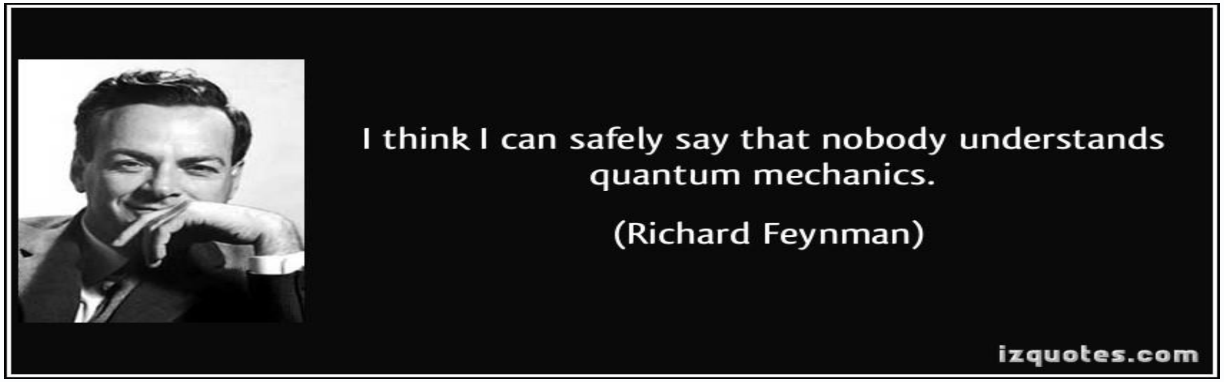
Quantum Mechanics

Unit : I

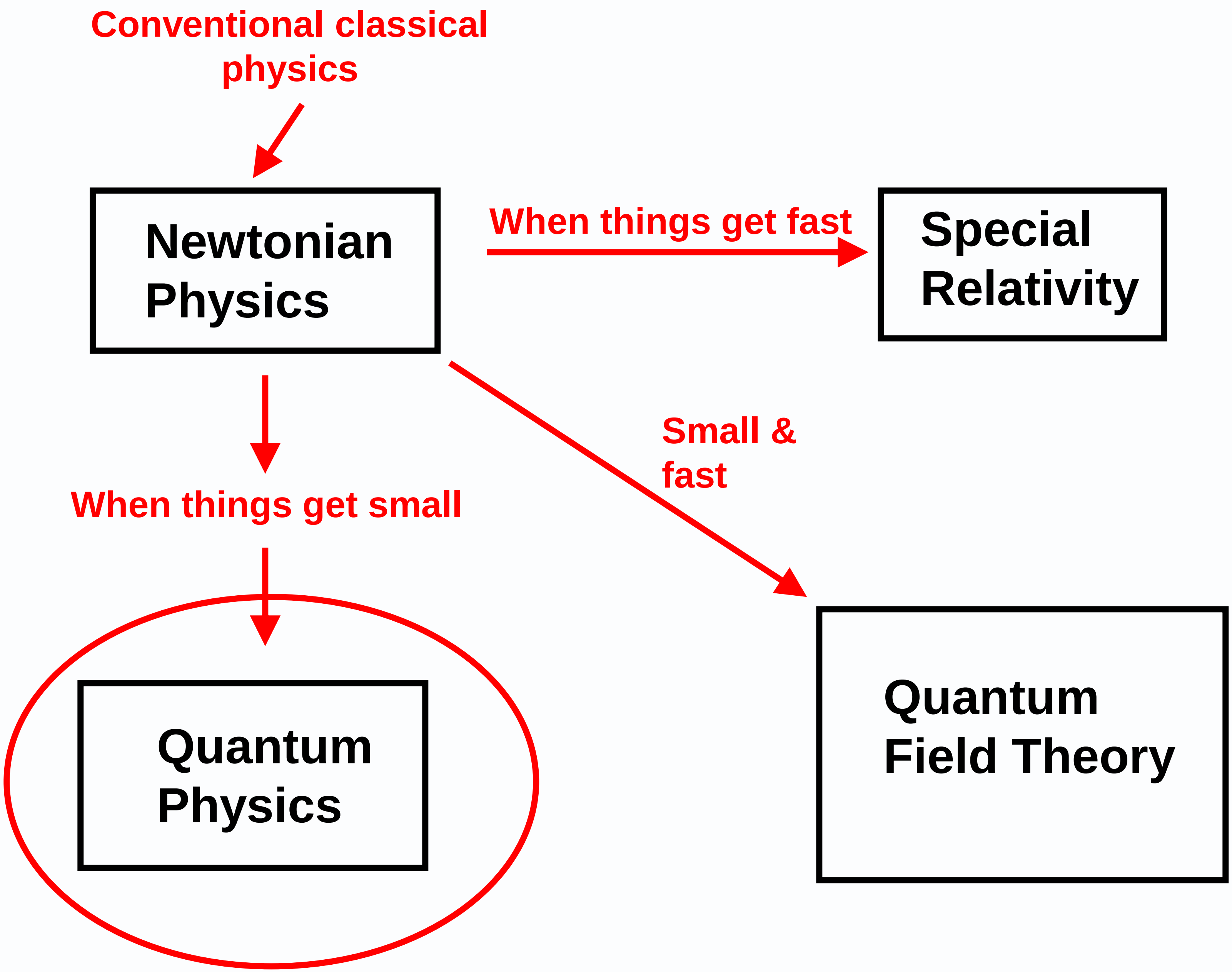


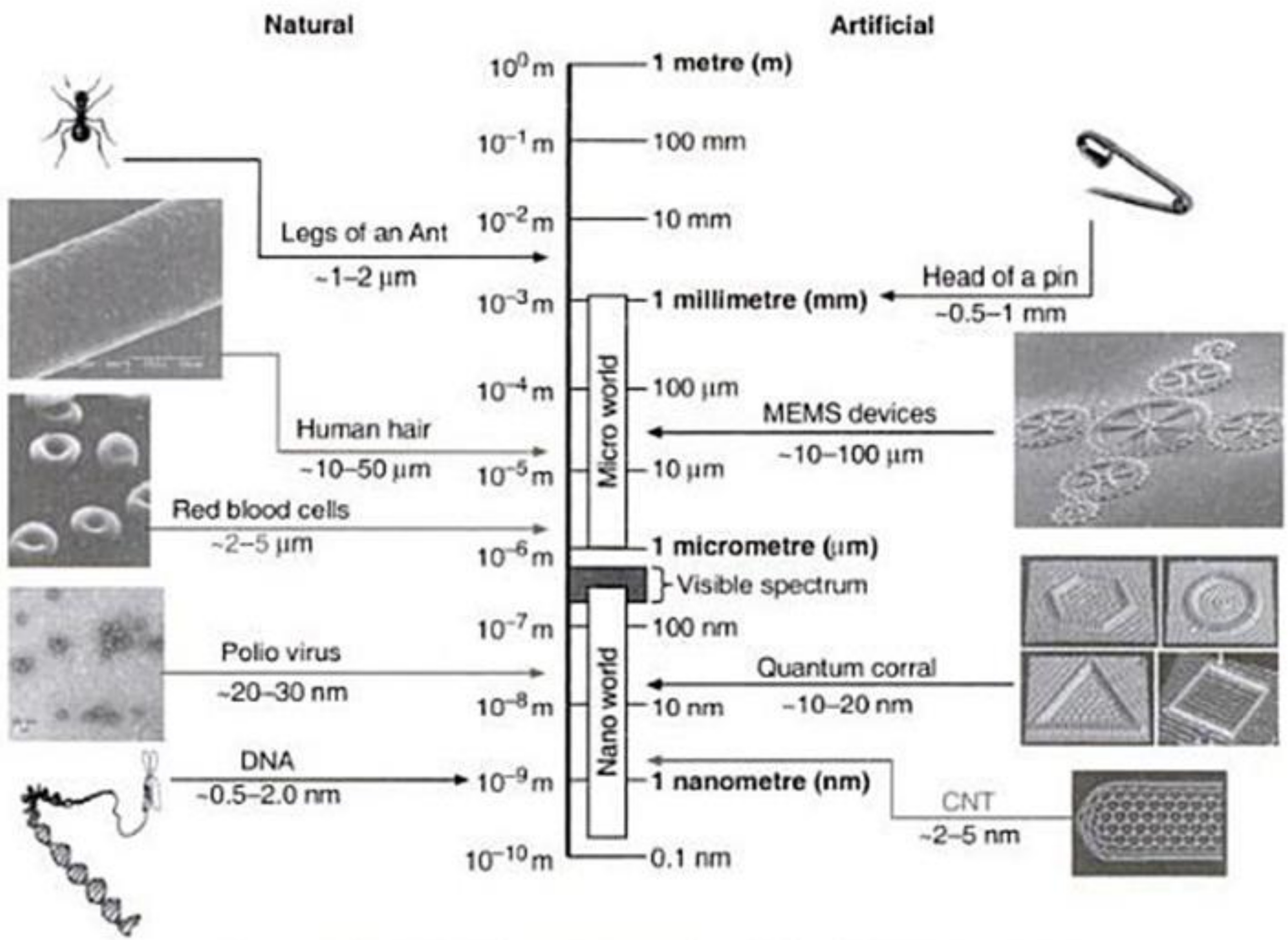
Why Quantum Mechanics is essential for Engineers?

Quantum Mechanics plays a vital role in engineering developments : VLSI, Photonics, Communications, etc.

As an engineer you should have at least little bit of understanding of Quantum Mechanics.
If you don't, you'll be left behind.

One day we may succeed in building Quantum Computers. When that day comes, it will bring a technological revolution which is hard to imagine right at this moment. As for example, Shor's algorithm factors numbers, will make current RSA cryptography insecure.
Quantum cryptography will allow private communication, ensuring that you and your communication partner are not eavesdropped on. To be ready for this inevitable revolution - you'll definitely need to understand the basics of quantum theory.


Conventional classical physics
Newtonian Physics
When things get fast
Special Relativity
Small & fast
When things get small
Quantum Physics
Quantum Field Theory



Description of nano-regime (from Forbes Nanotech Report).

Faster response time of miniaturized simple pendulum

The resonance frequency of a simple pendulum is

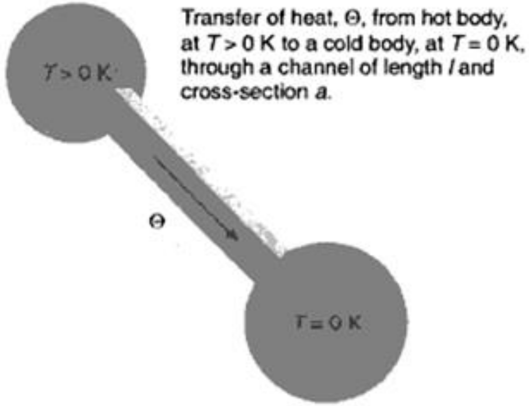
$$\nu = \frac{1}{2\pi}\sqrt{\frac{g}{L}}$$

g = gravitational acceleration
L = Length of the pendulum

$L = 1\,\mu m$ $\nu = 1000$ Hz
↳ τ (time period) = 1 ms

The miniature version of the simple pendulum has a much faster response time with respect to a normal grandfather pendulum which would have a resolution of 1s for a pendulum length of 1m.

Thermal time constants in smaller systems



Heat transfer from a hot body to a cold body through a heat-channel.

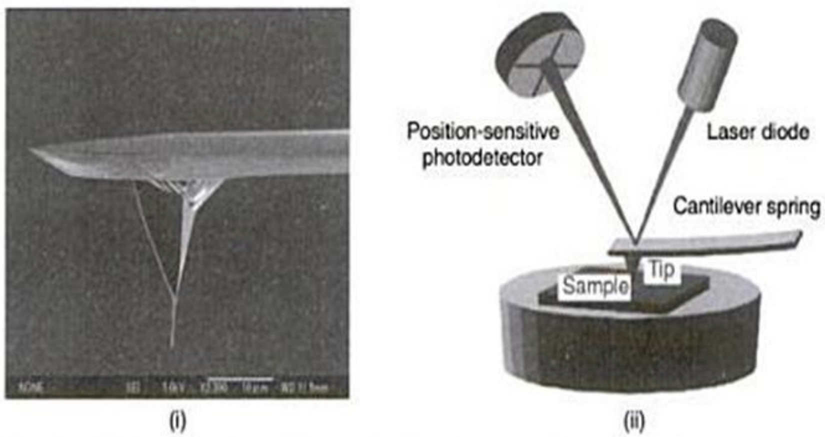
A hot body (at T>0K) of heat capacity per unit volume C, is connected to a cold body (at T=0K) through a heat channel of length L, cross section a, and thermal heat capacity K_{Th},

$$T = T_0 e^{-t/\tau_{th}}$$

τ_{th}, thermal time constant

$$= \frac{LCV}{K_{Th}a}, \quad \text{where } V = \text{volume}$$

Under isotropic environment it is proportional to $[L^2]$. Therefore, the thermal time constant strongly decreases with the size of the system. This phenomenon is used in data storage systems where the data bits are recorded with a resistively heated AFM tip and are detected by an integrated piezoelectric sensor. Such a system consumes less power and responds much faster.



