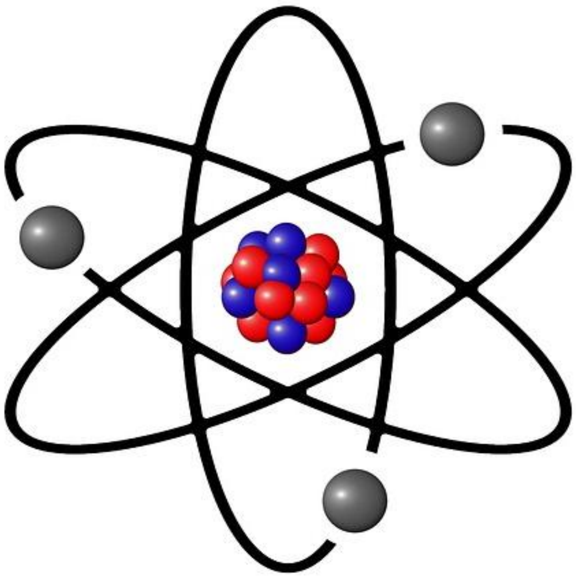
Classical mechanics (known as **Newtonian** mechanics) **describes** the **motion** of **macroscopic objects** and provides extremely **accurate results** as long as the domain of study is restricted to **large objects** and **the speeds** involved do not approach the **speed of light**.

If the **present state** of the **macroscopic object** is known, it is **possible** to **predict** by **the laws of classical mechanics how it will move in the future and how it have moved in the past**



Macroscopic objects

After the discovery of the presence of **molecules**, **atoms** and **sub-atomic particles**, a **new theories** are needed to **describe the motion** of these extremely **small objects** (**microscopic objects**) that **moves** at **very high speed** as the classical theories **failed** to **explain** many of the **phenomena** associated with these **microscopic objects**



Microscopic objects

Quantum Mechanics has much more complicated theories than **classical mechanics**, but provides **accurate results** for the **microscopic particles** and handles the wave-particle duality of atoms and molecules

- **Quantum Chemistry** is a **branch** of **chemistry** whose primary focus on the application of quantum mechanics in chemical systems. It is also called molecular quantum mechanics

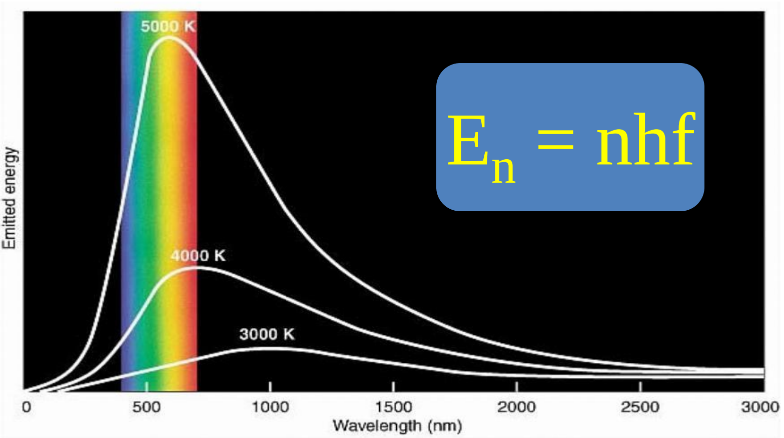
- Quantum chemistry answer questions such as

Why the chemical changes occurs? **How chemical changes occurs**?

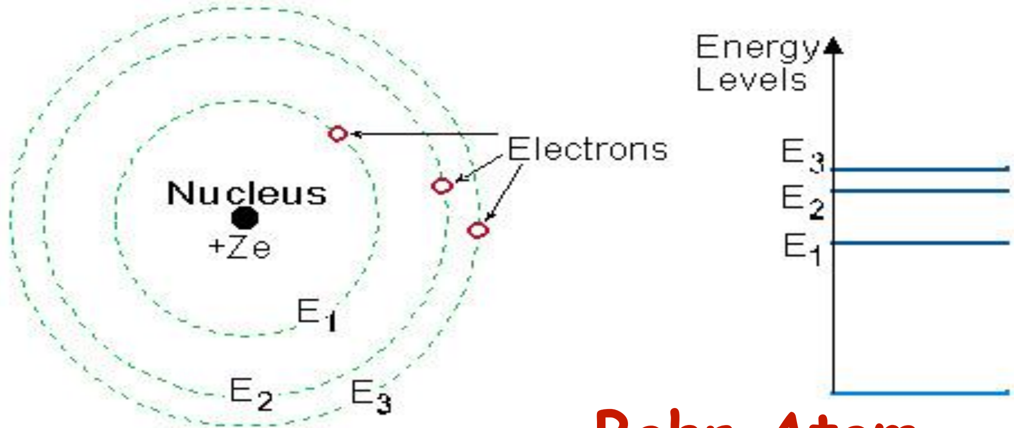
- Quantum mechanics can be applied for both macro and microscopic **objects**, and the **classical mechanics** can be considered as a **special case** of **quantum mechanics**

- Quantum chemistry is now essential for the **understanding** of the **results** of the **chemical experiments** in all chemistry branches

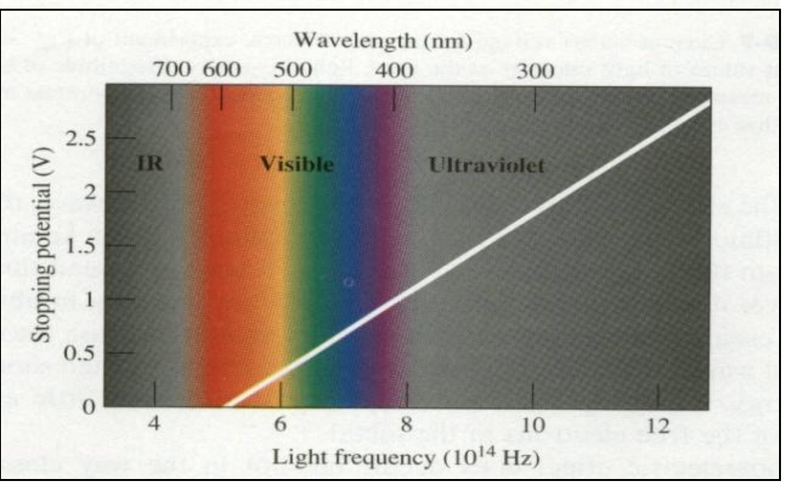
Origin of Quantum Theory



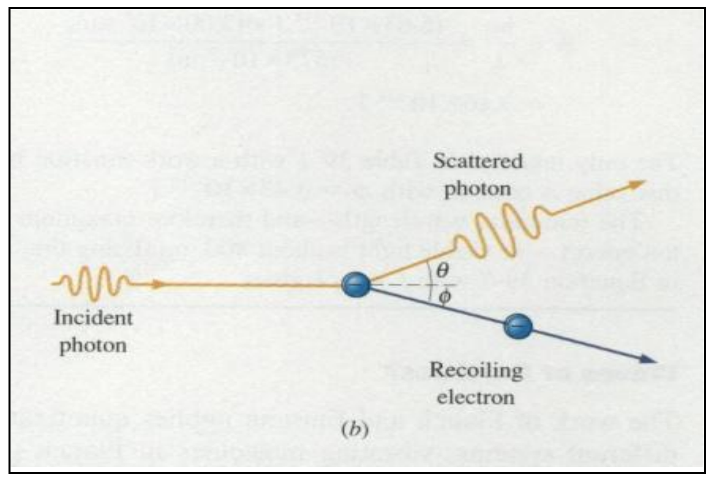
Black body Radiation
Planck (1900)

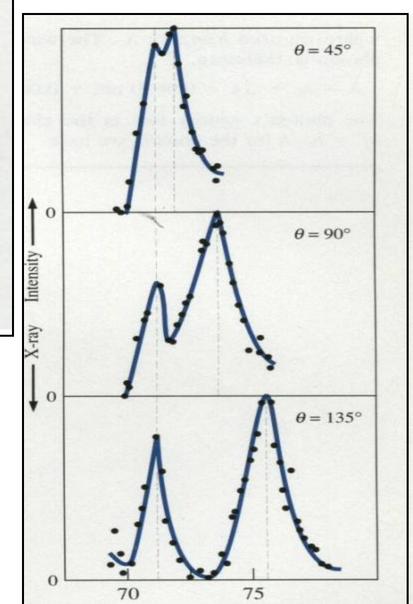


Bohr Atom
N. Bohr (1911)



Photoelectric Effect
A. Einstein
(1905)





Compton scattering
Compton
(1923)

Origin of Quantum Theory

- While the **classical 'mechanical theory'** of **matter** considered matter to be made of **discrete particles** (**atoms, electrons, protons** etc.), another theory called the '**Wave theory**' was necessary to interpret the **nature** of **radiations** like **X-rays** and **light**.

- According to the **wave theory**, **radiations** as **X-rays** and **light**, consisted of **continuous collection of waves travelling in space.**

- The **wave nature** of **ligh**t, however, **failed completely** to **explain** the **photoelectric effect** i.e. the **emission** of **electron** from **metal surfaces** by the action of **light**.

