

# Quantum Mechanics (Unit IV)

**Please read from any  
standard text book**

**Engineering Physics, Second Edition (H.K.Malik & A.K.Singh). :  
Chapter 15 (Development of Quantum Mechanics) and Chapter 16  
(Quantum Mechanics)**



**Both Chapters Included**

**Why Quantum Mechanics??????**

**Failure of Classical Mechanics**



**Need for Another Mechanics  
(Theory) ??????????????????**



**Development of Quantum  
Mechanics**

# Classical Mechanics-A Brief History Behind QM



Library of Congress

**Newton, Sir Isaac, PRS,**  
(1643 – 1727), English  
physicist and  
mathematician

$$\vec{F} = m \frac{d^2 \vec{x}}{dt^2}$$

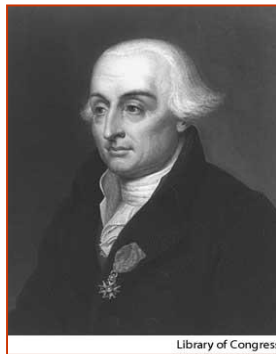
$$\vec{F} = -G \frac{m_1 m_2}{|\vec{x} - \vec{x}'|^3} (\vec{x} - \vec{x}')$$

$$G = 6.6726 \times 10^{-11} \text{m}^3 \cdot \text{s}^{-2} \cdot \text{kg}^{-1}$$

$$g = 9.8067 \text{m} \cdot \text{s}^{-2}$$



**Euler, Leonhard**  
(1707 -- 1783),  
Swiss  
mathematician.



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**Lagrange, Joseph Louis**  
(1736 -- 1813),  
Italian-French mathematician,  
astronomer and physicist.

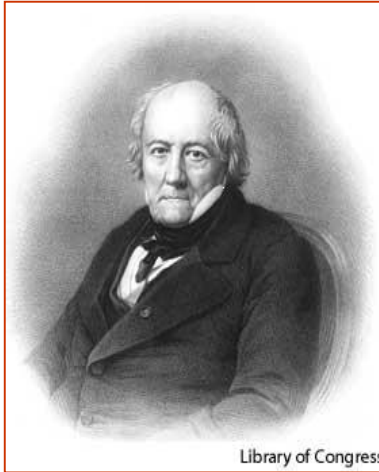


**Hamilton, William Rowan (1805 -- 1865),**  
Irish mathematician and  
astronomer.

# Classical Electrodynamics



**Coulomb, Charles Augustin (1736 – 1806), French physicist**



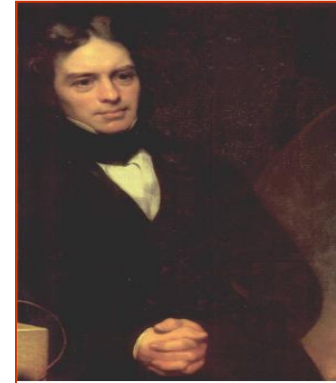
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**Biot, Jean Baptiste (1774 --1862), French Physicist;  
Savart, Félix (1791 -- 1841), French Physicist**



b / André Marie Ampère (1775-1836).

**Ampere, Andre Marie (1775 -- 1836), French Physicist**



h / Michael Faraday (1791-1867), the son of a poor blacksmith, discovered induction experimentally.

**Faraday, Michael (1791 -- 1867), English Physicist**



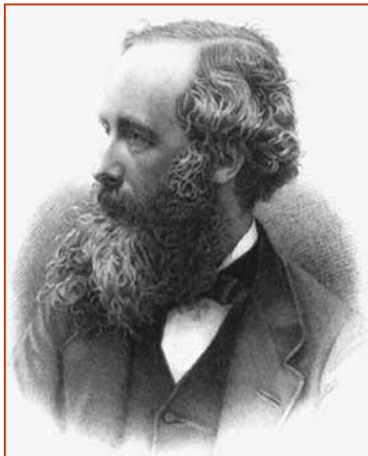
**Hendrik Antoon Lorentz**

1/2 of the prize the Netherlands

Leiden University Leiden, the Netherlands

b. 1853  
d. 1928

**Lorentz, Hendrik Antoon (1853 -- 1928), Dutch Physicist**



Library of Congress

$$\rho(\vec{x}, t) = \sum_{\alpha} q_{\alpha} \delta(\vec{x} - \vec{x}_{\alpha}(t)),$$