(i) SEM image of AFM tip, and (ii) schematic diagram of the working principle of AFM.

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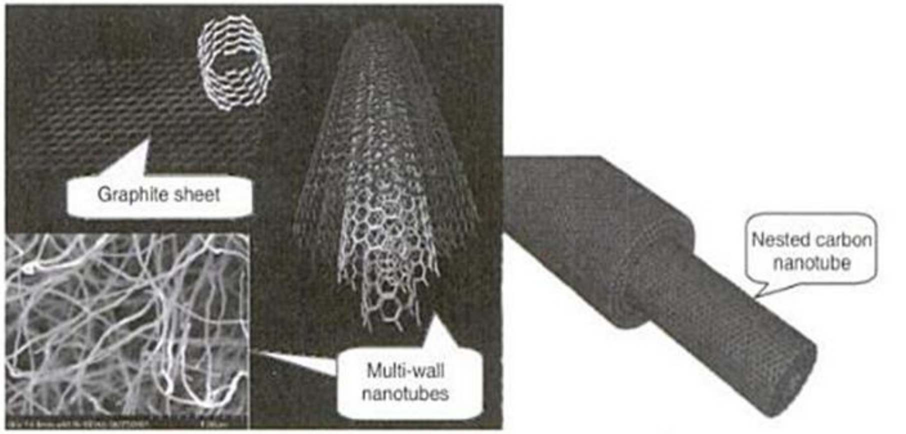
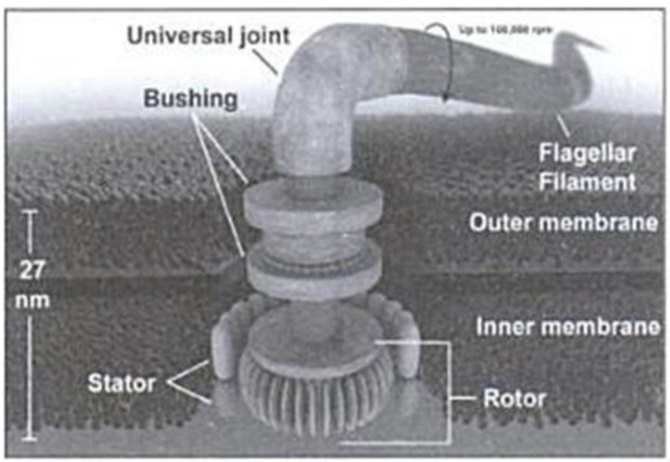
Disappearance of friction in highly symmetric molecular systems



(a) (b)

Schematic representation of **(a)** multi-wall carbon nanotubes formed from graphite sheets, and **(b)** computer generated model of nested carbon nanotube.



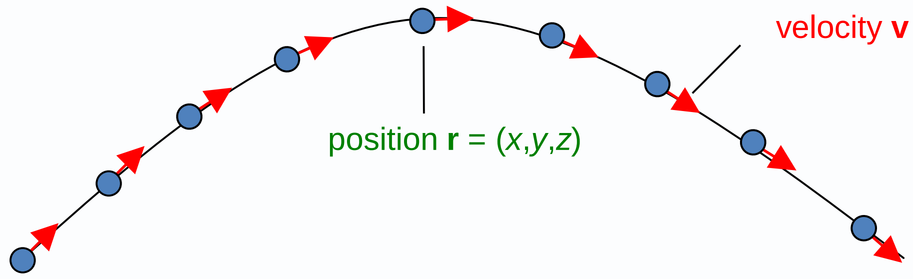
Schematic representation of *E.coli* bacterial flagella rotary motor.

Classical Mechanics (CM)

- *Do the electrons in atoms and molecules obey Newton's classical laws of motion?*
- We shall see that the answer to this question is "No".
- This has led to the development of Bohr's model of nuclear atom.

Features of Classical Mechanics

1) CM predicts a precise trajectory for a particle.



- The exact position (**r**)and velocity (**v**) (and hence the momentum **p** = m**v**) of a particle (mass = m) can be known simultaneously at each point in time.

- Note: position (r),velocity (**v**) and momentum (**p**) are vectors, having magnitude **and** direction ⇒ **v** = (v_x, v_y, v_z).

2) Any type of motion (translation, vibration, rotation) can have any value of energy associated with it

   – i.e. there is a continuum of energy states.

3) Particles and waves are distinguishable phenomena, with different, characteristic properties and behaviour.

	Property		Behaviour
Particles	mass position velocity	⇒	momentum collisions
Waves	wavelength frequency	⇒	diffraction interference

Revision of Some Relevant Equations in CM

Total energy of particle :

E = **Kinetic Energy (T)** + **Potential Energy (U)**

$\boxed{\mathbf{T} \text{ - depends on } \mathbf{v}}$ $\boxed{\mathbf{U} \text{ - depends on the position } (\mathbf{r})}$

U depends on the system
e.g., positional, electrostatic

$$E = \tfrac{1}{2}mv^2 + U$$

$$\Rightarrow \qquad E = p^2/2m + U \qquad (\mathbf{p} = m\mathbf{v})$$

Note: E, T, U (and **r**, **v**, **p**) are all defined at a particular time (t), *viz*, E(t) etc.

- Consider a 1-dimensional system (straight line translational motion of a particle under the influence of a potential acting parallel to the direction of motion) :

- **Define :**

position	$r = x$
velocity	$v = dx/dt$
momentum	$p = mv = m(dx/dt)$
PE	U
force	$F = -(dU/dx)$

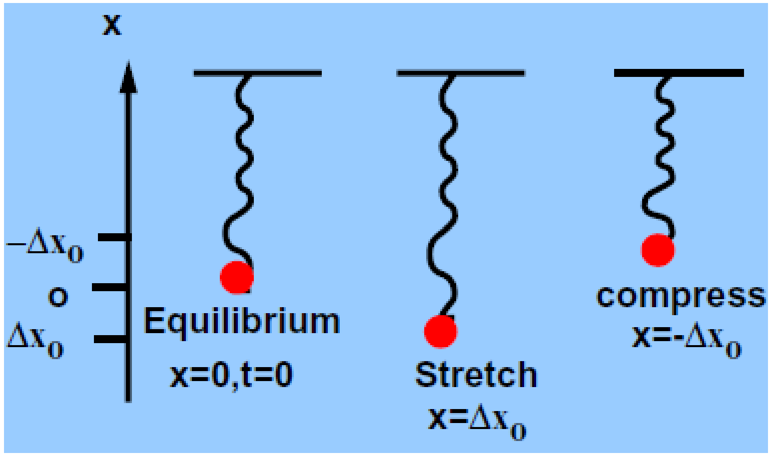
- **Newton's 2nd Law of Motion :**

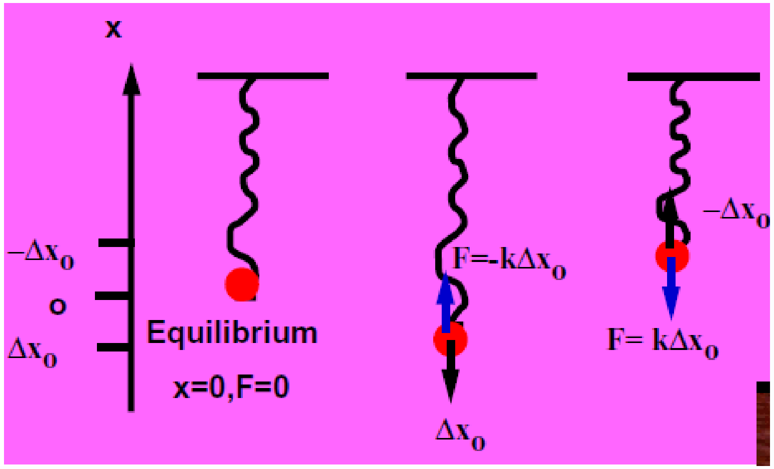
$$\mathbf{F = \underbrace{ma}_{\text{acceleration}} = m(dv/dt) = m(d^2x/dt^2)}$$

- Therefore, if we know the forces acting on a particle we can solve a differential equation to determine it's trajectory $\{x(t),p(t)\}$.

Classical Harmonic Oscillator

Let us consider a particle of mass **'m'** attached to a spring





At t = o, the particle is at equilibrium, and there is no force working on it , F = 0

According to Hooke's Law :

$$F = -k\,x$$

i.e., the force is proportional to displacement and pointing in the opposite direction k is the force constant and x is the displacement.

Classically, a harmonic oscillator follows Hooke's law.

Newton's second law says

$$F = ma$$

Therefore,

$$-k\,x = m\,\frac{d^2x}{dt^2}\,.$$

$$m\,\frac{d^2x}{dt^2} + k\,x = 0\,.$$

The solution to this differential equation is of the form

$$x(t) = A\sin(wt)$$

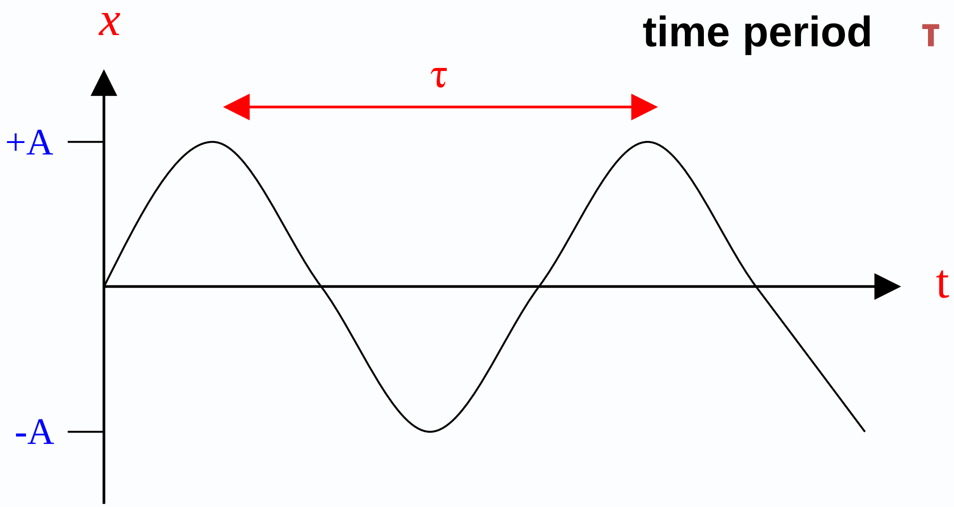
where the angular frequency of oscillation is **‘ω’** in radians per second

$$\boldsymbol{\omega = \sqrt{\frac{k}{m}}}$$

Also, **ω = 2πυ,** where **‘υ’** is frequency of oscillation

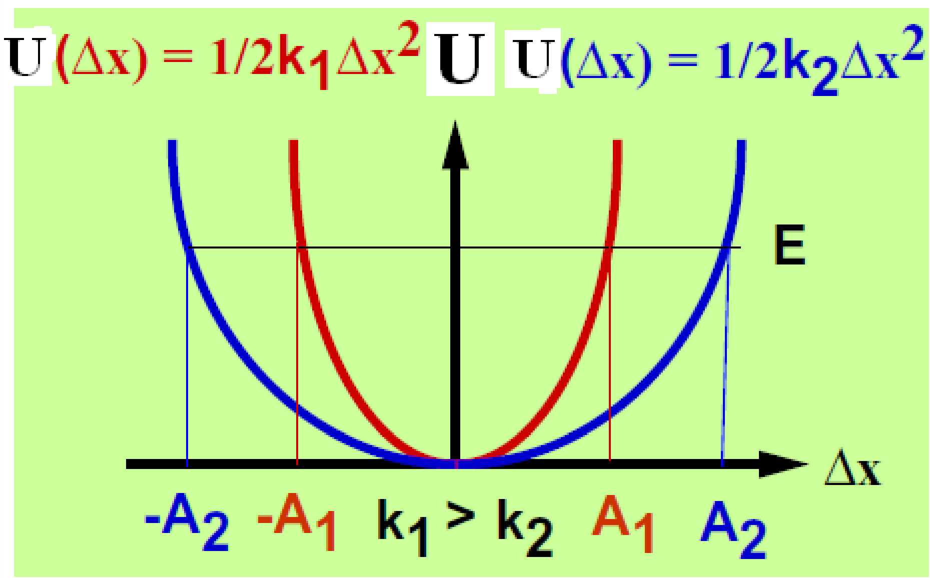
Note : frequency depends only on the characteristics of the system (m, *k*) – not the amplitude (A)!

time period $\tau = 1/\nu$



Potential Energy

$$U = \int dU = \int -F dx = \frac{1}{2}kx^2 = \frac{1}{2}kA^2 \sin^2 wt$$



➢The **parabolic potential energy U = ½ *kx*²** *of a harmonic oscillator, where x is* the displacement from equilibrium.

➢The **narrowness of the curve depends on the force constant *k***: *the larger the* value of *k, the narrower the well.*

- As the amplitude (A) can take any value, this means the total energy (U) can also take any value, – *i.e.*, energy is continuous.

- At any time (t), the position {$x(t)$} and velocity {$\mathbf{v}(t)$} can be determined exactly, – *i.e.*, the particle trajectory can be specified precisely.

- We shall see that these ideas of classical mechanics fail when we go to the atomic regime (where U and m are very small) – then we need to consider Quantum Mechanics.