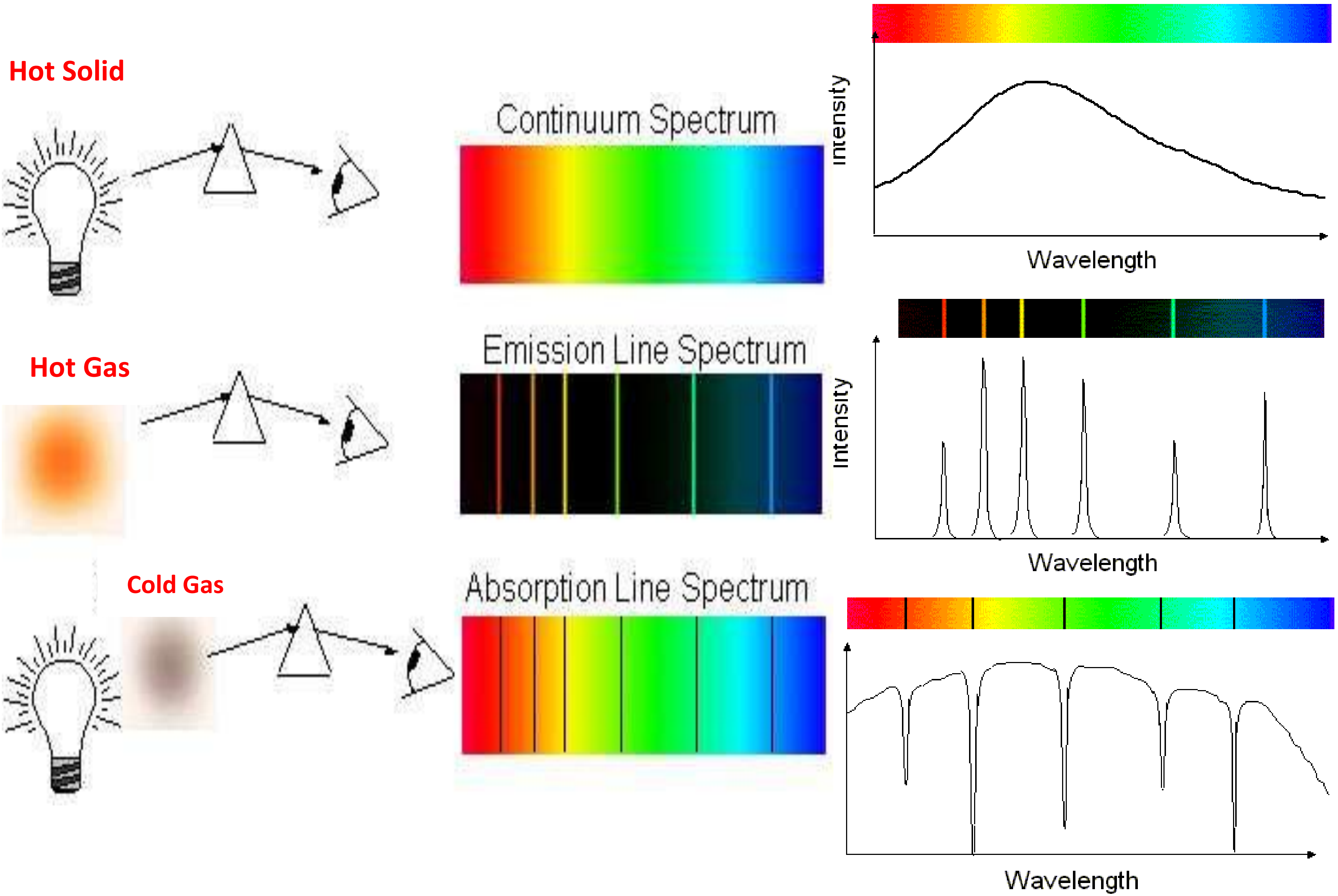
Origin of Quantum Theory

- In their attempt to find a plausible **explanation** of **radiations** from **heated bodies** as also the **photoelectric effect**, **Planck** and **Einstein** (1905) proposed that **energy radiations**, including those of **heat** and **light**, are **emitted discontinuously** as **little** **quanta**, or **photons**.

- According to it, **light** **exhibits** both a **wave** and a **particle nature**.

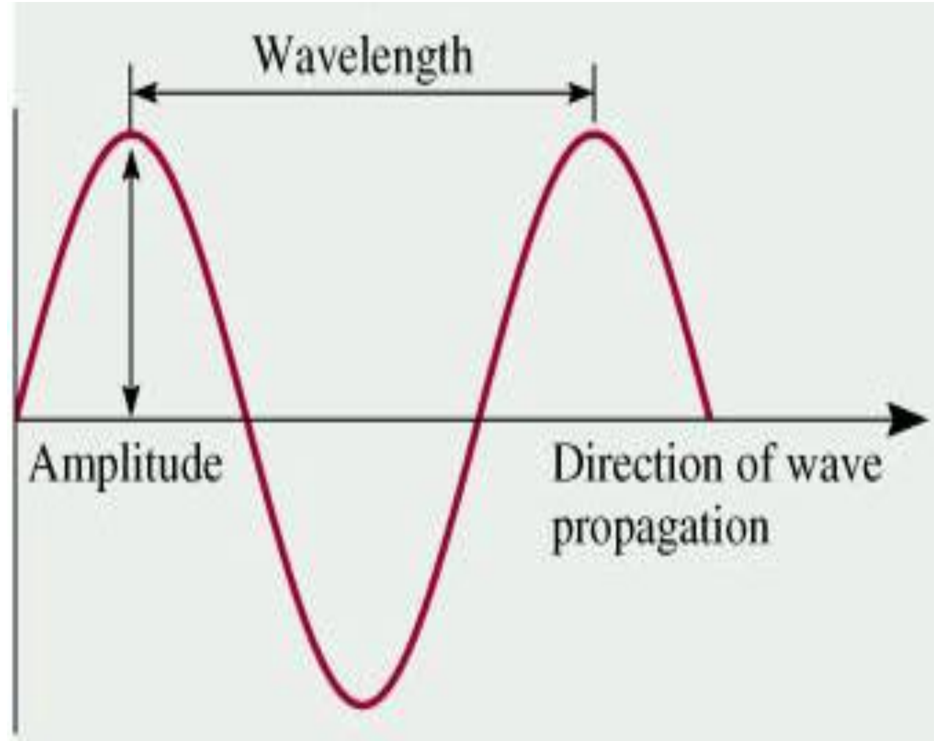
- This theory which **applies** to all **radiations**, is often referred to as the '**Wave Mechanical Theory**'.

Introduction to Radiation



Waves

Wavelength (λ) is the distance between identical points on successive waves



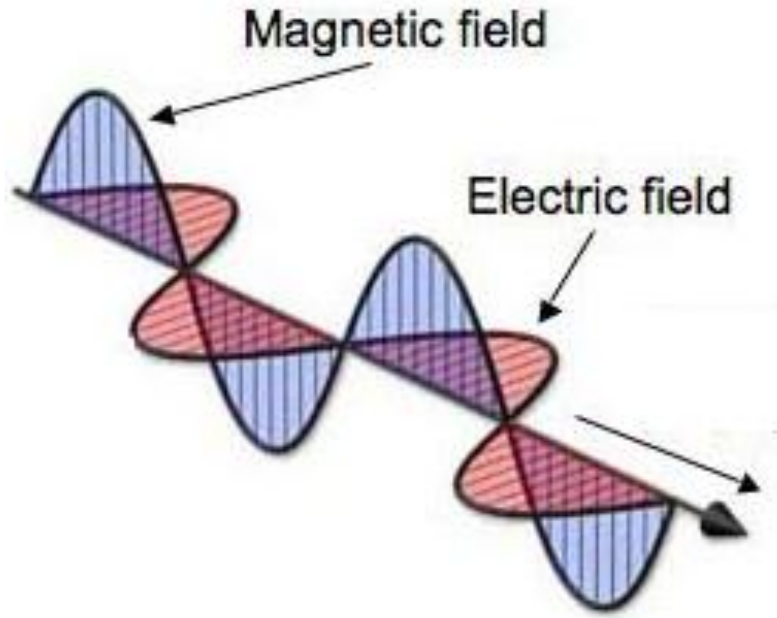
Wave amplitude is the vertical distance from the midline of a wave to the peak