$$\vec{j}(\vec{x}, t) = \sum_{\alpha} q_{\alpha} \vec{v}_{\alpha}(t) \delta(\vec{x} - \vec{x}_{\alpha}(t)),$$

$$m_{\alpha} \ddot{\vec{x}}_{\alpha}(t) = q_{\alpha} \left[ \vec{E}(\vec{x}_{\alpha}(t), t) + \frac{\vec{v}_{\alpha}(t) \times \vec{B}(\vec{x}_{\alpha}(t), t)}{c} \right].$$

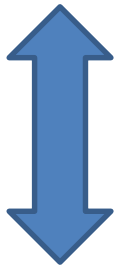
**Maxwell, James Clerk (1831 – 1879), Scottish physicist**

# **Experiments and Ideas Prior to Quantum Theory**

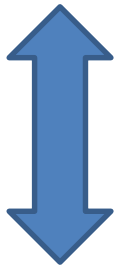
**(Before 1913)**

# **Blackbody Radiation and Quanta of Energy**

# Ultra-violate Catastrophe



## Failure of Classical Physics

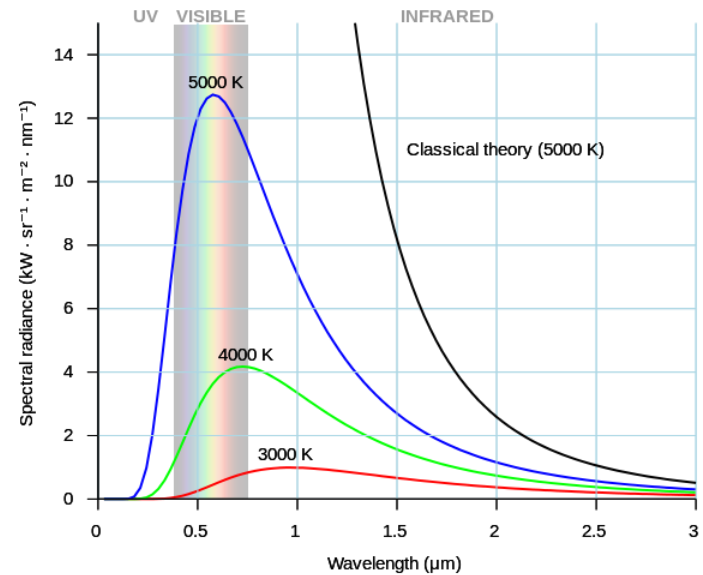


## Rayleigh-Jeans Law



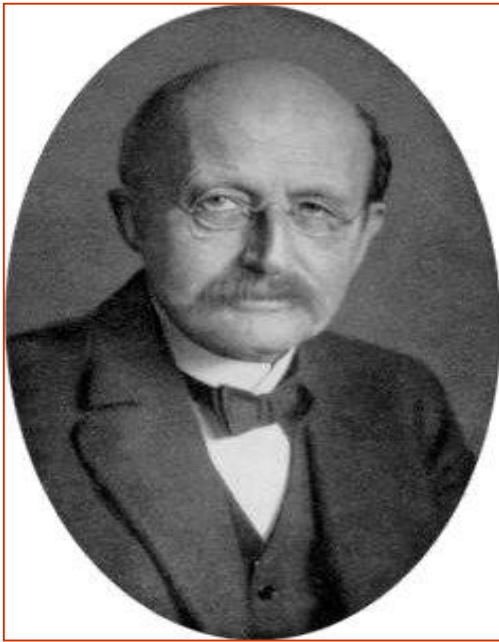
$$E(\nu)d\nu \propto \nu^2 KT d\nu$$

There will be infinite amount of energy at higher frequency (UV-Region) or at higher temperature: **Wrong, it never happens.**



Blue, Green, Red: Experimentally Observed Spectrum.