- CM also fails when velocity is very large (as $v \rightarrow c$), due to relativistic effects.

Experimental Evidence of the Breakdown of Classical Mechanics

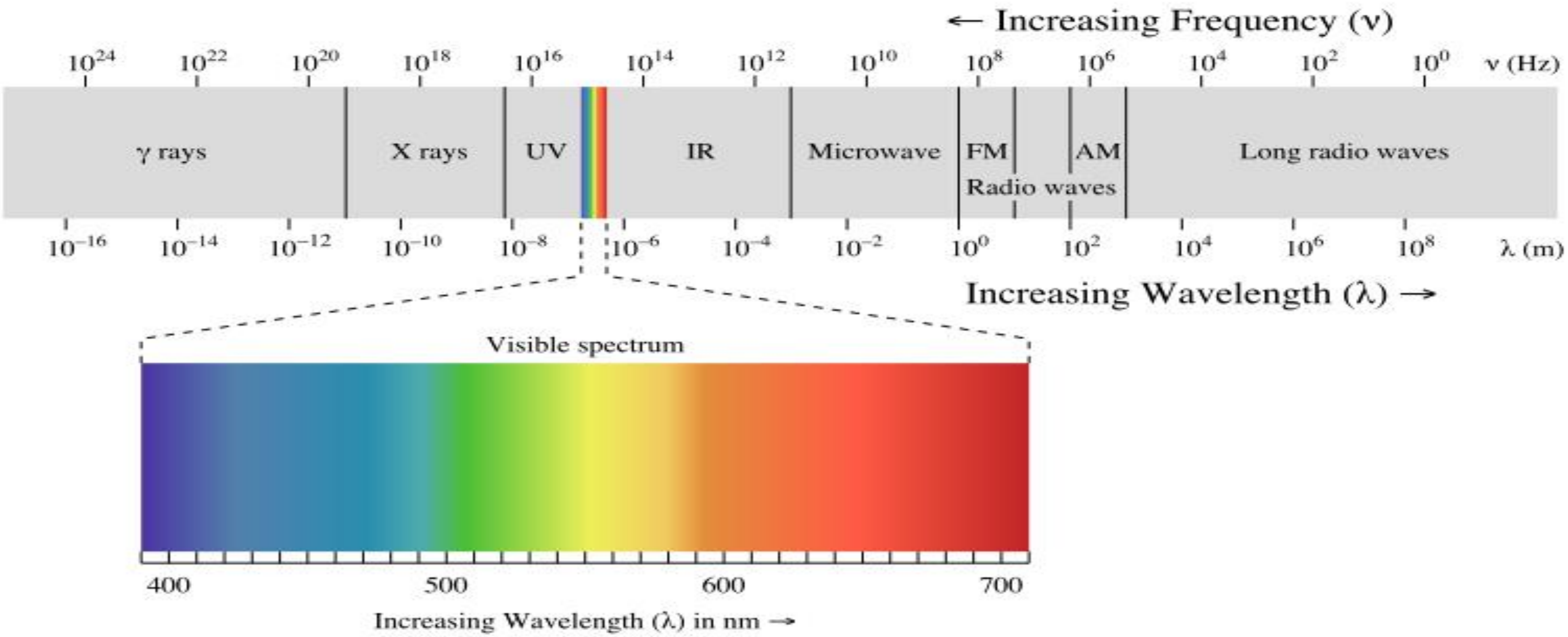
- By the early 20th century, there were a number of experimental phenomena that could not be explained by classical mechanics.

a) Black Body Radiation
b) Photoelectric effect
c) Dual nature of light
d) Discrete nature of atomic and molecular spectra
e) Compton scattering

Genius Minds of 20th Century

What is LIGHT?

- Light is an electromagnetic wave.
- Visible Light is simply the name for a range of electromagnetic radiation that can be detected by the human eye.



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Waves and Particles

Wavelength or Freque
ncy

Waves

Spread in space and
time

Can be superposed – show
interference effects

Pass through each
other

Particles

Localized in space and
time

Cannot pass through each
other -
they bounce or shatter.

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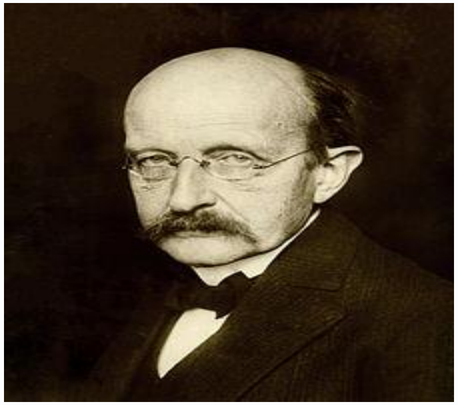
“Necessity is the mother of invention” — Plato

Thomas Alva Edison's first successful light bulb model, used in public demonstration at Menlo Park, December 1879.



Max Planck (1858–1947), a German physicist considered to be the founder of quantum theory.

Planck's Quantum Theory

- **Planck (1900)** proposed that the light energy emitted by the black body is quantized in units of $h\nu$ (ν = frequency of light).

$$E = nh\nu \quad (n = 1, 2, 3, \ldots)$$

- High frequency light is only emitted from the black body if thermal energy $kT \geq h\nu$.

- $h\nu$ – a quantum of energy.

- Planck's constant $h \sim 6.626 \times 10^{-34}$ J.s

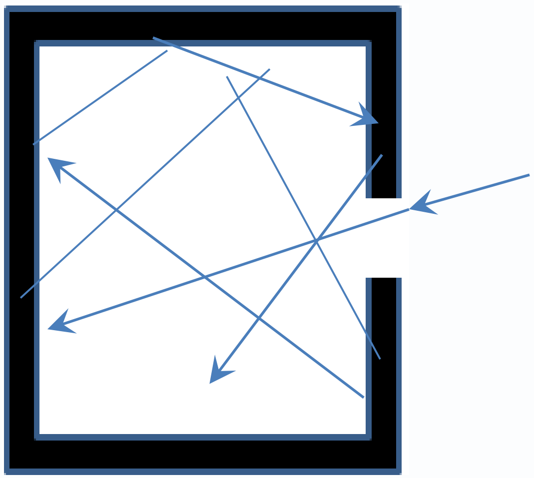
- If $h \to 0$ we regain classical mechanics.

- Planck (1900) : Vibrating atoms that emit light do so in discrete amounts.
- Einstein (1905) : Light propagates in discrete wave packets called photons, with the energy of each photon being related to the wave frequency by Planck's relation.

Black Body Radiation

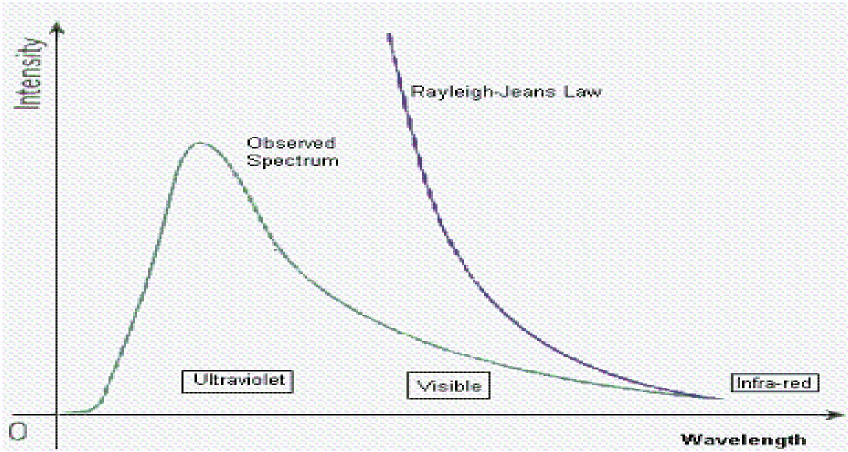
A black body is an ideal body which allows the whole of the incident radiation to pass into itself (without reflecting the energy) and absorbs within itself the whole incident radiation (without passing on the energy).

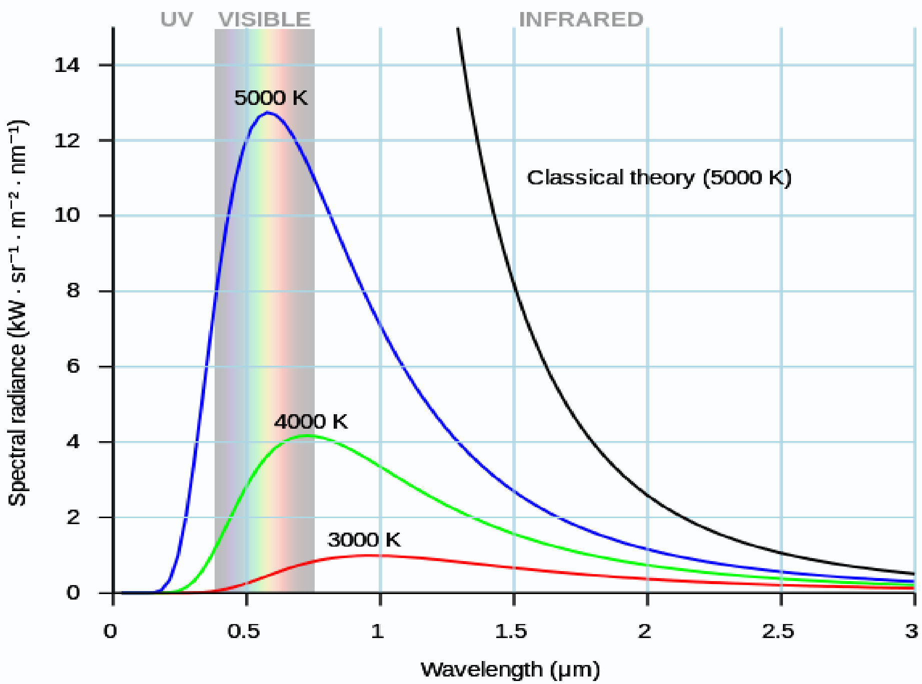
This propety is valid for radiation corresponding to **all wavelengths and to all angles of incidence**. Therefore, the black body is an ideal absorber of incident radiation.



Kirchhoff's design of black body (1859).

Experimental Characteristics of Black Body Radiation





As the temperature increases peak wavelength emitted by black body decreases .

Spectral radiance: Power per unit area per unit wavelength

Image Source: https://en.wikipedia.org/wiki/Planck's_law#/media/File:Black_body.svg

Classical Explanation

Stefan–Boltzmann law

In 1879, J. Stefan found experimentally that the total intensity (or the total power per unit surface area) radiated by a glowing object of temperature T is given by

$$I = a\sigma T^4$$

which is known as the **Stefan–Boltzmann law**.

Where, $\sigma = 5.67 \times 10^{-8}\ Wm^{-2}\ K^{-4}$ is the Stefan–Boltzmann constant, and a is a coefficient which is less than or equal to 1; in the case of a blackbody a = 1.

Wien's law

In 1894, Wien extended it.

$$\lambda_{max} T = \text{constant} = 2898\ \mu mK$$

Although Wien's formula fits the high-frequency/low wavelength data remarkably well, it fails badly at low frequencies.

Rayleigh-Jeans Law

* It agrees with experimental measurements for long wavelengths.
* It predicts an energy output that **diverges towards infinity as wavelengths grow smaller.**
* The failure has become known as the **ultraviolet catastrophe**.