Frequency (ν) is the number of peaks that pass at a given point in a second

Speed of wave = Frequency x Wavelength = λ ν

Electromagnetic waves

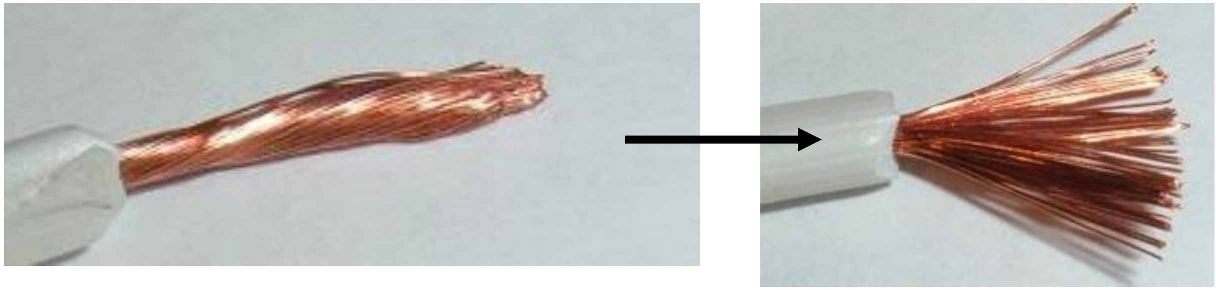
► **Electromagnetic radiations** the emission and transmission of <u>energy</u> in the form of electromagnetic waves

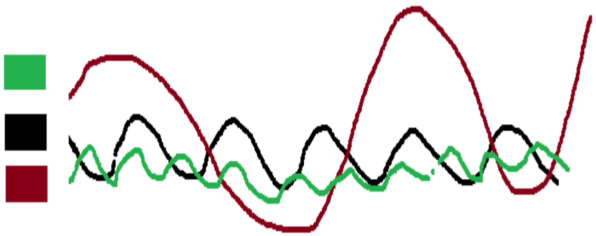


► For all **electromagnetic radiation**

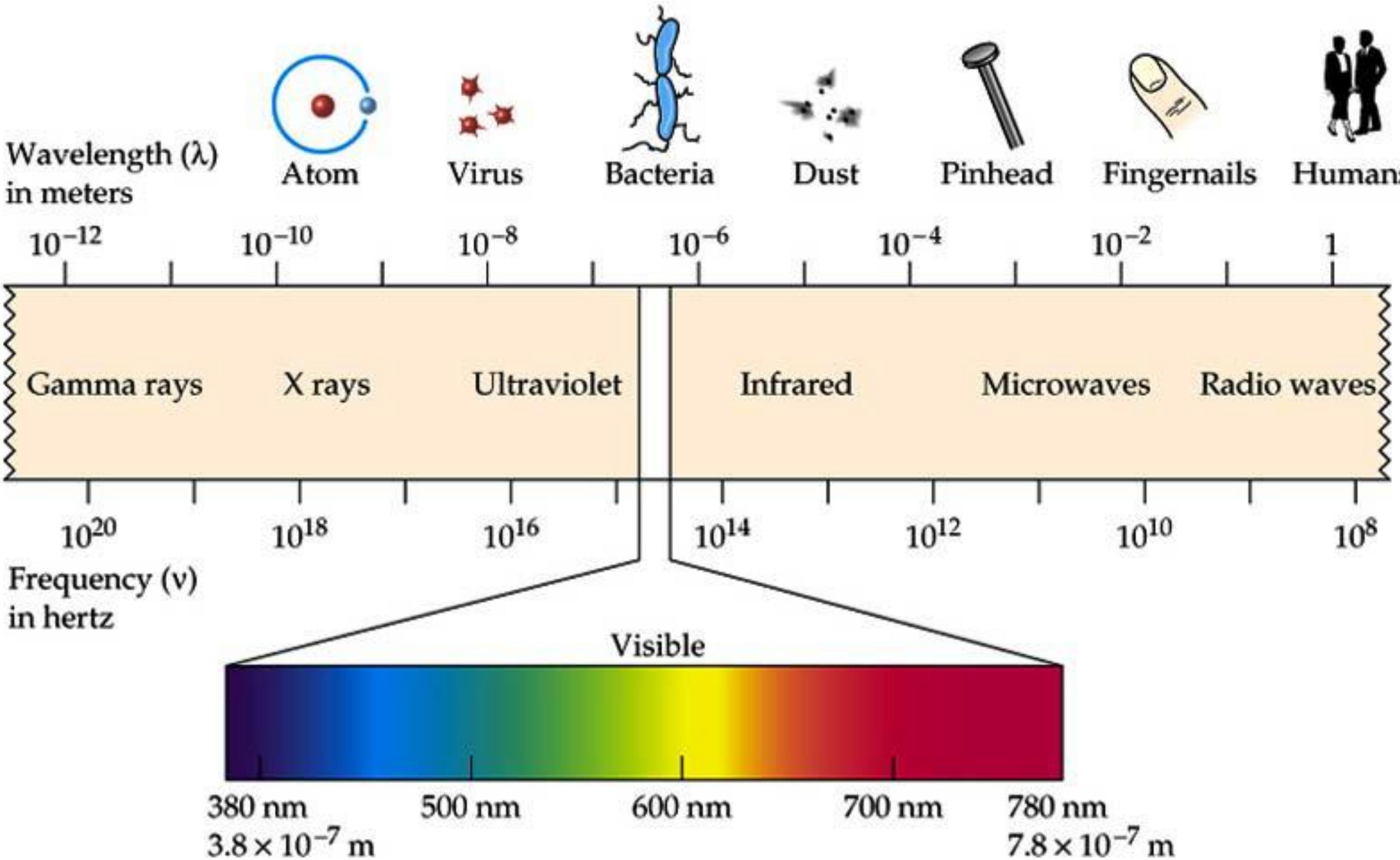
$$\lambda \times \nu = C$$

► <u>C</u> is the speed of light = 3.00×10^{8} m/s





Electromagnetic radiations



(3) Failures of classical mechanics

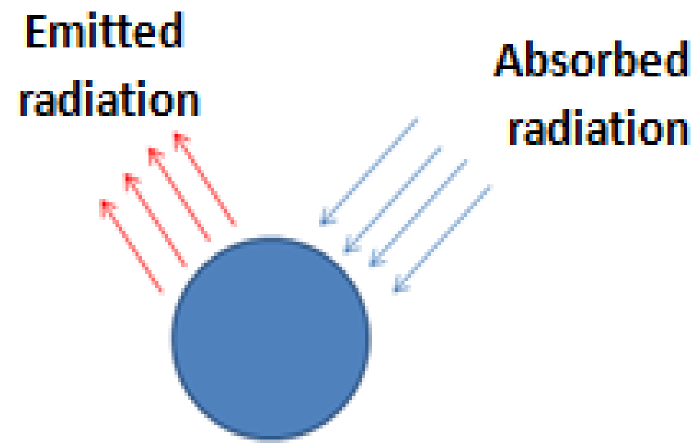
At the end of the eighteenth century, many experiments were conducted, the results of which differed with the conclusions of classical mechanics.

The only solution was to assume the failure of classical mechanics with these experiments and to search for new theories that could explain these results.

Black-Body Radiation

What is the black body?

According to the law of thermal radiation, for an object that is in thermal equilibrium with its surroundings:



$$\frac{E_\lambda}{A_\lambda} = K_\lambda(T) \quad (1)$$

A_λ denote the **percentage** of the **radiation absorbed**

E_λ denote **amount** of the **radiation emitted**

$K_\lambda(T)$ is a constant that depends only on the object's temperature **T** and the wavelength **λ**

From the relation between E_λ and A_λ we can see that **poor absorbers** are also **poor emitters**

For an absolutely absorbing body (**ideal absorber**), which **absorbs all the incident radiation**, $A_\lambda = 1$ for all wavelengths. Then it follows that:

$$K_\lambda(T) = E_\lambda \quad \textbf{(2)}$$

This **absolutely absorbing body** is called **black body**

Since the absorption by a black body is the **maximum** and the ratio of the emitted to absorbed amounts of radiation is the same for all materials, then the emittance of the black body is also the **maximum** among all objects

From equation 2, we see that the constant $K_\lambda(T)$ (at a given wavelength) equals to the density of radiation emitted by a black body at this wavelength

A good approximation to the **black body** is a **tiny hole made in a cavity** with **no other openings**

✓Any ray of radiation entering the hole will be reflected by the cavity's walls and absorbed by them.

✓On the other hand, the **molecules** of the **walls emit some radiation**.