Black: Predicted By Rayleigh-Jeans



### The Nobel Prize in Physics 1918

"in recognition of the services he rendered to the advancement of Physics by his discovery of energy quanta"

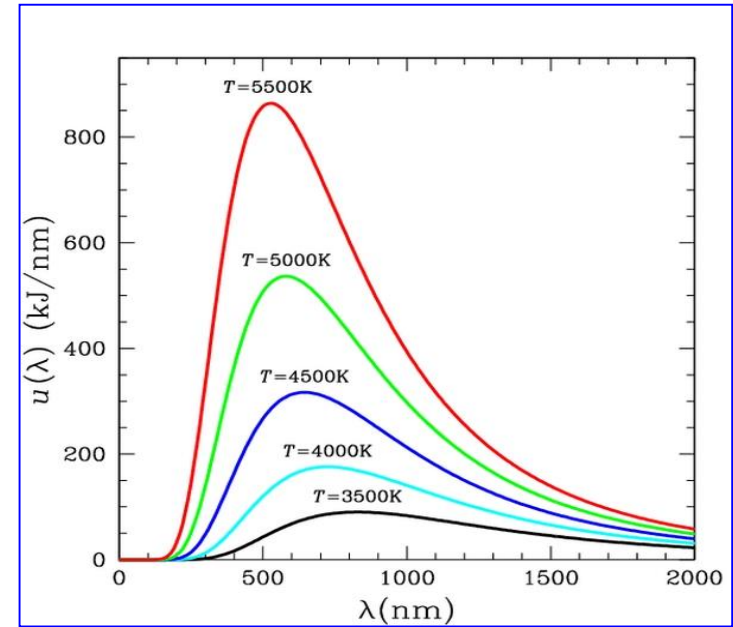


**Max Karl Ernst Ludwig Planck**

Germany

Berlin University  
Berlin, Germany

b. 1858  
d. 1947



**Planck (1858 -- 1947), German physicist.**

**Planck's law of black body radiation (1900)**

$$u_\nu d\nu = \frac{8\pi\nu^2}{c^3} \frac{h\nu}{e^{h\nu/K_B T} - 1} d\nu$$

**Planck's assumption (1900): Radiation of a given frequency  $\nu$  could only be emitted and absorbed in "quanta" of energy  $E=h\nu$**



# Failure of Classical Theory 1

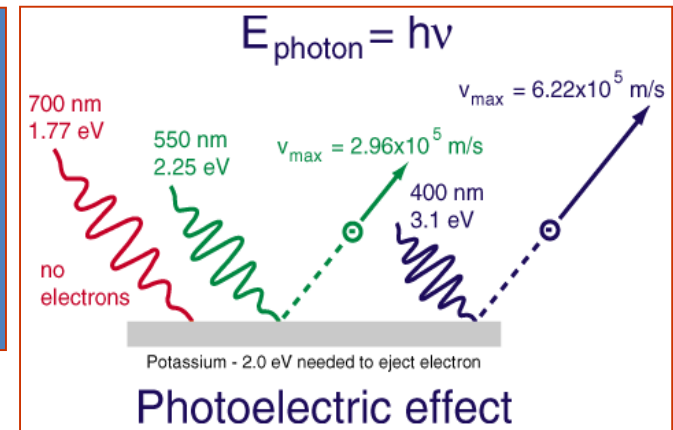
Classical theory suggested a “UV catastrophe,” leading to obviously nonsensical infinite energy radiating from hot body.

Max Planck solved this problem by postulating light quanta (now often called the father of quantum mechanics).

# **Radiation interaction with matter: Photoelectric Effect and Quanta of Light**

In 1839, Alexandre Edmond Becquerel observed the photoelectric effect via an electrode in a conductive solution exposed to light.