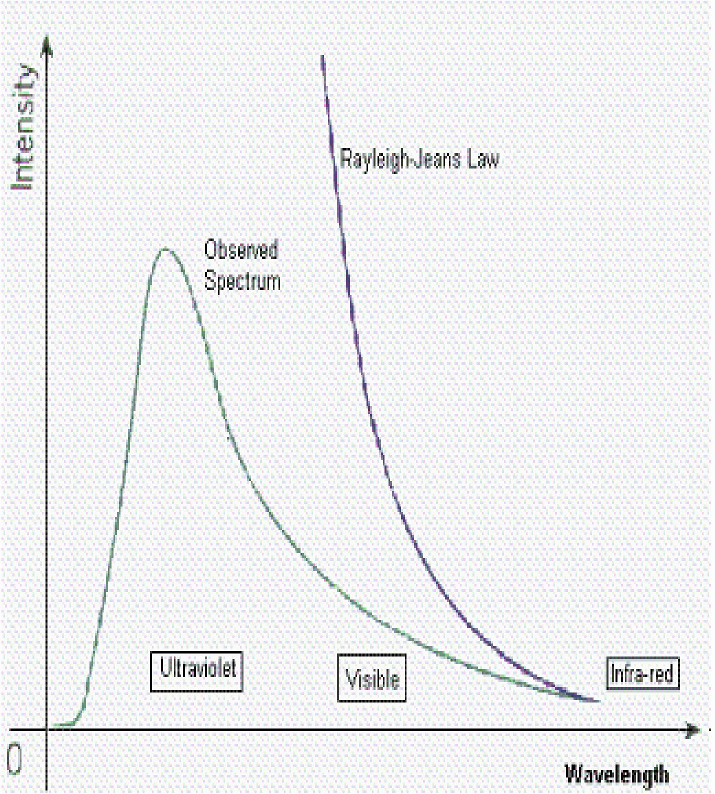
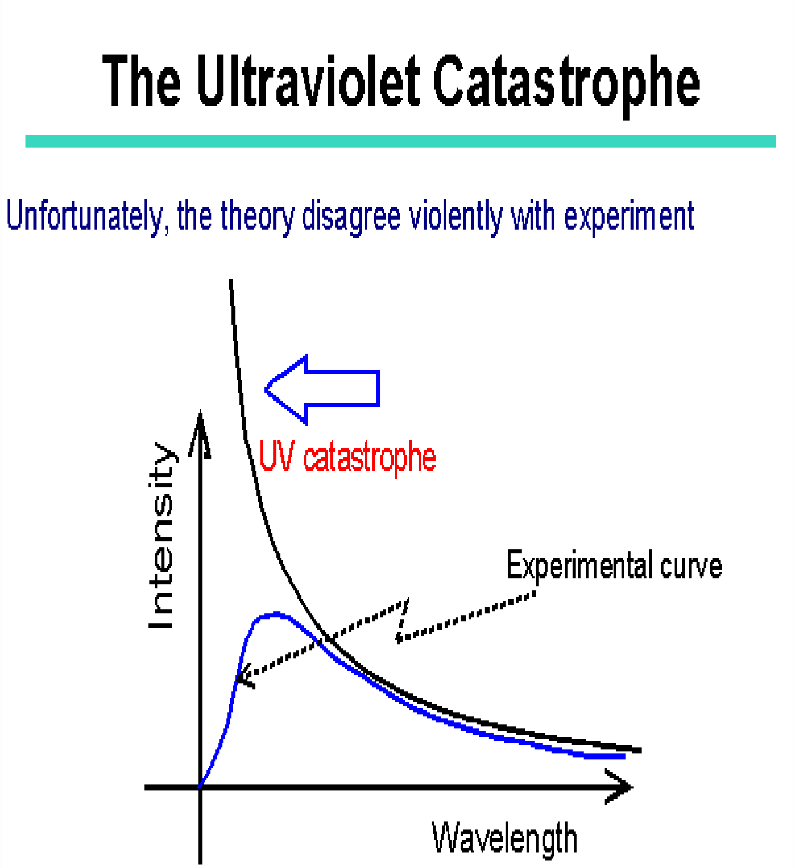


Image Source: http://www.egglescliffe.org.uk/physics/astronomy/blackbody/Image22c.gif

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

- This formula also had a problem. The problem was with the λ term in the denominator.
- For large wavelengths it fitted the experimental data but it had major problems at shorter wavelengths.

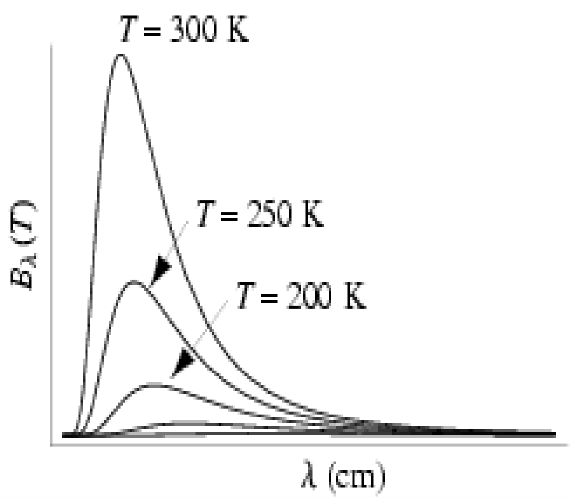


http://theory.uwinnipeg.ca/users/gabor/foundations/quantum/images/slide5.gif

Quantum Mechanical Explanation

In 1900, Max Planck suggested that oscillating atoms could emit or absorb energy in the tiny bursts of energy called quanta. Planck's suggestion imparts a discrete or particle nature to radiation.

E= *hv* (h is Planck's constant)

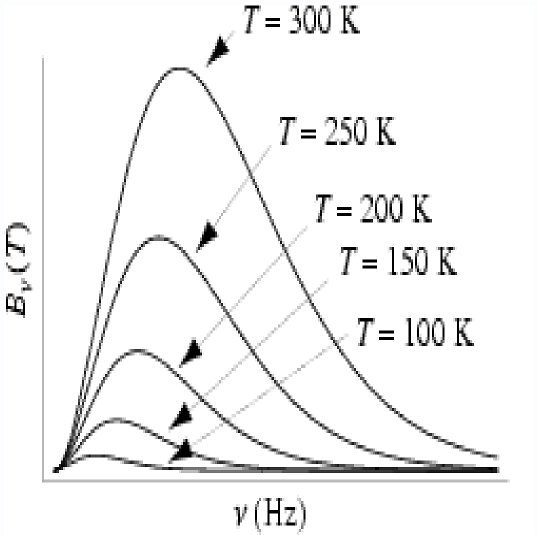


As a function of wavelength.

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

As a function of frequency

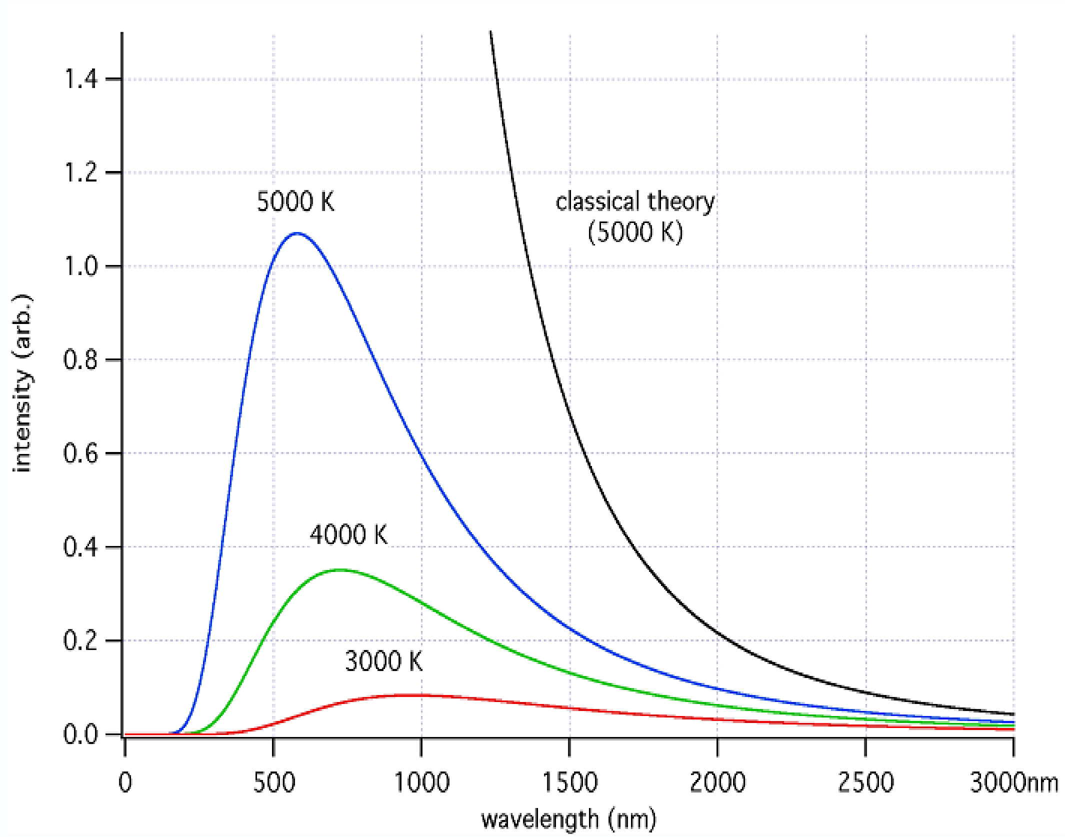
$$I(\nu, T) = \frac{2h\nu^3}{c^2} \frac{1}{e^{\frac{h\nu}{kT}} - 1}$$

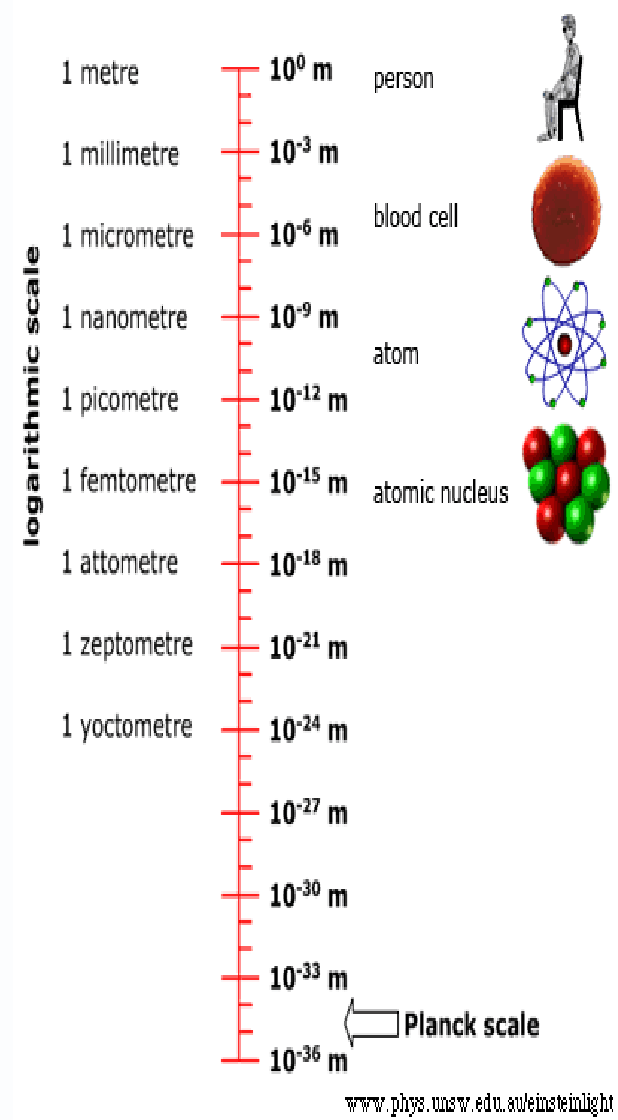


The Planck's Law gives a distribution that peaks at a certain wavelength, the peak shifts to shorter wavelengths for higher temperatures, and the area under the curve grows rapidly with increasing temperature.

http://scienceworld.wolfram.com/physics/PlanckLaw.html

Comparison between Classical and Quantum viewpoints

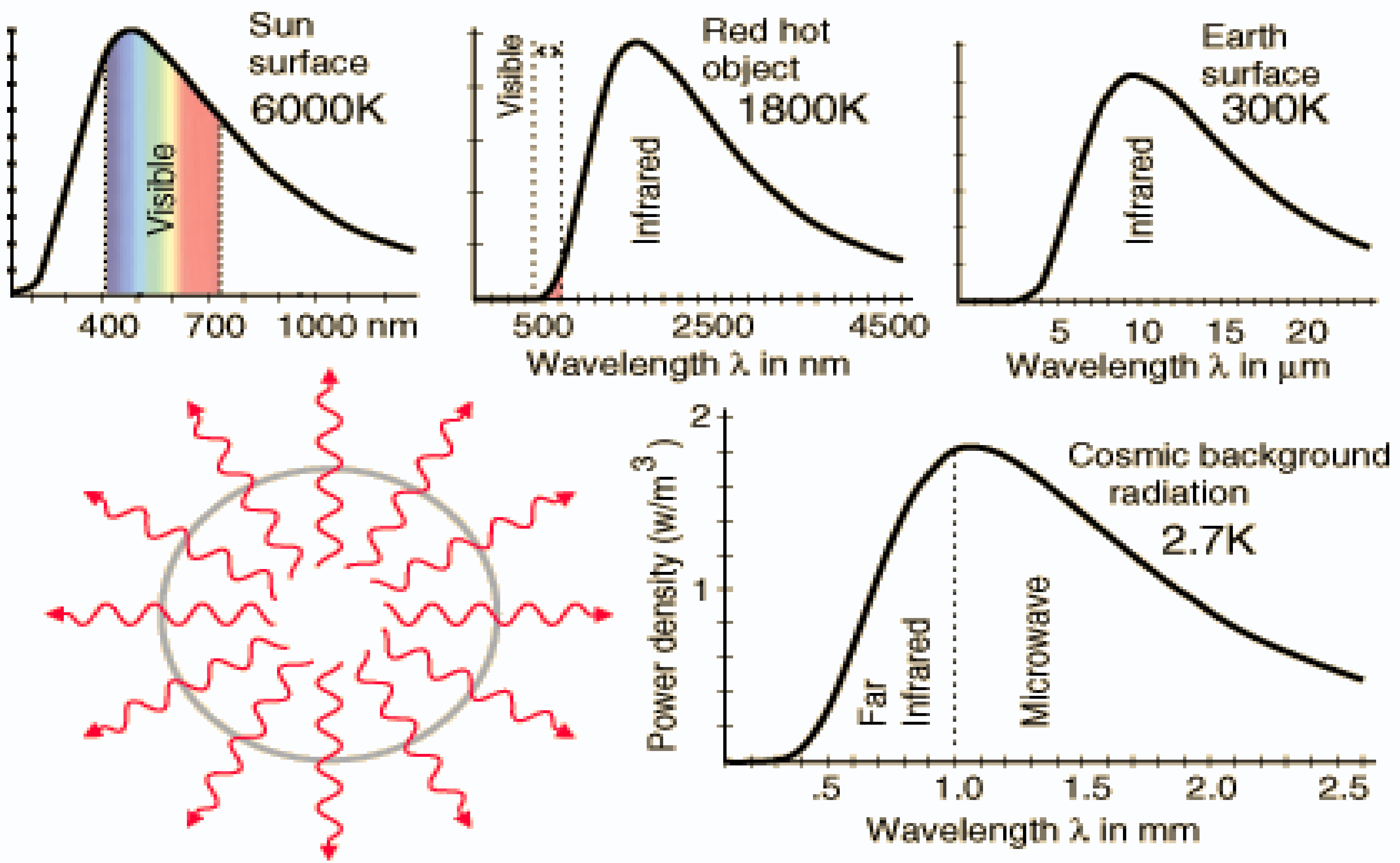




There is a good fit at long wavelengths, but at short wavlengths there is a major disagreement. Rayleigh-Jeans $\longrightarrow \infty$, but Black-body $\longrightarrow$ 0.