✓When **equilibrium** between the walls and the radiation inside the cavity is **reached**, the **amount** of the **emitted radiation** of a given wavelength equals the **amount** of **absorbed radiation**

Stars

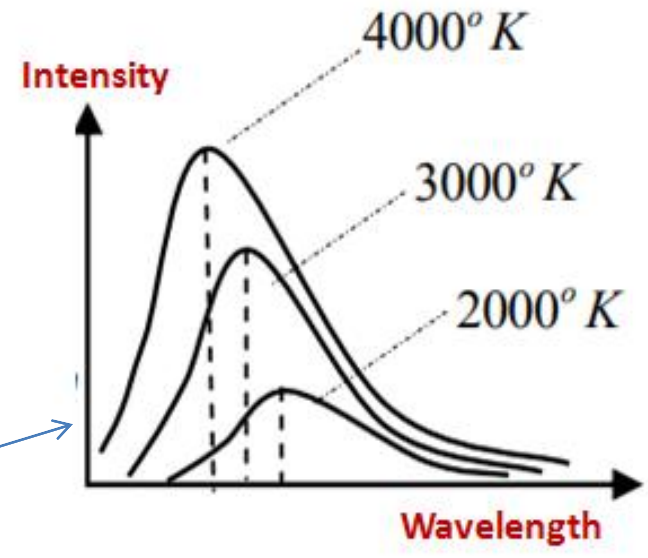
Hot iron

Molten Lava

Examples of Black Bodies

Black body radiation

The heated black body emits electromagnetic radiation. Experimentally, it was found that the wavelength distribution is a function of temperature and the intensity of the radiation is a function of wavelength as shown:



►The total power of the emitted radiation increases with temperature

►The peak of the wavelength distribution shifts to shorter wavelengths as the temperature increases

The basic problem was in understanding the observed distribution of the black body radiation

Classical prediction (Rayleigh-Jeans law)

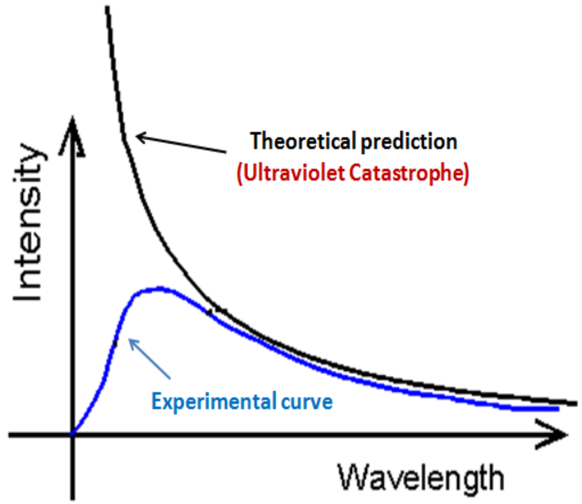
An early classical attempt to explain blackbody radiation was the Rayleigh-Jeans law. According to this law, for a given temperature **T** and wavelength **λ** the radiation intensity is given by:

$$I(\lambda, T) = \frac{2\pi c k_B T}{\lambda^4}$$

C is the speed of light and K_B is the Boltzmann constant

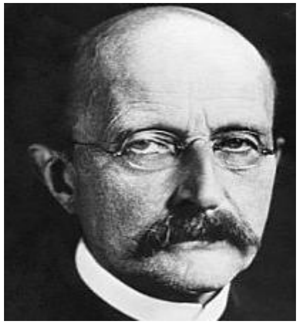
This law matched the experimental results fairly well at long wavelengths

At short wavelengths, there was a major disagreement between this law and the experimental results



This mismatch became known as the ultraviolet catastrophe as you would have infinite energy as the wavelength approaches zero

Planck's Theory of Blackbody Radiation



Plank assumed that the cavity radiation came from atomic oscillators in the cavity walls and made two assumptions about the nature of these oscillators

►First Assumption

The energy of an oscillator can have only certain discrete values E_n (The energy is quantized).

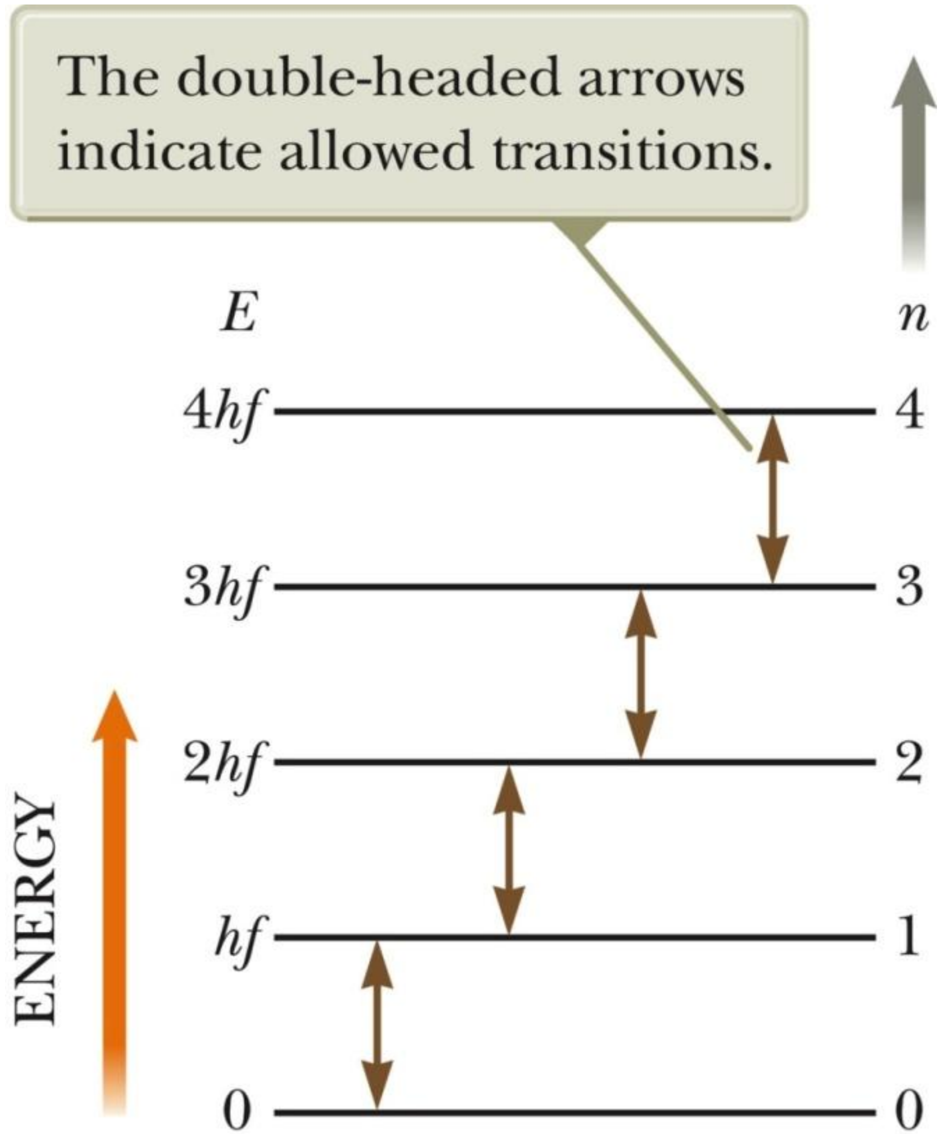
Quantized stair

Continuous stair

$$E_n = n h f$$

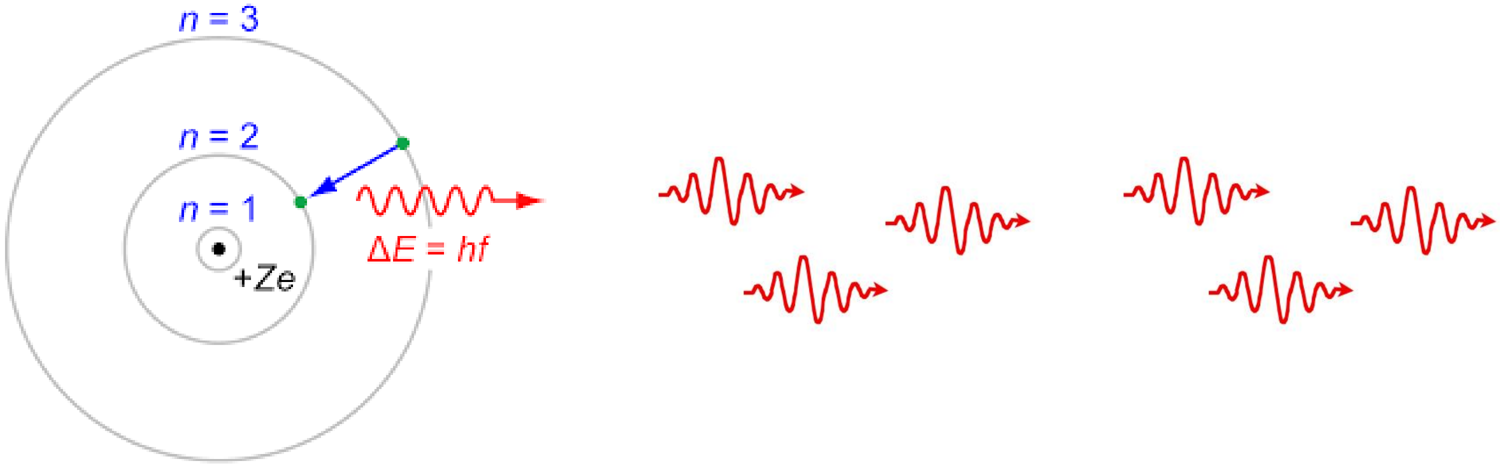
- n is a positive integer called the quantum number
- f is the frequency of oscillation
- h is Planck's constant