In 1905, Albert Einstein proposed the well-known Einstein's equation for photoelectric effect. Wins Nobel Prize (1921)



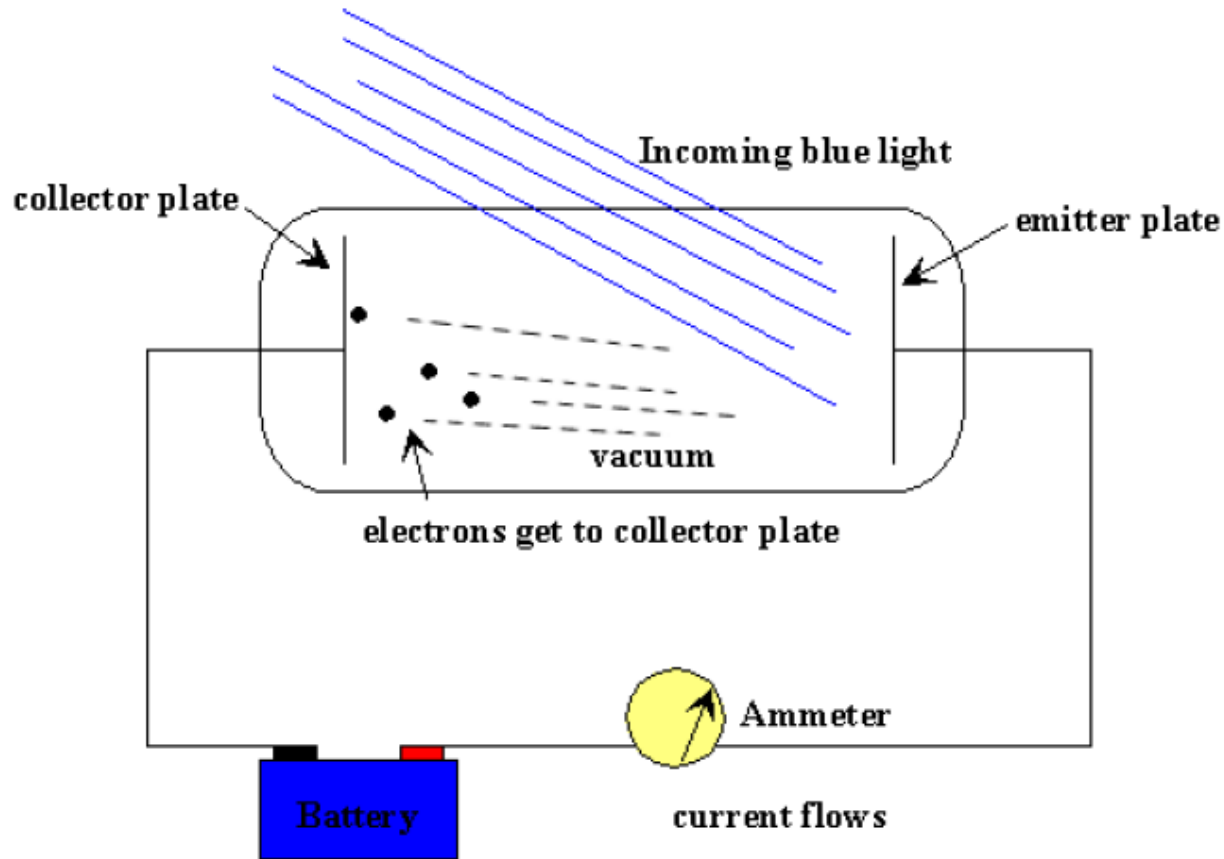
$$\frac{1}{2} m_e v_k^2 = E_k = h\nu - W$$

In 1916, Robert Andrews Millikan finished a decade-long experiment to confirm Einstein's explanation of photoelectric effect. Wins Nobel Prize (1923)