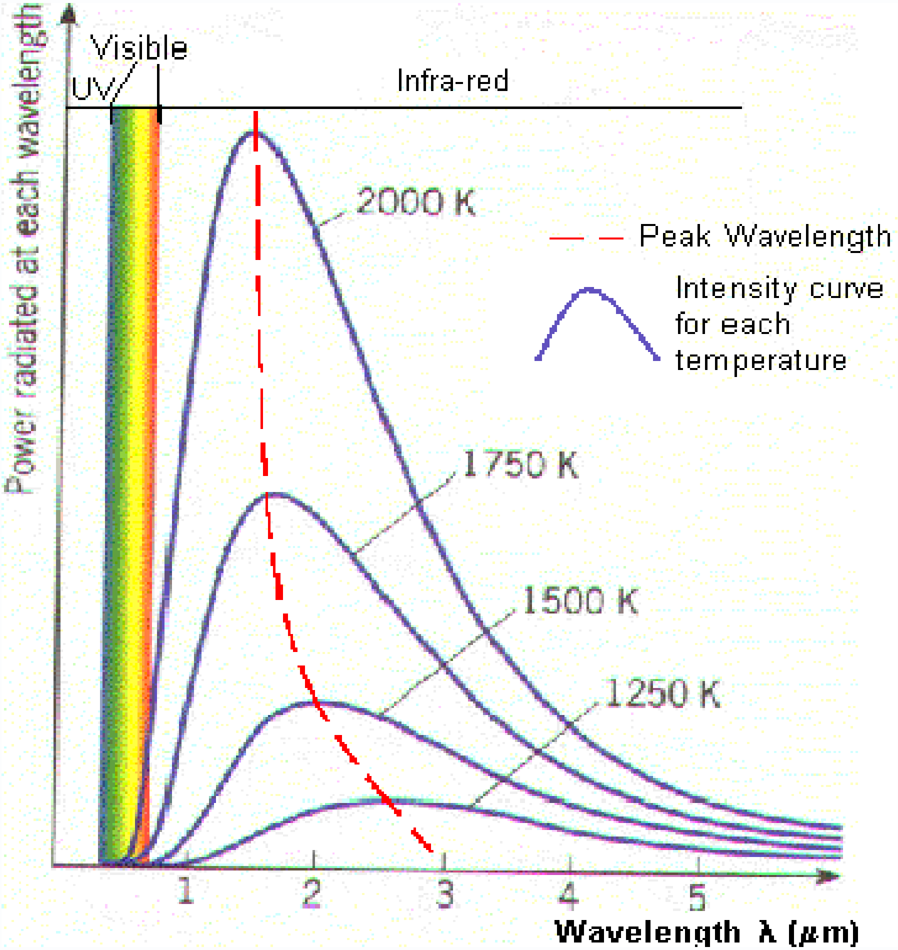
http://upload.wikimedia.org/wikipedia/commons/a/a1/Blackbody-lg.png

Radiation Curves



Conclusions

- As the temperature increases, the peak wavelength emitted by the black body decreases.
- As temperature increases, the total energy emitted increases, because the total area under the curve increases.
- The curve gets infinitely close to the x-axis but never touches it.



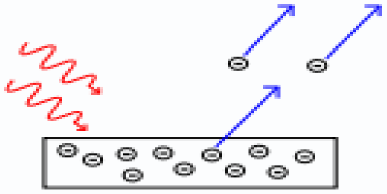
https://phet.colorado.edu/sims/blackbody-spectrum/blackbody-spectrum_en.html

http://www.astro.ufl.edu/~oliver/ast3722/lectures/BasicDetectors/BlackBody.gif

Photoelectric Effect

Classical wave explanation

In 1887 Hertz discovered the photoelectric effect: electrons (confirmed by J.J. Thomson) were observed to be ejected from metals when irradiated with light. Moreover, the following experimental laws were discovered prior to 1905:



(Image Source: Wikipedia)

❖Intensity of light (radiation) should have a proportional relationship with the resulting maximum kinetic energy of photo electron.

❖Photo electric current occur for any light regardless of frequency or wavelength.

❖There should be delay on the order of seconds between the radiation contact with the metal and initial release of photo electron.

Quantum Mechanical Explanation

In 1905, Albert Einstein solved this apparent paradox by describing light as composed of discrete quanta, now called photons, rather than continuous waves.

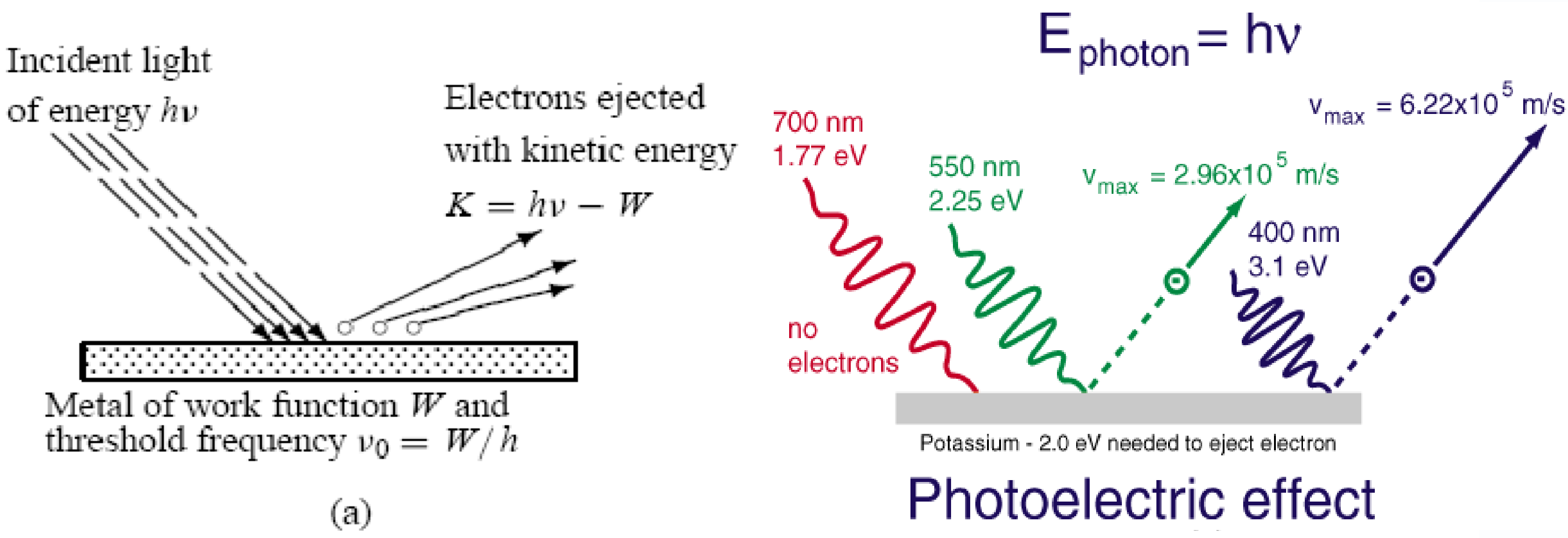
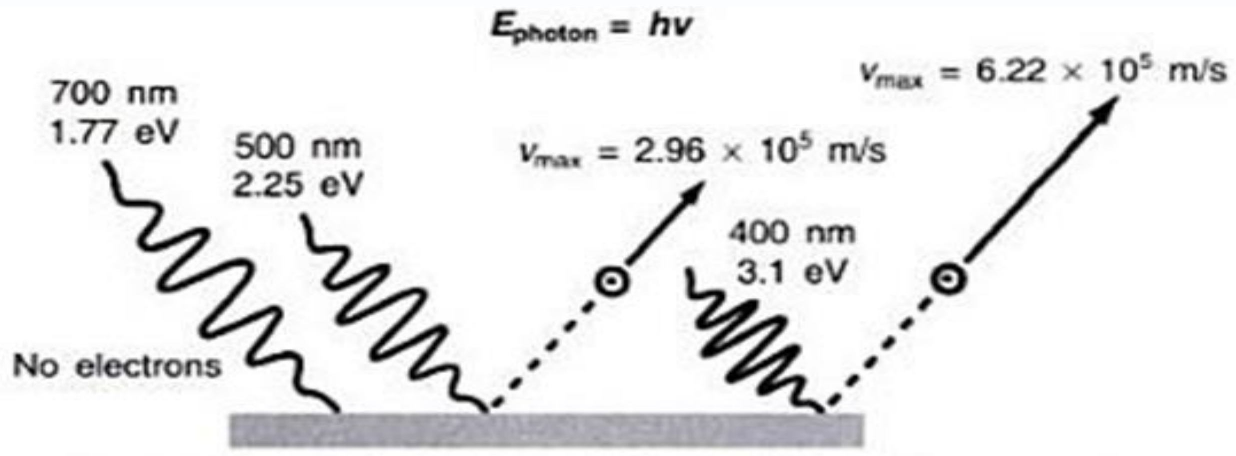


Figure 1.3 (a) Photoelectric effect: when a metal is irradiated with light, electrons may get emitted. (b) Kinetic energy K of the electron leaving the metal when irradiated with a light of frequency ν; when $\nu < \nu_0$ no electron is ejected from the metal regardless of the intensity of the radiation.

$$K = h\nu - W = h(\nu - \nu_0),$$

where *K* represents kinetic energy of the electron leaving the metal surface.

Reference: Quantum mechanics: Concepts and Applications by N. Zettili



Potassium –2.0 eV energy is needed to eject a photoelectron

Explanation of particle nature of light in photoelectric effect. The following algebraic relation $h\nu = \phi + KE_{max}$ explains that a part of the incident photon energy is used to overcome the work function ($\phi = h\nu_0$, ν_0 = threshold frequency) of the material to extract a photoelectron and rest is converted to the kinetic energy of the photoelectron ($1/2\ mv^2_{max}$). Therefore, one can rewrite the above relation as $h\nu = h\nu_0 + (1/2)\ mv^2_{max} \Rightarrow h(\nu - \nu_0) = (1/2)\ mv^2_{max}$. Therefore, below the threshold frequency there will be no photo-electron emission, however, intense the incident light might be.

Albert Einstein awarded the Nobel prize in 1921 for his discovery of the law of photoelectric effect.

Experimental Result

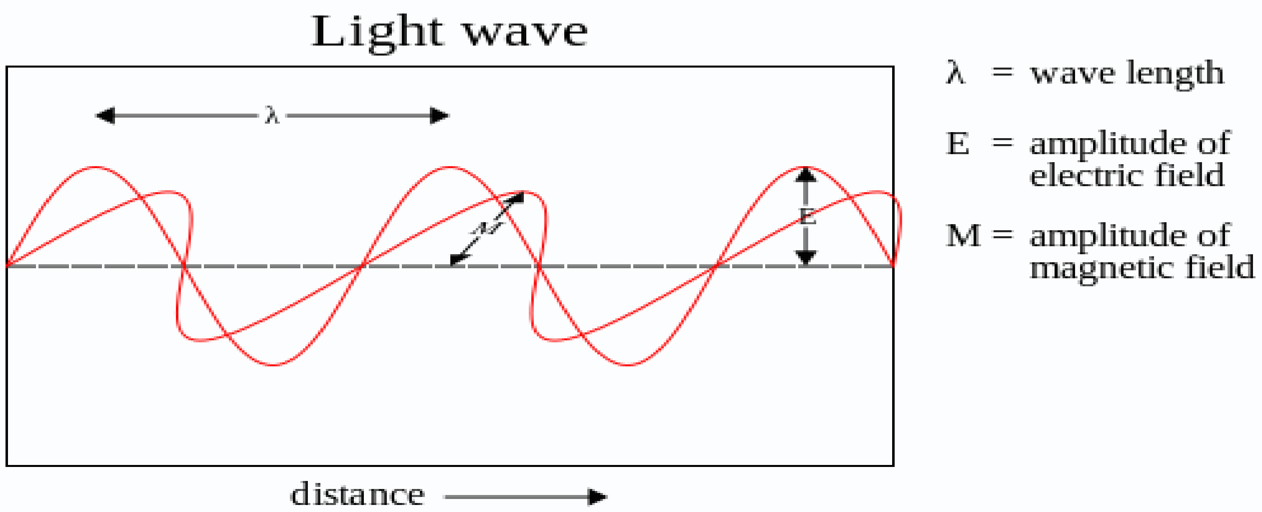
1. The photoelectric effect provides evidence for the particle nature of light.