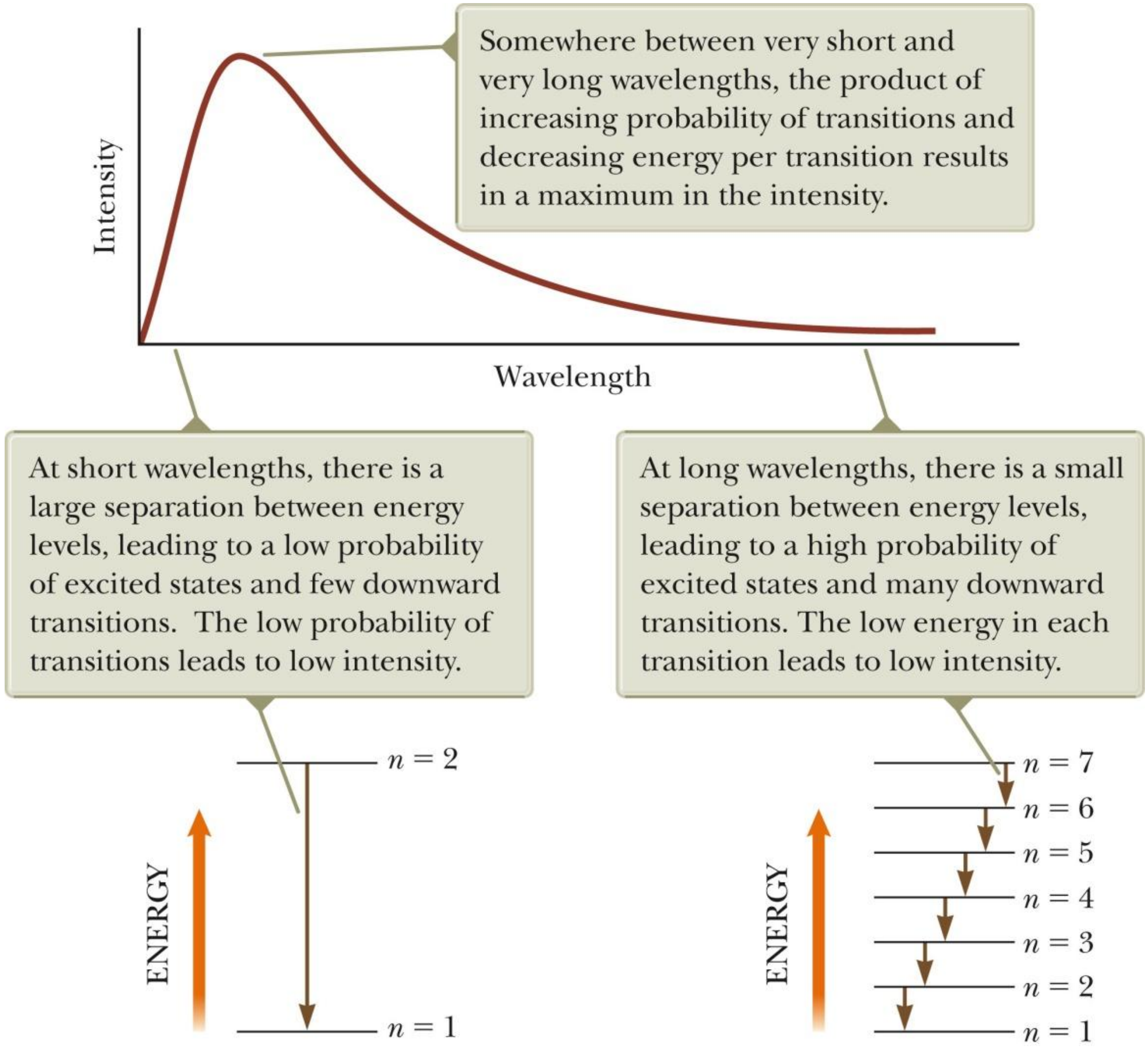
Each discrete energy value corresponds to a different quantum state and each quantum state is represented by the quantum number, n.



►Second Assumption

The oscillators emit or absorb energy when making a transition from one quantum state to another and the entire energy difference between the initial and final states in the transition is emitted or absorbed as a single quantum of radiation (quantum). The energy carried by the quantum of radiation is E = h ƒ




Somewhere between very short and very long wavelengths, the product of increasing probability of transitions and decreasing energy per transition results in a maximum in the intensity.
Intensity
Wavelength
At short wavelengths, there is a large separation between energy levels, leading to a low probability of excited states and few downward transitions. The low probability of transitions leads to low intensity.
At long wavelengths, there is a small separation between energy levels, leading to a high probability of excited states and many downward transitions. The low energy in each transition leads to low intensity.
n = 2
n = 1
ENERGY
n = 7
n = 6
n = 5
n = 4
n = 3
n = 2
n = 1
ENERGY

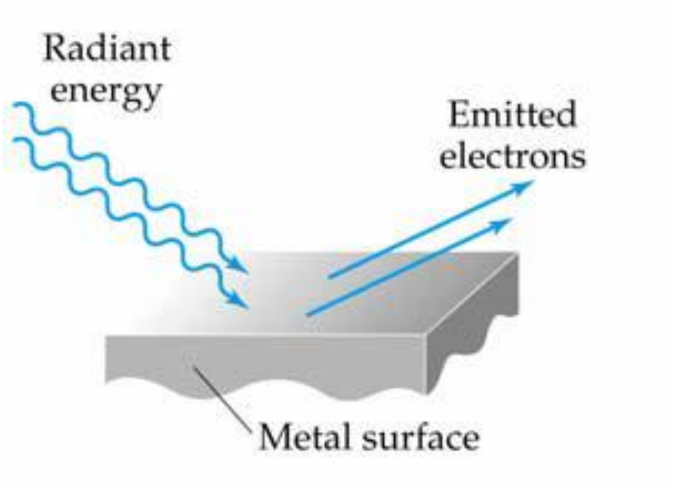
Planck generated a theoretical expression for the wavelength distribution

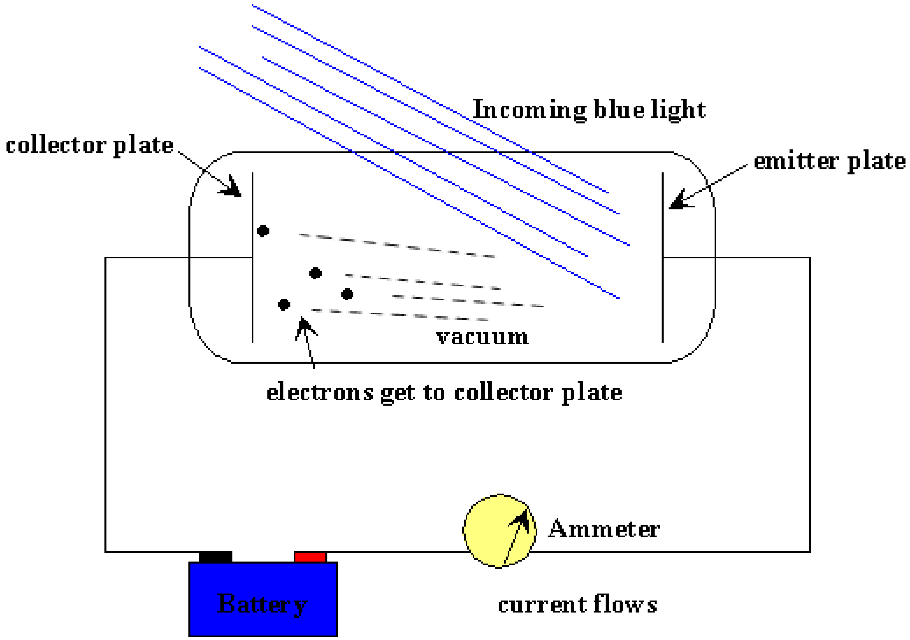
$$I(\lambda, T) = \frac{2hc^2}{\lambda^5} \frac{1}{e^{\frac{hc}{\lambda k_B T}} - 1}$$

C is the speed of light and **K_B** is the Boltzmann constant and **h** is Plank's constant

2-2 Photoelectric Effect

The phenomenon of emission of electrons (**photoelectrons**) from metal surfaces exposed to electromagnetic radiation energy (X – rays, γ – rays, UV rays, Visible light and even Infra Red rays) to produce **a photoelectric current**



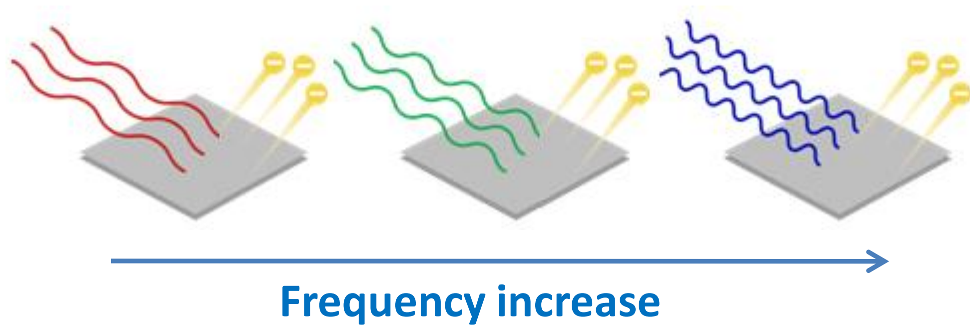


The experimental results contradict all classical predictions concerning the photoelectric effect

► Dependence of ejection of electrons on light frequency (ν)