**Electric Charge of an electron**

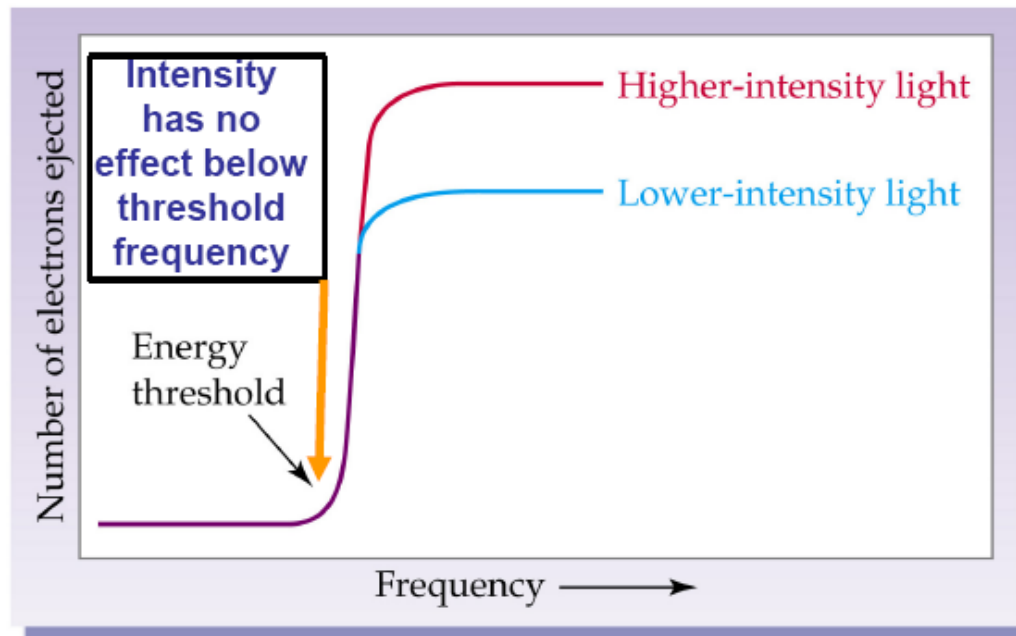
# Photoelectric Effect

A Photocell is Used to Study the Photoelectric Effect



# Photoelectric Effect

## Influence of Light Intensity on the Photoelectric Effect



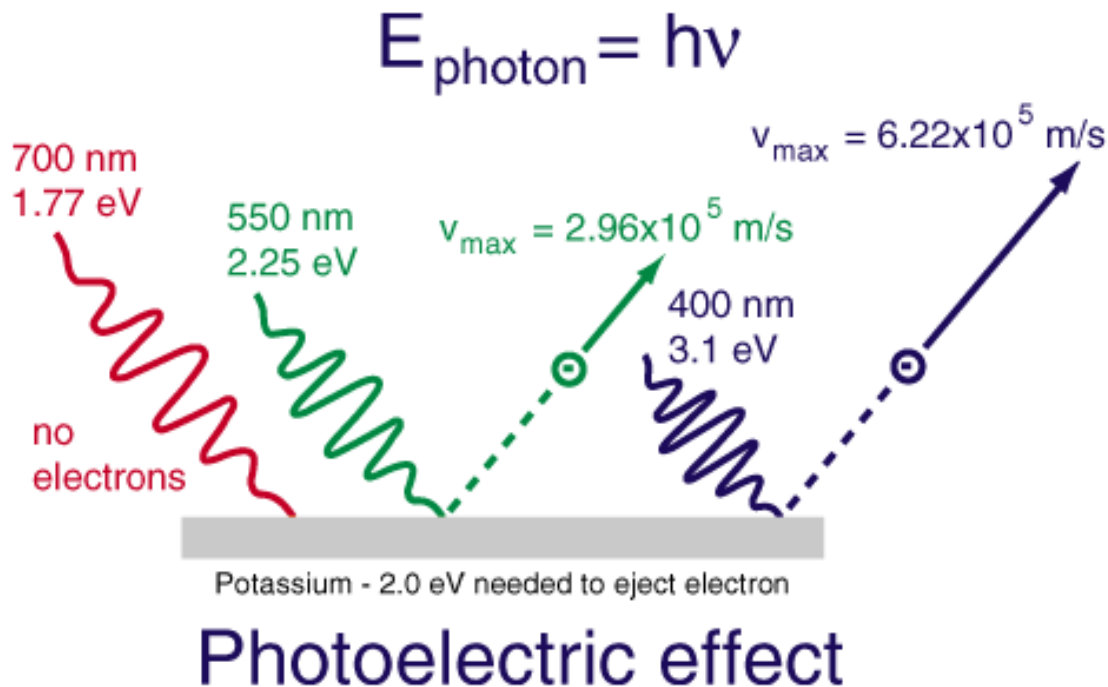
Larger light intensity means larger number of photons at a given frequency (Energy).