1. It also provides evidence for quantization.

1. The intensity of light source had no effect on the maximal kinetic energy of the photo electrons.

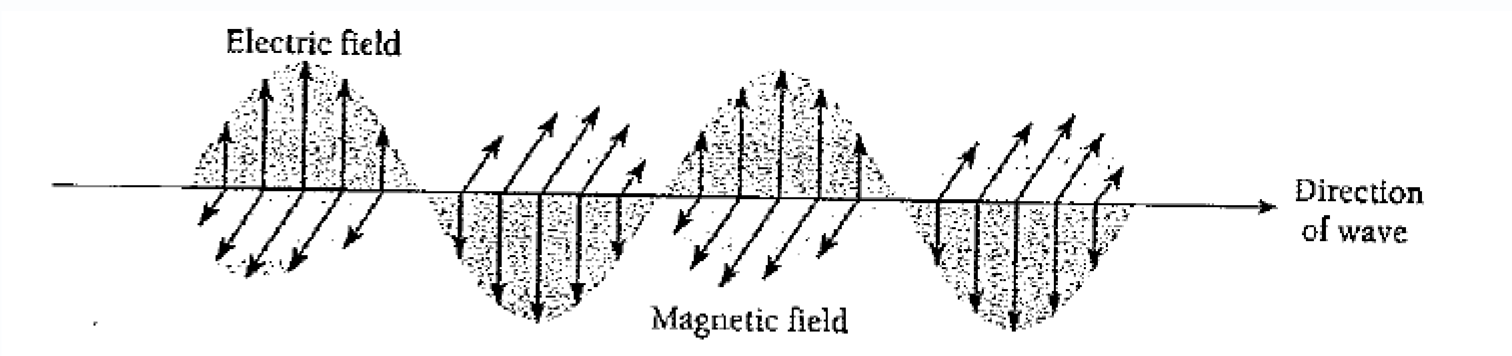
1. Below a certain frequency the photoelectric effect does not occur at all.

1. There is no significant delay (less than 10-9 second) between the light source activation and the emission of the first photo electrons.



Light comes in packets or “quanta”.

Light waves carry energy only in packets, with high frequency light consisting of large packets of energy and low frequency light consisting of small packets of energy.



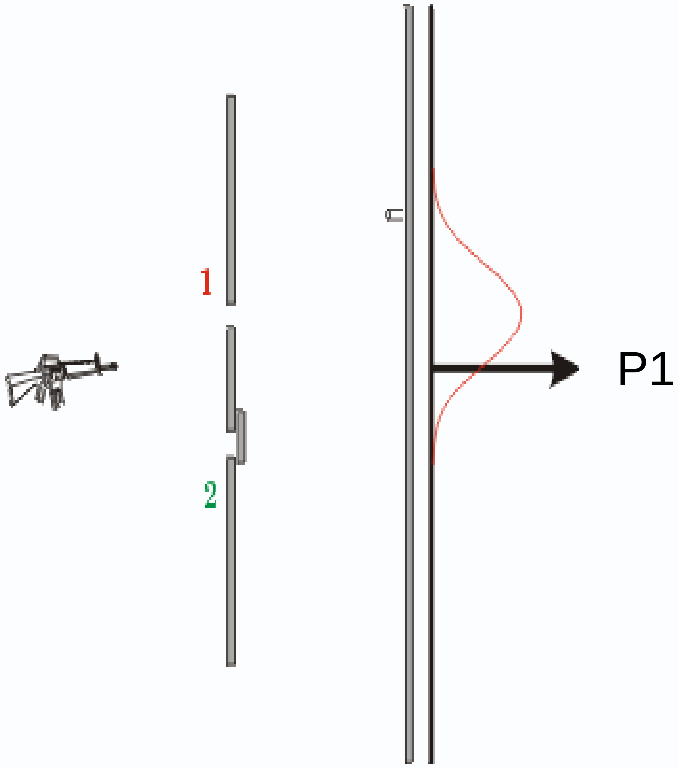
Light: A Particle or Wave

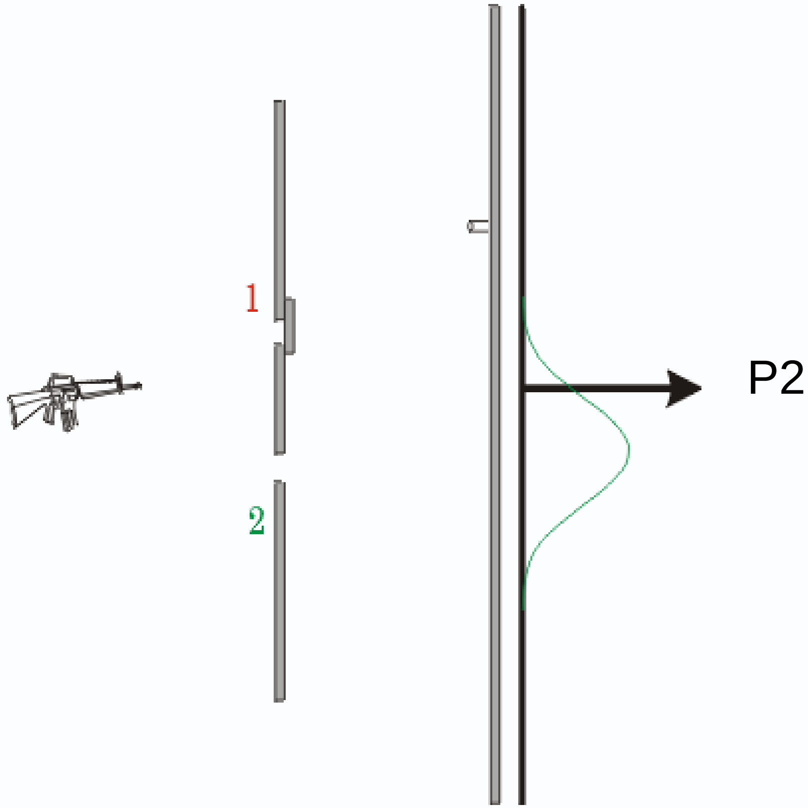
- Different tests support different sides of the argument
- Today : Wave particle duality.

2-slit experiments with bullets (Particles)

Particles through single slit :

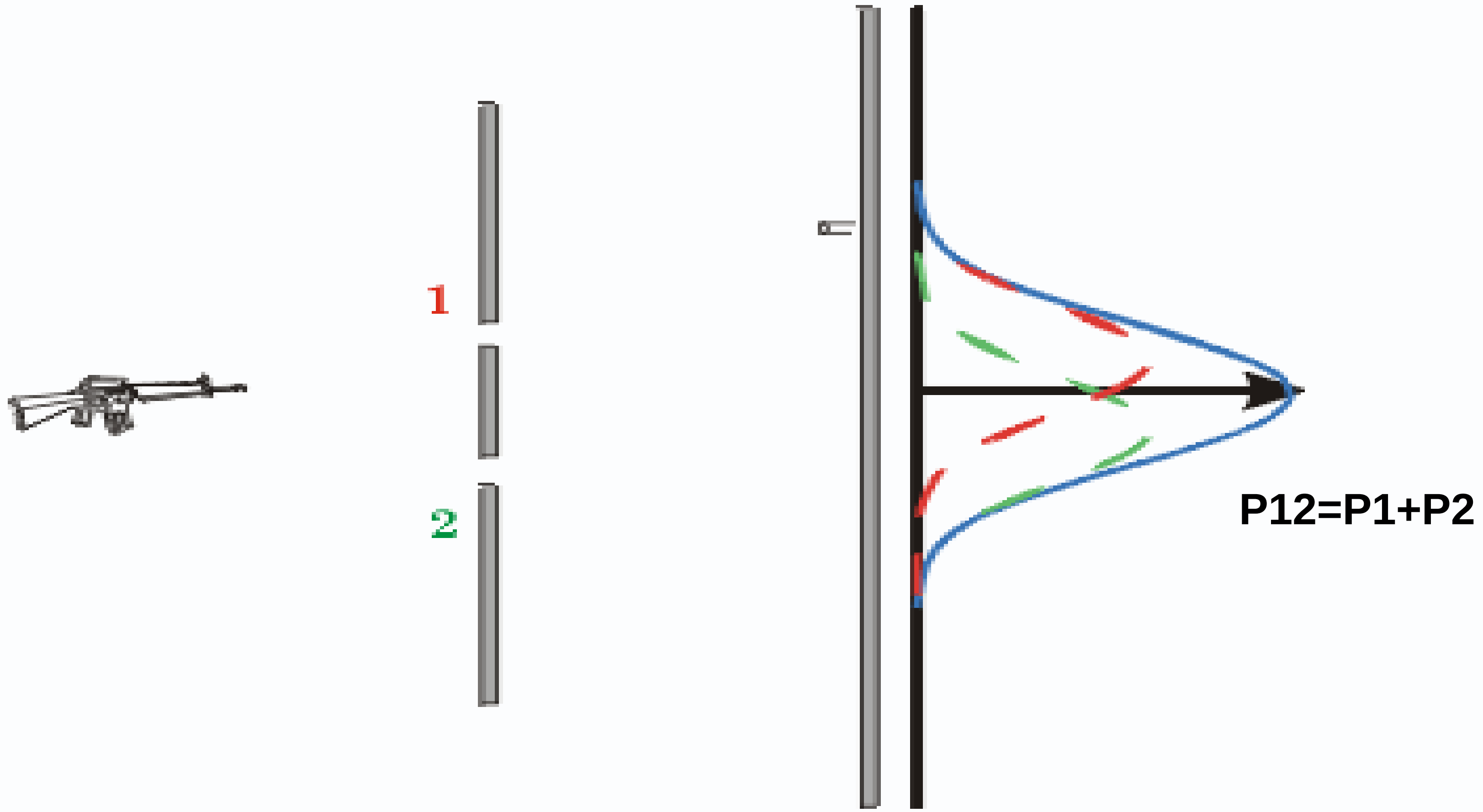
Bullets always come in "lumps" -- identical size and mass.





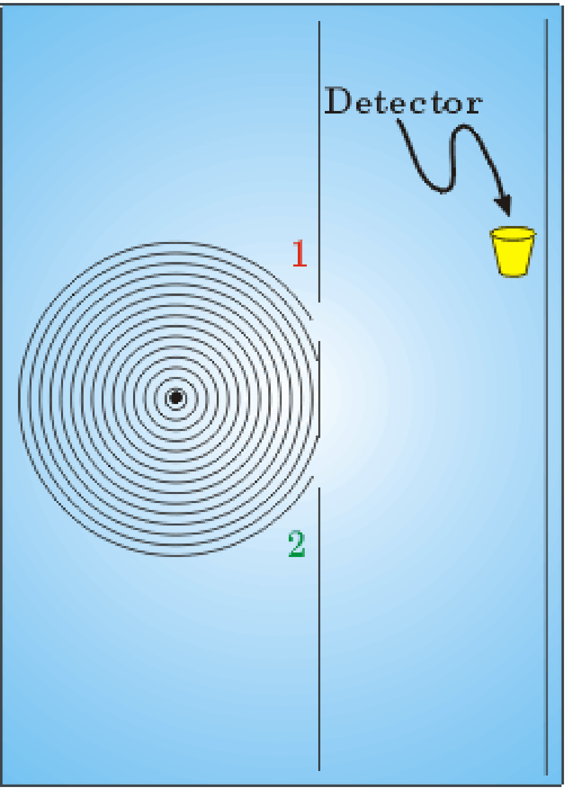
“God does not play dice with the universe.” — Albert Einstein

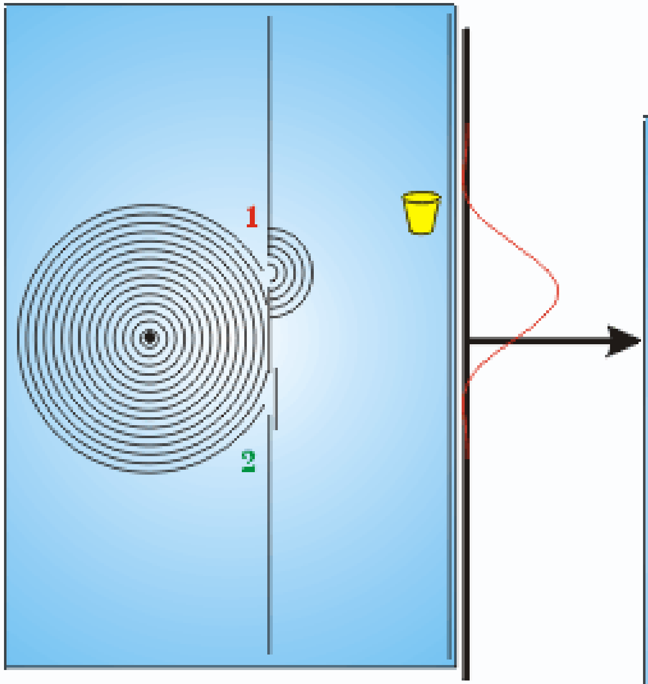
Particles through both slits :



No interference: Probability to arrive at screen is sum of probability to go through slit 1 and probability to go through slit 2, smooth distribution.