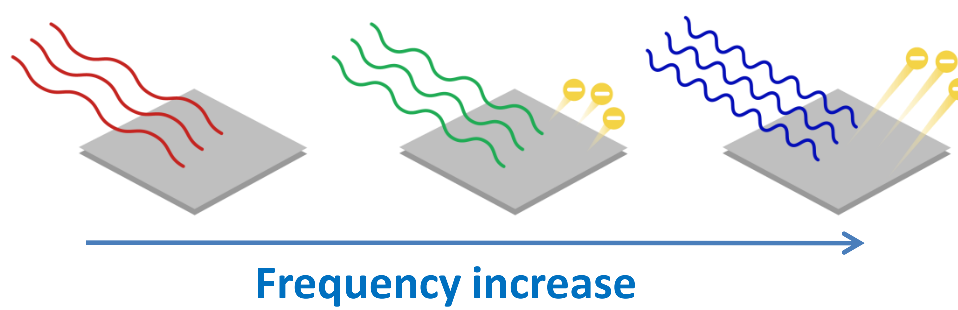
Classical Prediction

Electrons should be ejected at any frequency as long as the light intensity is high enough



Experimental Result

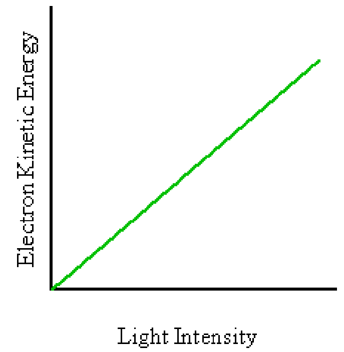
There is a minimum value of frequency called threshold frequency **(ν_0)** (cutoff frequency) below which photoelectric emission is not possible however high the intensity of incident light may be. The cutoff frequency depends on the nature of the metal emitting photoelectrons.



► Dependence of photoelectron kinetic energy on light intensity

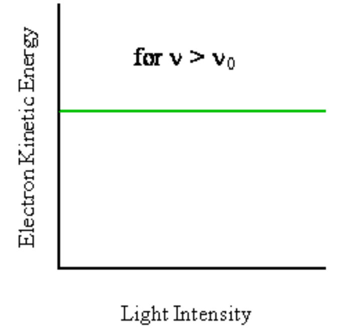
Classical Prediction

Electrons should absorb energy continually from the electromagnetic waves and as the light intensity incident on the metal is increased, the electrons should be ejected with more kinetic energy

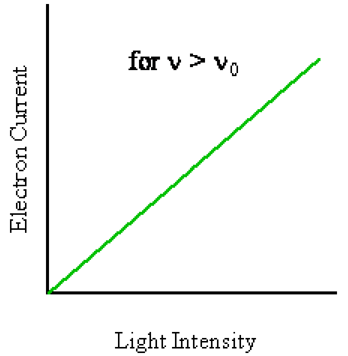


Experimental Result

According to the experimental results, for a frequency higher than the cutoff frequency, the kinetic energy is independent of light intensity



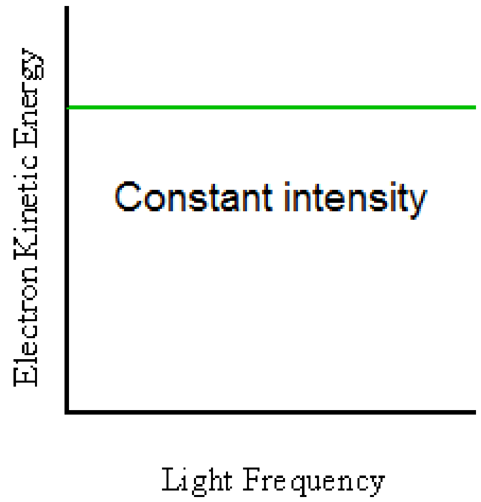
Note that the number of photoelectrons emitted per second (i.e. photoelectric current) is directly proportional to the intensity of incident light provided the frequency is above the threshold frequency



► Dependence of photoelectron kinetic energy on light frequency

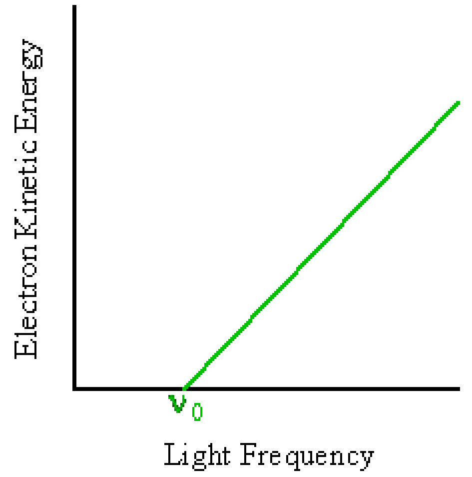
Classical Prediction

There should be no relationship between the frequency of the light and the kinetic energy of the photoelectron.



Experimental Result

For a frequency higher than the cutoff frequency, the kinetic energy of the photoelectrons increases with increasing light frequency



► Time interval between incidence of light and ejection of photoelectrons

Classical Prediction

At low light intensities, a measurable time interval should pass between the instant the light is turned on and the time an electron is ejected from the metal. This time interval is required for the electron to absorb the incident radiation before it acquires enough energy to escape from the metal

Experimental Result

Electrons are emitted almost instantaneously, even at very low light intensities.

Einstein’s explanation of Photoelectric effect

Einstein extended Planck's assumption to light and described light as composed of discrete quanta (now called photons) as opposed to continuous waves. In addition, he agreed with Planck and proposed that the energy in each quantum of light was equal to the frequency multiplied by a constant (Plank’s constant).

$$E = h\nu$$

h = Plank’s constant
ν = Frequency

In addition, Einstein proposed that light is not only a wave but also a particle and proposed that each photon has a mass m (**duality of photons**) where:

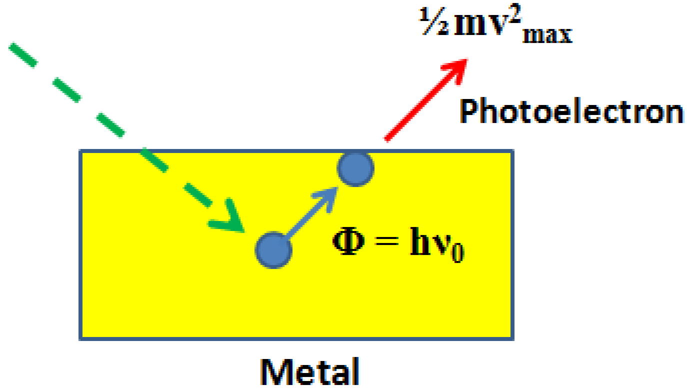
$$E = mc^2$$

m = mass of photon
c = speed of light

According to Einstein

When a photon of energy hν falls on a metal surface, the energy of the photon is absorbed by the electron and is used in two ways:

► A part of energy is used to overcome the surface barrier and come out of the metal surface. This part of the energy is called 'work function' ($\Phi = h\nu_0$).



► The remaining part of the energy is used in giving a velocity 'v' to the emitted photoelectron. This is equal to the maximum kinetic energy of the photoelectrons ($\frac{1}{2} mv^2_{max}$) where 'm' is mass of the photoelectron.

According to law of conservation of energy

$$h\nu = \Phi + \frac{1}{2} mv^2_{max} = h\nu_0 + \frac{1}{2} mv^2_{max} \Rightarrow \frac{1}{2} mv^2_{max} = h(\nu - \nu_0)$$

● If $\nu < \nu_0$, then $\frac{1}{2}mv^2_{max}$ is negative, which is not possible. Therefore, for photoelectric emission to take place $\nu > \nu_0$.

● Since one photon emits one electron, so the number photoelectrons emitted per second is directly proportional to the intensity of incident light

● It is clear that $\frac{1}{2} mv^2_{max} \alpha \nu$ as h and ν_0 are constant. This shows that K.E. of the photoelectrons is directly proportional to the frequency of the incident light.

● Photoelectric emission is due to collision between a photon and an electron. So that, there is no expected delay between the incidence of photon and emission of photoelectron. It is found that delay is only 10^{-8} seconds

Q1: If the work function (Φ) of Cs metal is 3.43 x 10^{-19} J, what will be the kinetic energy and the speed of an electron emitted from its surface by a light with wavelength of 550 nm?

(speed of light c = 3 x 10^{8} m/sec, Plank's constant h =6.63 x 10^{-34} J.sec.), The mass of electron = 9.11 x 10^{-31}Kg.