# Photoelectric Effect

- The photoelectric effect provides evidence for the particle nature of light.
- It also provides evidence for quantization.
- The electrons will only be ejected once the threshold frequency is reached .
- Below the threshold frequency, no electrons are ejected.
- Above the threshold frequency, the number of electrons ejected depend on the intensity of the light.

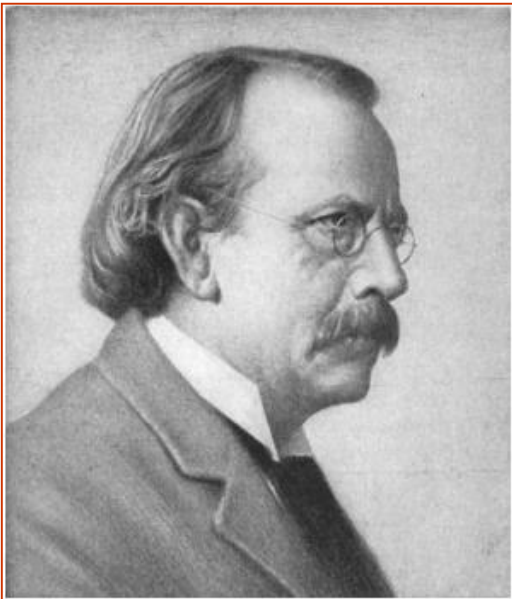
# Failure of Classical Theory 2

- Why was red light incapable of knocking electrons out of certain materials, no matter how bright (more intensity)
  - yet blue light could readily do so even at modest intensities
  - called the photoelectric effect
  - Einstein explained in terms of photons, and won Nobel Prize



# **Atomic Structure**

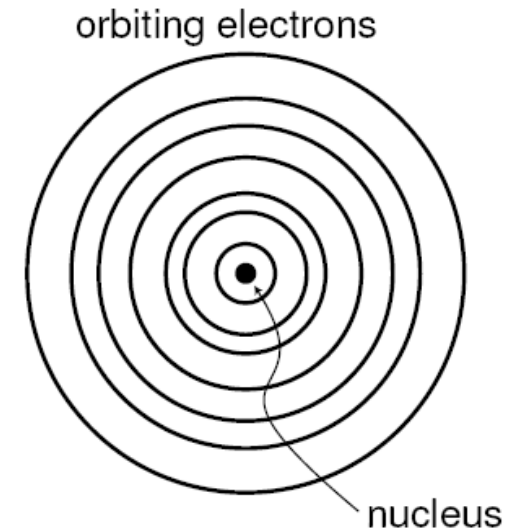




j / J.J. Thomson in the lab.



e / Ernest Rutherford (1871-1937).