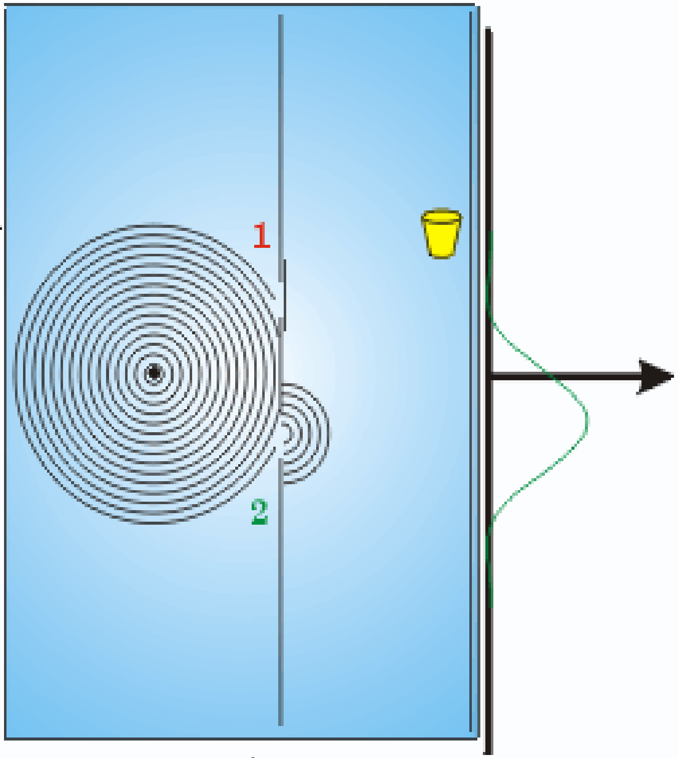
2-slit experiments with water waves





When 1st Slit open

$I_1=|h1|^2$

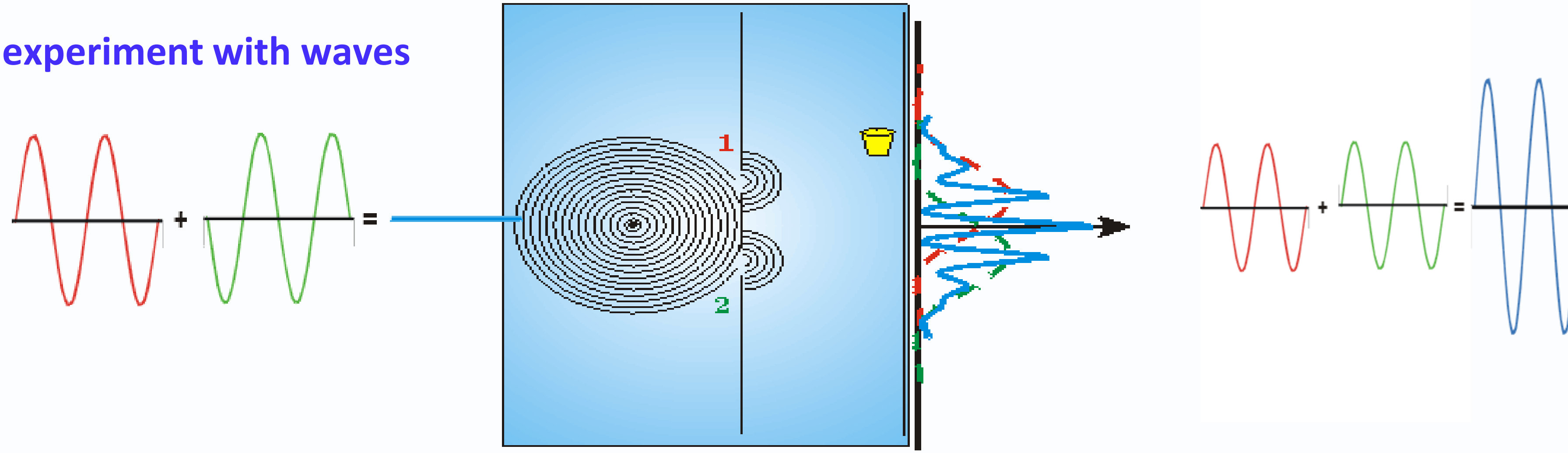


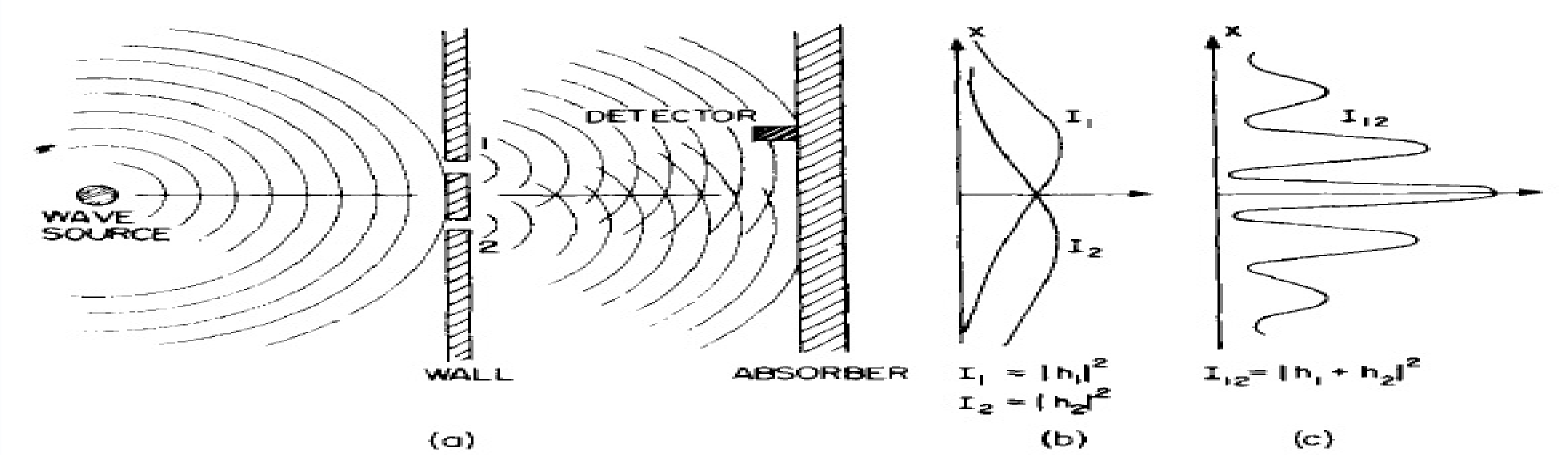
When 2nd Slit open

$I_2=|h2|^2$

Intensity of water waves proportional to square of height.

An experiment with waves





$$I_1 = |h_1|^2, \quad I_2 = |h_2|^2, \quad I_{12} = |h_1 + h_2|^2.$$

$$I_{12} = I_1 + I_2 + 2\sqrt{I_1 I_2}\cos\delta.$$

where δ is the phase difference between h_1 and h_2

2-slit experiment with electrons

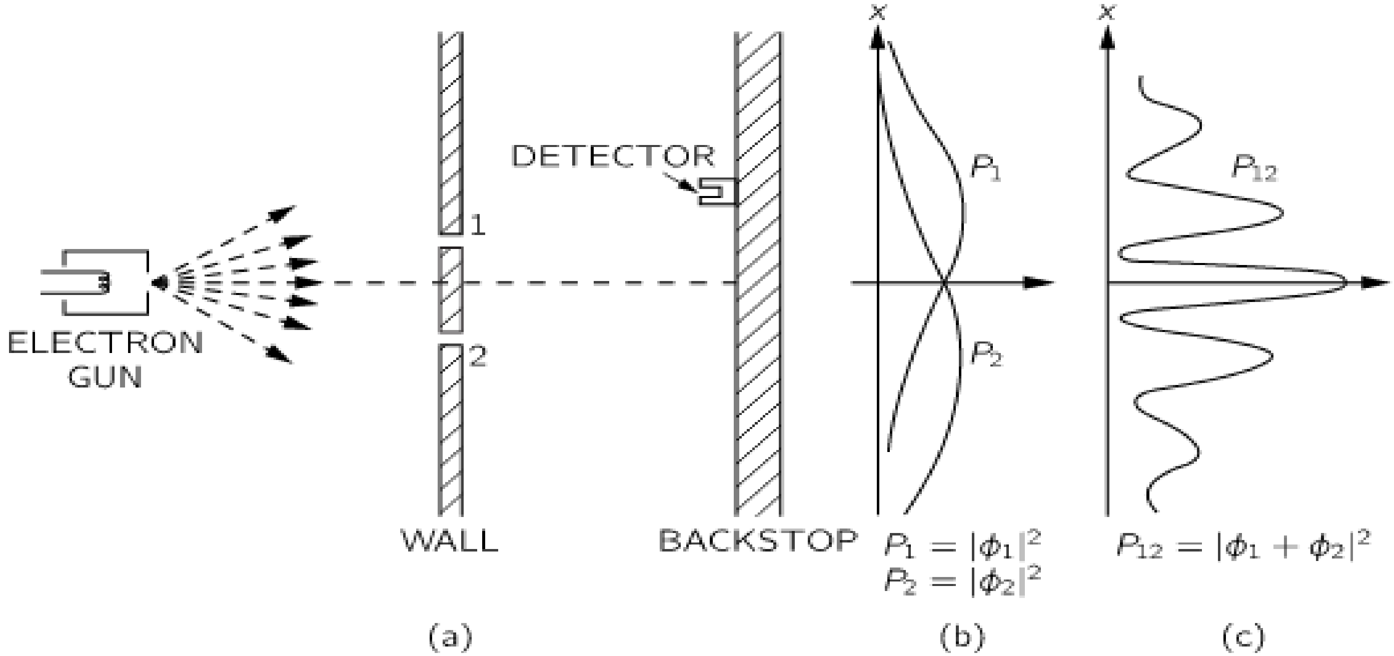


Fig. 1–3. Interference experiment with electrons.

What is the relative probability that an electron 'lump' will arrive at the backstop at various distances from the center?

The results of our experiment is the interesting curve marked *P*12 in part (c). This is the way electrons go.

The interference of electron waves

Proposition A :	**Each electron *either* goes through hole 1 *or* it goes through hole 2.**

The result P_{12} obtained with both holes open is clearly not the sum of P_1 and P_2, the probabilities for each hole alone. *In* analogy with our water wave experiment, we say, "There is interference"

For electrons: $$P_{12} \neq P_1 + P_2.$$

Undoubtedly we should conclude that *Proposition A is false*. It is *not* true that the electrons go *either* through hole 1 or hole 2. But before taking the conclusion, let us test it by another experiment.

If electrons can be seen to go through one slit or the other, how can they interfere with themselves? Let's try to determine which slit they pass through with a "camera“.

Watching the electrons

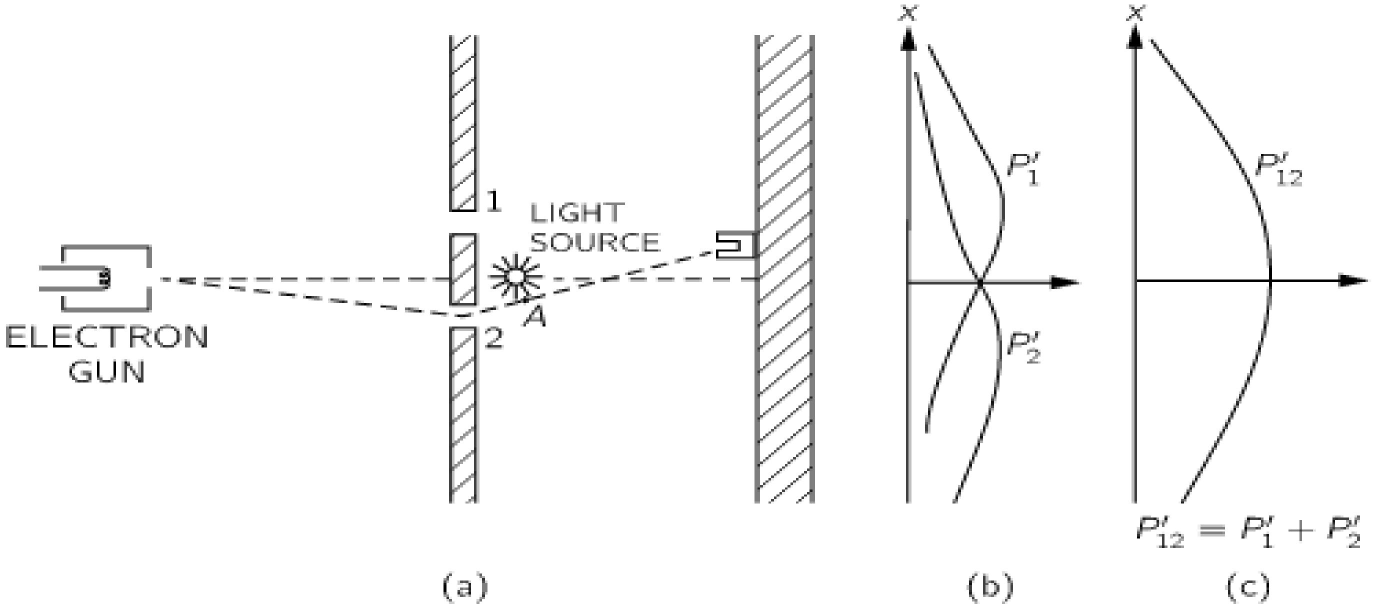


Fig. 1–4. A different electron experiment.