Solution:

The energy E of the incident photon = hν = hc/λ

$$= \frac{(6.63 \times 10^{-34}\ J.\ sec.)\ \times\ (3 \times 10^{8}\ m.\ sec^{-1})}{550 \times 10^{-9}\ m} = 3.62 \times 10^{-19}\ J$$

$$\Rightarrow\ E\ (photon) = \Phi + \tfrac{1}{2} mv^2_{max}$$

$$\Rightarrow\ 3.62 \times 10^{-19}\ J = 3.43 \times 10^{-19}\ J + \tfrac{1}{2} mv^2_{max}$$

$$\Rightarrow\ \tfrac{1}{2} mv^2_{max} = 3.62 \times 10^{-19}\ J - 3.43 \times 10^{-19}\ J = \boxed{1.9 \times 10^{-20}\ J}$$

$$\frac{1}{2} \times 9.11 \times 10^{-31}\ \text{Kg} \times v^2_{max} = 1.9 \times 10^{-20}\ \text{J}$$

$$v^2_{max} = \frac{1.9 \times 10^{-20}\ \text{Kg. m}^2\text{. sec}^{-2})}{\frac{1}{2} \times 9.11 \times 10^{-31}\ \text{Kg.}} = 4.17 \times 10^{10}\ \text{m}^2\text{.sec.}^{-2}$$

$$V_{max} = \boxed{2.04 \times 10^5\ \text{m.sec}}$$

(4) de Broglie's equation

In 1924, Louis de Broglie postulated that as the photons have dual characteristics (wave and particle characteristics), all forms of matter also have both wave and particle characteristics and the frequency and wavelength of matter waves can be determined

According to Planck, the photon energy 'E' is given by the equation

$E = h\nu \quad ...(i)$ **where h is Planck's constant and v the frequency of radiation**

By applying Einstein's mass-energy relationship, the energy associated with photon of mass 'm' is given as

$E = mc^2 \quad ...(ii)$ **where c is the velocity of radiation**

Comparing equations (i) and (ii)

$$mc^2 = h\nu = h\frac{c}{\lambda} \quad \left(\because \ \nu = \frac{c}{\lambda}\right) \xrightarrow{\text{or}} mc = \frac{h}{\lambda} \xrightarrow{\text{or}} \boxed{\lambda = \frac{h}{mc}} \quad ...(iii)$$

The equation (iii) is called de Broglie's equation. This expression of the equation is applied only to electromagnetic radiation, i.e. to a beam of photons

De Broglie suggested that the wave length of beams of other particles could be calculated from the following parallel relation

$$\boxed{\lambda = \frac{h}{mv}} \quad (iv)$$

where v is the velocity of the particles and m its mass

The de Broglie's equation is true for all particles, but it is only with very small particles, such as electrons, that the associated wavelength is measurable

(a) For a large mass

Let us consider a stone of mass 100 g moving with a velocity of 1000 cm/sec. The de Broglie's wavelength λ will be given as follows :

$$\lambda = \frac{6.6256 \times 10^{-27}}{100 \times 1000} \qquad \left(\lambda = \frac{h}{\text{momentum}}\right) \qquad = 6.6256 \times 10^{-32}\ \text{cm}$$

This is too small to be measurable by any instrument and hence no significance

(b) For a small mass

Let us now consider an electron in a hydrogen atom. It has a mass = 9.1091×10^{-28} g and moves with a velocity 2.188×10^{-8} cm/sec. The de Broglie's wavelength λ is given as

$$\lambda = \frac{6.6256 \times 10^{-27}}{9.1091 \times 10^{-28} \times 2.188 \times 10^{-8}} = 3.32 \times 10^{-8}\ \text{cm}$$

This value is quite comparable to the wavelength of X-rays and hence detectable

Q2: What is the wavelength of an electron moving at 5.31×10^{6} m/sec?

The mass of electron = 9.11×10^{-31} Kg. ► h = 6.63×10^{-34} J.sec.

Solution:

de Broglie's equation is

$$\lambda = \frac{h}{mv} = \frac{6.63\,x10^{-34}\ J.Sec}{(9.11\,x10^{-31}Kg)x(5.31\,x10^{6}\,m.Sec^{-1})}$$

$$= \frac{6.63 \times 10^{-34}\ (Kg.m^{2}.sec^{-2})\ sec.}{(9.11 \times 10^{-31}Kg.)\ \ X\ (5.31 \times 10^{6}\ m.sec^{-1})}$$

$= 13.7 \times 10^{-11}$ m

Q3- How can you calculate the wave length of a beam of electrons if you know that:

► The kinetic energy of each electron = 1.6×10^{-15} J

► The mass of electron = 9.11×10^{-31}Kg.

► $h = 6.63 \times 10^{-34}$ J.sec.

Solution:

$$E = \tfrac{1}{2} mv^2 \Rightarrow v^2 = \frac{2E}{m} = \frac{2 \times 1.6 \times 10^{-15}\ Kg.\ m^2.sec^{-2}}{9.11 \times 10^{-31}\ Kg}$$

kinetic energy of electron (E)

$$v^2 = 0.351 \times 10^{16}\ m^2.sec^{-2}$$

$$v = 0.59 \times 10^{8}\ m.sec^{-1}$$

$$\lambda = \frac{h}{mv} = \frac{6.63 \times 10^{-34}\ J.Sec}{(9.11 \times 10^{-31} Kg) x (0.59 \times 10^{8} m.Sec^{-1})}$$

$$\lambda = 12.3 x 10^{-12} m$$

Q4: What is the weight of a car moving with a speed of 35.84 m/s and a wave with wavelengths of 1.85×10^{-38} m ? ► $h = 6.63 \times 10^{-34}\ Kg.\ m^2.\ sec^{-1}$

Solution:

de Broglie's equation is

$$\lambda = \frac{h}{mv} \Longrightarrow m = \frac{h}{\lambda v}$$

$$= \frac{6.63 \times 10^{-34}\ Kg.m^2.sec^{-1}}{(1.85 \times 10^{-38}\ m) \ \ X\ (35.84\ m.sec^{-1})}$$

= 1000 Kg

(5) Heisenberg's uncertainty principle

One of the most important consequences of the dual nature of matter is the uncertainty principle developed by Werner Heisenberg in 1927. According to the uncertainty principle, it is impossible to determine two independent properties accurately at the same time. For example, both the position and the momentum of a moving particle at any instant cannot be determined with absolute exactness. If the momentum (or velocity) be measured very accurately, a measurement of the position becomes less precise and if position is determined with accuracy the momentum becomes less accurately known

The uncertainty in measurement of position, Δx, and the uncertainty of determination of momentum, Δp (or Δmv), are related by Heisenberg's relationship as

$$\Delta x \times \Delta p \geq \frac{h}{2\pi} \qquad \text{or} \qquad \Delta x \times m\,\Delta v \geq \frac{h}{2\pi}$$

Where h is Planck's constant

There is a clear difference between the behavior of large objects like a stone and small particles such as electrons. The uncertainty product is negligible in case of large objects

For a moving ball of iron weighing 500 g, the uncertainty expression assumes the form

$$\Delta x \times m\, \Delta v \geq \frac{h}{2\pi} \quad \text{or} \quad \Delta x \times \Delta v \geq \frac{h}{2\pi m} \geq \frac{6.625 \times 10^{-27}}{2 \times 3.14 \times 500} \approx 5 \times 10^{-31} \text{ erg sec g}^{-1}$$

which is negligible value. Therefore for large objects, the uncertainty of measurements is practically nil

But for an electron of mass m = 9.109 × 10^{-28} g, the product of the uncertainty of measurements is quite large as

$$\Delta x \times \Delta v \geq \frac{h}{2\pi m} \geq \frac{6.625 \times 10^{-27}}{2 \times 3.14 \times 9.109 \times 10^{-28}} \approx 0.3 \text{ erg sec g}^{-1}$$

This value is large enough in comparison with the size of the electron and can not be neglected

Q5: Calculate the uncertainty in position of an electron if the uncertainty in velocity is 5.7×10^5 m sec^{-1}.

Solution

According to Heisenberg's uncertainty principle

$$\Delta x \times \Delta p = \frac{h}{2\pi} \longrightarrow \Delta x \times m\,\Delta v = \frac{h}{2\pi} \longrightarrow \Delta x = \frac{h}{2\pi\,m \times \Delta v}$$

$\Delta v = 5.7 \times 10^5\ \text{m sec}^{-1}$ $h = 6.6 \times 10^{-34}\ \text{kg}\ m^2\ \text{sec}^{-1}$ $m = 9.1 \times 10^{-31}\ \text{kg}$

On substitution we get:

$$\Delta x = \frac{6.6 \times 10^{-34}\ \text{kg m}^2\ \text{sec}^{-1}}{2 \times 3.14 \times \left(9.1 \times 10^{-31}\ \text{kg}\right)\left(5.7 \times 10^5\ \text{m sec}^{-1}\right)}$$

$$= \frac{6.6 \times 10^{-8}}{2 \times 3.14 \times 9.1 \times 5.7}\,m = \mathbf{2 \times 10^{-10}\ m}$$

Q6: The uncertainty in the position and velocity of a particle are 10^{-10} m and 5.27 × 10^{-24} m sec^{-1} respectively. Calculate the mass of the particle.