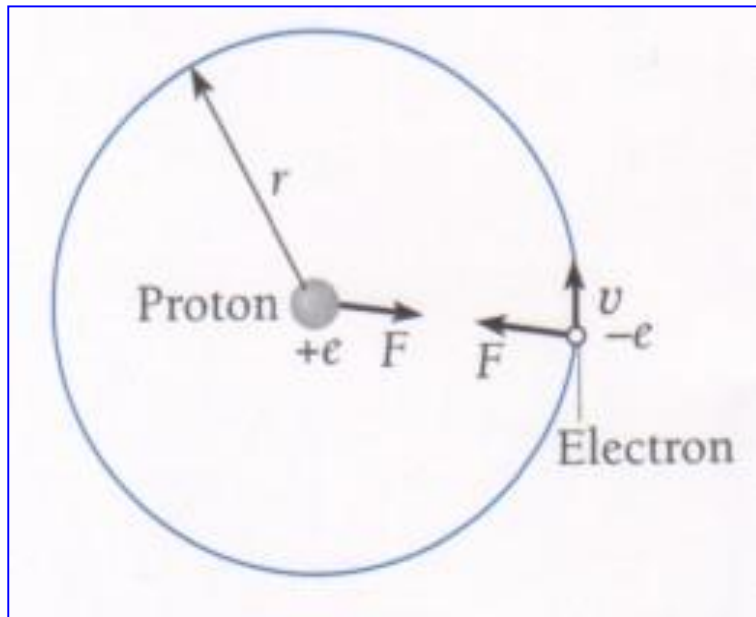


h / The planetary model of the atom.

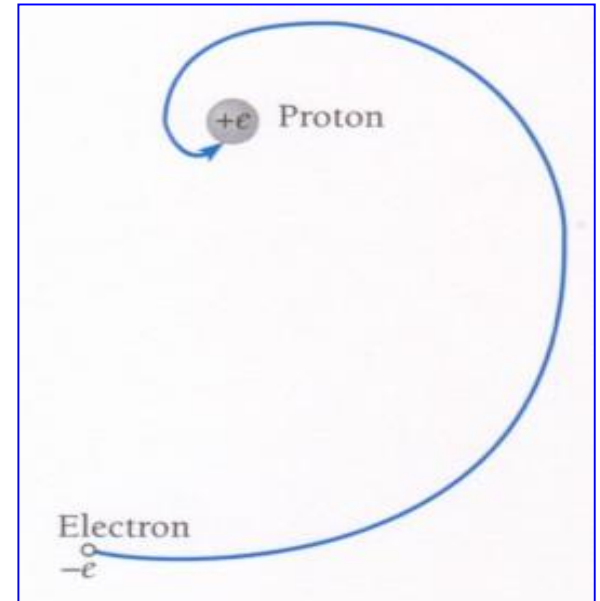
## **Nuclear atom model (1911): Ernest Rutherford**

**Rutherford, Ernest, FRS (1871 -- 1937), New Zealand-English nuclear physicist.**

# Failure of Classical Theory 3



This means  
an electron  
should fall  
into the  
nucleus.



**Classical Electrodynamics:**  
Charged particles radiate EM energy (photons) when their velocity vector changes (e.g. they accelerate).

**New mechanics is needed!**

# **Atomic Spectra**

# Spectroscopy

Balmer, Johann Jakob (1825 -- 1898), Swiss mathematician and an honorary physicist.



Rydberg, Johannes Robert (1854 -- 1919), Swedish physicist.

from  $n \geq 3$  to  $n = 2$



Balmer series  
(1885)