If the motion of all matter—as well as electrons—must be described in terms of **waves**, what about the bullets in the previous experiment? **Why didn't we see an interference pattern there?**

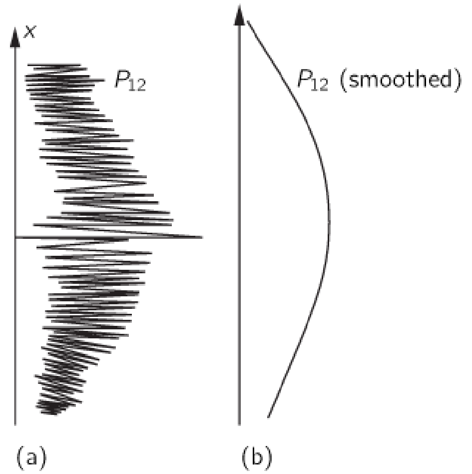
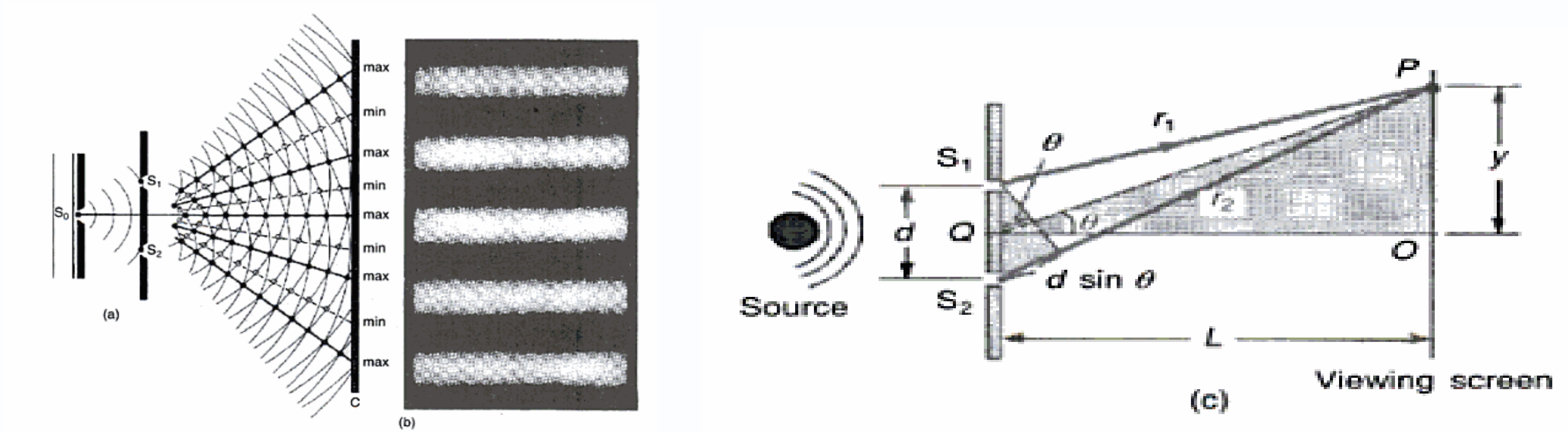


Fig. 1–5. Interference pattern with bullets: (a) actual (schematic), (b) observed.

We conclude in the following way : The electrons arrive in lumps, like particles, and the probability of arrival of these lumps is distributed like the distribution of intensity of a wave. It is in this sense that an electron behaves "sometimes like a particle and sometimes like a wave."

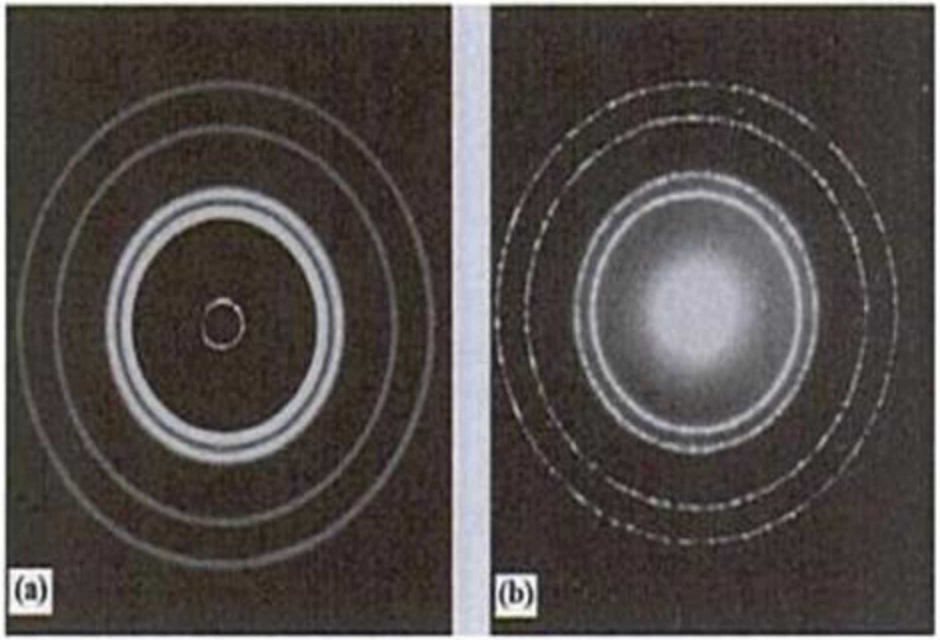
Young's Double Slit Experiment of Light



Schematic representation of Young's double slit experiment showing interference pattern.

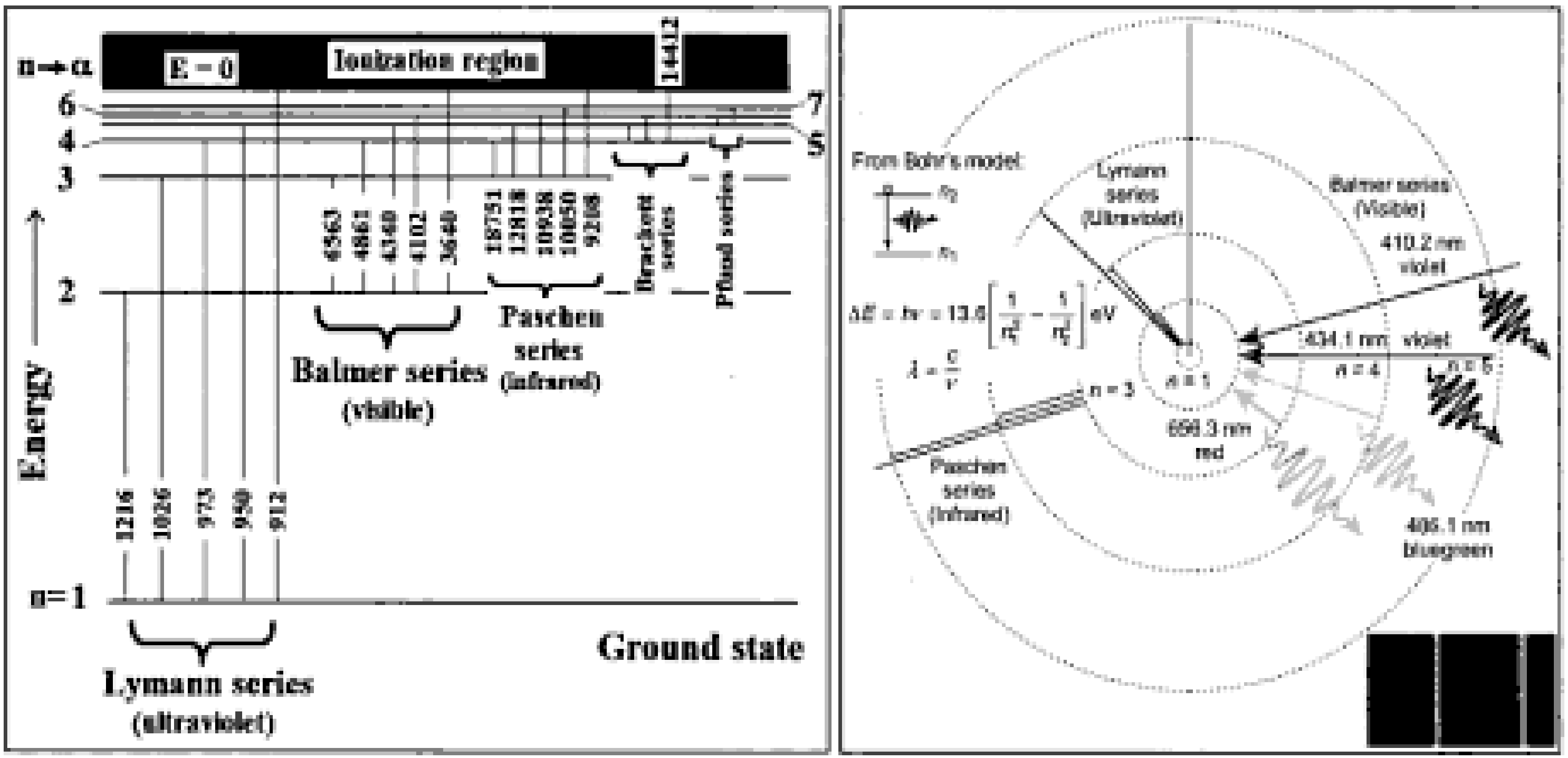
The wave nature of light was established by Young's double slit experiment where the sinusoidal interference pattern of coherence light falling on a screen behind two linear slits of small spacing d, is guided by $n\lambda = d \sin\theta$, where λ is the wavelength of light and θ is the angular position of the appearance of maxima on the interference pattern and n is an integral number.

The path difference of the light from two slits shall be an integral multiple of light wavelength $n\lambda$.



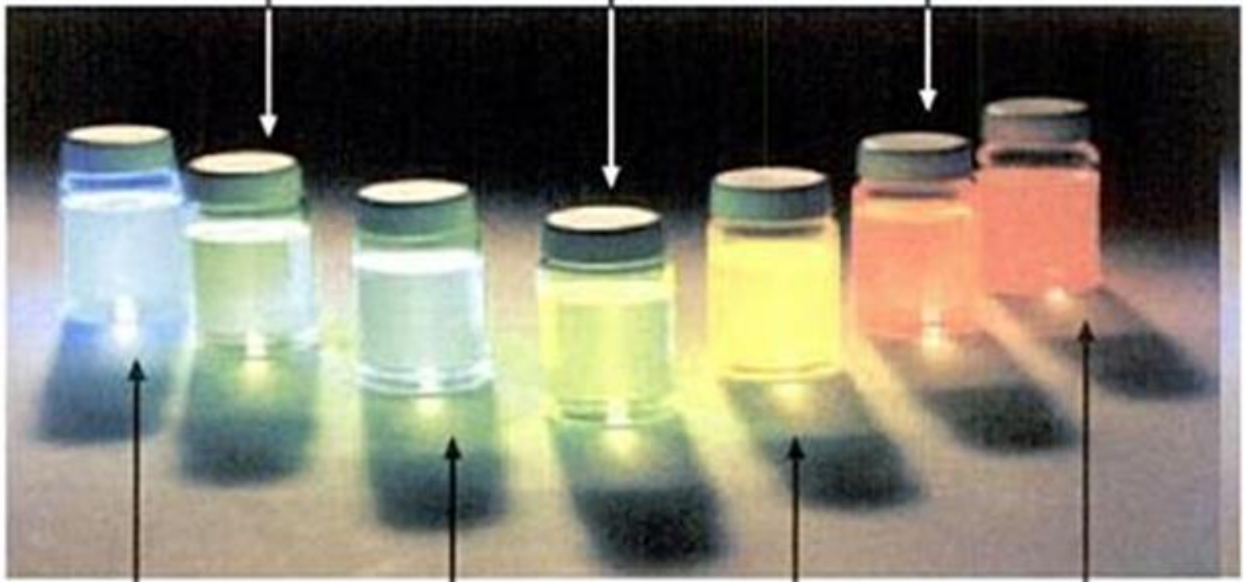
Diffraction pattern of **(a)** a beam of X-ray passing through thin aluminium foil, and **(b)** by a beam of electrons passing through the same foil.

Bohr's model of Hydrogen Atom



(a) (b)

Fig. 5.5 **(a)** Hydrogen line spectra, and **(b)** description of the transitions various Bohr orbits.



Images of core-shell CdSe/ZnS quantum dots stored in vials, showing emission of different colours with change in the size of the QDs.