Solution

According to Heisenberg's uncertainty principle

$$\Delta x \times \Delta p = \frac{h}{2\pi} \longrightarrow \Delta x \times m\,\Delta v = \frac{h}{2\pi} \longrightarrow m = \frac{h}{2\pi \times \Delta x \times \Delta v}$$

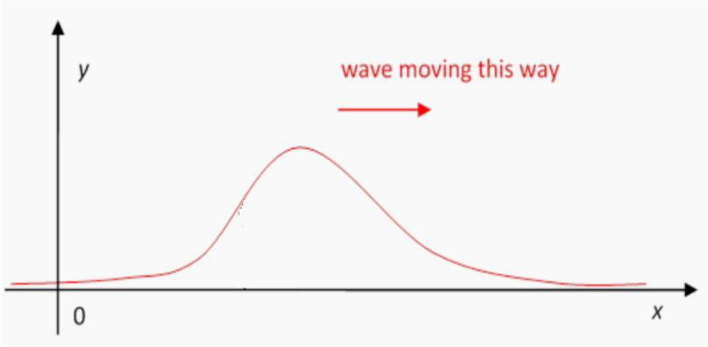
$$h = 6.6 \times 10^{-34}\ \text{kg m}^2\ \text{sec}^{-1} \qquad \Delta x = 1 \times 10^{-10}\ \text{m} \qquad \Delta v = 5.27 \times 10^{-24}\ \text{m sec}^{-1}$$

On substitution we get:

$$m = \frac{6.6 \times 10^{-34}\ \text{kg m}^2\ \text{sec}^{-1}}{2 \times 3.14 \times \left(1 \times 10^{-10}\ \text{m}\right)\left(5.27 \times 10^{-24}\ \text{m sec}^{-1}\right)} = 0.2\ \text{kg} = 200\ \text{g}$$

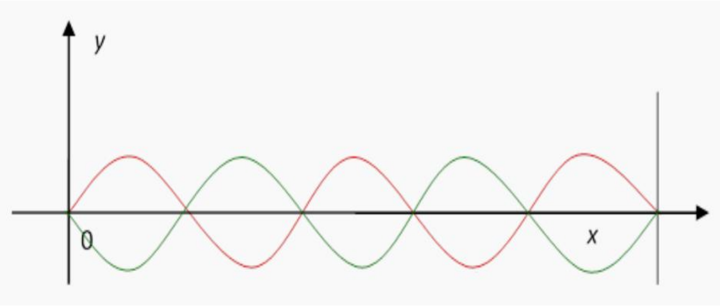
(6) The Wave Equation

Traveling and Standing Waves



Water waves

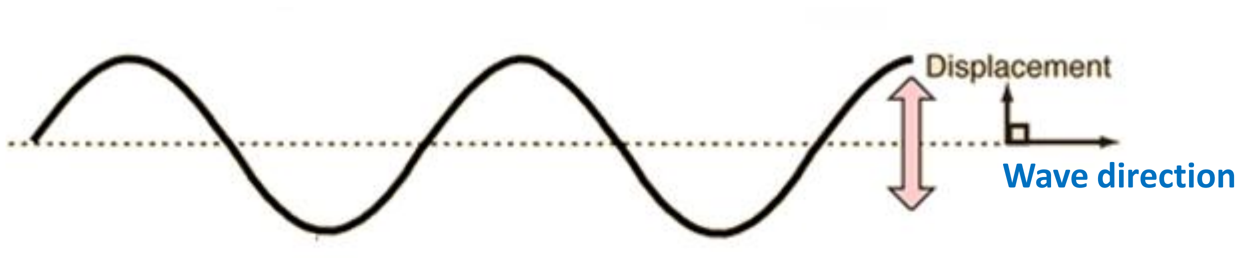
Electromagnetic waves, sound waves, and water waves are examples of traveling



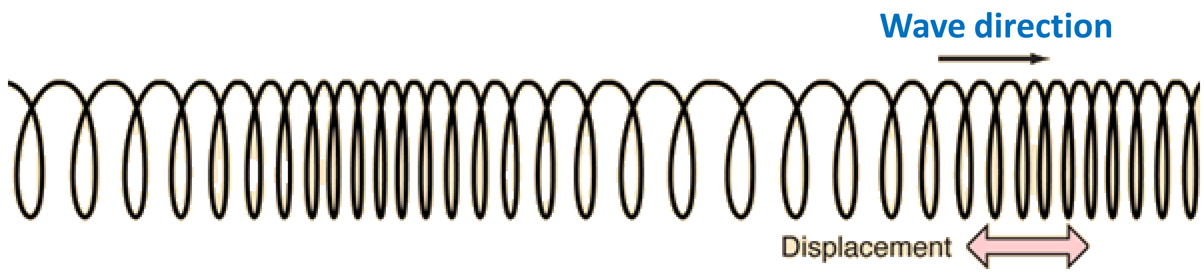
Gitar

The standing waves generated on a string fixed at both ends when it is made to vibrate. Almost all musical instruments generate standing waves

Transverse and Longitudinal Waves



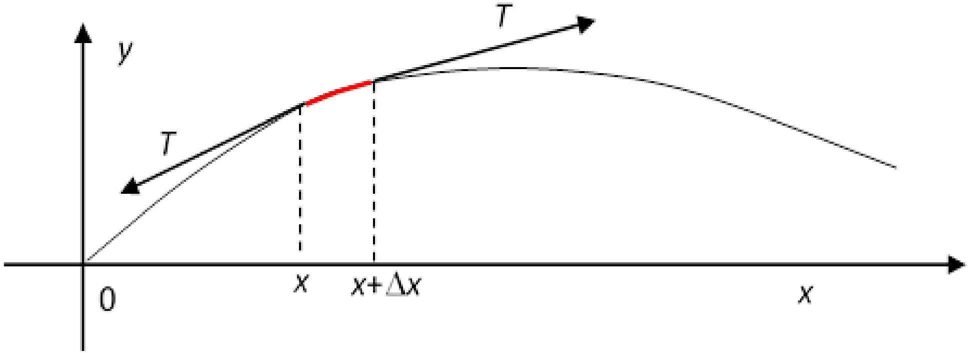
For transverse waves the displacement of the medium is perpendicular to the direction of the wave



For longitudinal waves the displacement of the medium is parallel to the wave direction

Derivation of the Wave Equation

By applying Newton's Second Law (F=ma) to one tiny bit of a uniform string



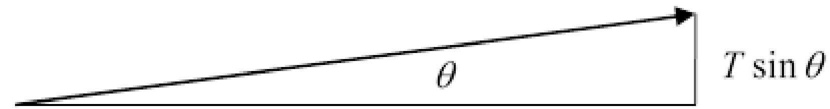
For the small length of string between x and x + Δx in the diagram above

If the mass density of the string is μ kg/m, so, **m = μΔx**

The forces on the bit of string (neglecting the tiny force of gravity, air resistance, etc.) are the tensions T at the two ends

As the string curves during waving, so the two T vectors at opposite ends of the bit of string do not quite cancel giving a net force F which is very close to vertical

The vertical component of the tension T at each of the two end of the bit of string is T sinθ.



By assuming that the wave amplitude is small, then θ is small, and we can take tanθ = sinθ = dy/dx , so that

The vertical component of the tension T at the x end is → $T\,\frac{dy\,(x)}{dx}$

The vertical component of the tension T at the x + Δx end is → $T\,\frac{dy\,(x+\Delta x)}{dx}$

And the total vertical force from the tensions at the two ends becomes

$$\vec{F} = T\left(\frac{dy\,(x+\Delta x)}{dx} - \frac{dy\,(x)}{dx}\right) \cong T\frac{d^2y\,(x)}{dx^2}\Delta x$$

Because y is a function of t as well as of x: **y = y(x,t).** So that, we replace d/dx with ∂/∂x for denoting differentiation with respect to one variable while the other is held constant (which is the case here—we're looking at the sum of forces at one instant of time) is to replace d/dx with ∂/∂x .

So we should write: $$\overrightarrow{F} = T\frac{\partial^2 y}{\partial x^2}\Delta x \quad \textbf{(1)}$$

But we know that: $$\overrightarrow{F} = m\,\overrightarrow{a} \quad \textbf{(2)}$$

The acceleration (a) of the bit of string is **$\partial^2 y/\partial t^2$** as it moves only up and down in the *y*-direction

And the mass of the bit of string is given by **m** = **μΔx**

So we can write equation 2 as follow: ⟶ $$\overrightarrow{F} = \mu\Delta x\frac{\partial^2 y}{\partial t^2} \quad \textbf{(3)}$$

From equations 1 and 3

$$T\frac{\partial^2 y}{\partial x^2}\Delta x = \mu\Delta x\frac{\partial^2 y}{\partial t^2} \longrightarrow T\frac{\partial^2 y}{\partial x^2} = \mu\frac{\partial^2 y}{\partial t^2} \quad \textbf{(4)}$$

If we know that $\longrightarrow$ $v^2 = \frac{T}{\mu}$ v is the wave speed

So that the equation 4 can be written as: $\longrightarrow$

$$\frac{\partial^2 y}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2 y}{\partial t^2} \quad \textbf{(5)}$$

Or in general

$$\frac{\partial^2 F}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2 F}{\partial t^2}$$

This is called the wave equation

F is called the wave function

The wave function F depends of x and t while υ is the speed of wave. For example, if we are studying a sound wave, in this case F will represent the change of compressions and rarefactions of air molecules and υ is sound speed, and if we are studying electromagnetic wave, F will represent the change in the magnetic and electric fields and υ is speed of light and so on.

Sound waves

Electromagnetic waves