visible spectrum

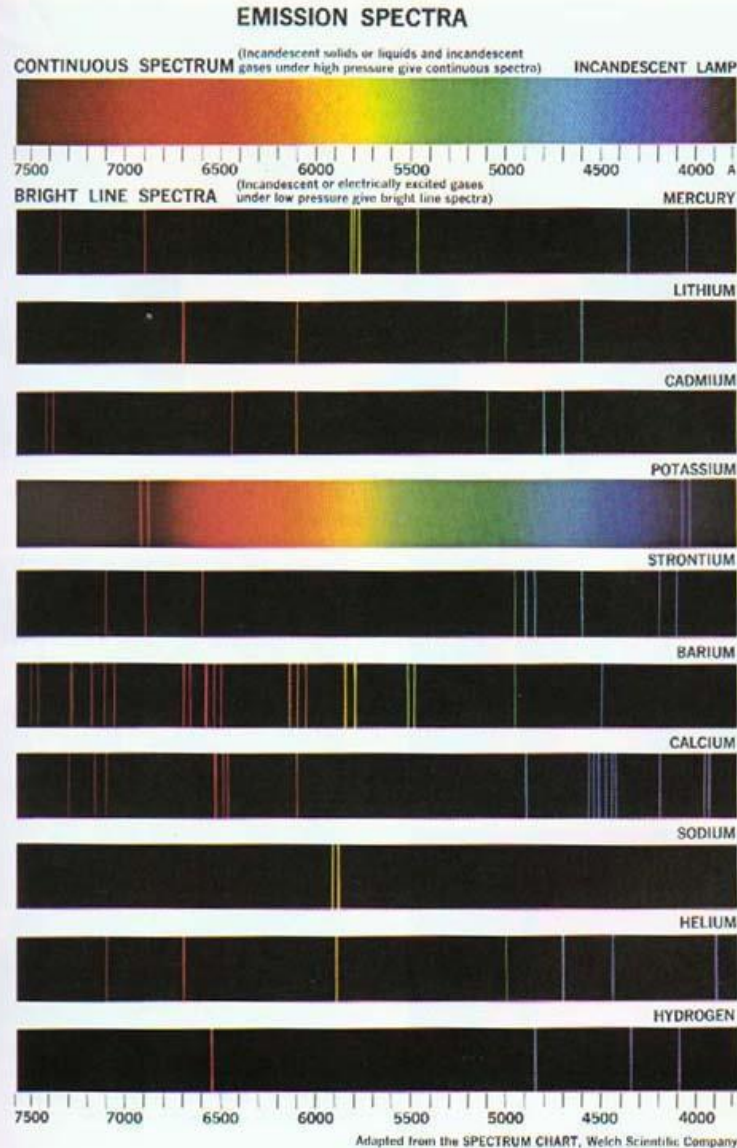
Rydberg formula for hydrogen  
(1888)

$$\frac{1}{\lambda_{\text{vac}}} = R_{\text{H}} \left( \frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$

Rydberg formula for all hydrogen-like atom (1888)

$$\frac{1}{\lambda_{\text{vac}}} = RZ^2 \left( \frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$

# Failure of Classical Theory 4



- What caused spectra of atoms to contain discrete “lines”
  - it was apparent that only a small set of optical frequencies (wavelengths) could be emitted or absorbed by atoms
- Each atom has a distinct “fingerprint”
- Light only comes off at very specific wavelengths
  - or frequencies
  - or energies
- Note that hydrogen (bottom), with only one electron and one proton, emits several wavelengths

# **Old Quantum Theory**

**(1913 -- 1924)**



The Nobel Prize in Physics 1922

"for his services in the investigation of the structure of atoms and of the radiation emanating from them"



Niels Henrik David Bohr

Denmark

Copenhagen University  
Copenhagen, Denmark

b. 1885  
d. 1962

Bohr, Niels Henrik David (1885 -- 1962),  
Danish physicist.

**Bohr's model of atomic structure, 1913**

The electron's orbital angular momentum  
is quantized

$$\mathbf{L} = n \cdot \hbar = n \cdot \frac{h}{2\pi}$$

$$E_n = \frac{-13.6 \text{ eV}}{n^2} = \frac{-m_e q_e^4}{8h^2 \epsilon_0^2} \frac{1}{n^2}$$

$$E = E_i - E_f = \frac{m_e e^4}{8h^2 \epsilon_0^2} \left( \frac{1}{n_f^2} - \frac{1}{n_i^2} \right)$$

$$\frac{1}{\lambda} = \frac{m_e e^4}{8ch^3 \epsilon_0^2} \left( \frac{1}{n_f^2} - \frac{1}{n_i^2} \right)$$

The theory that electrons travel in discrete orbits around the atom's nucleus.

The idea that an electron could drop from a higher-energy orbit to a lower one, emitting a photon (light quantum) of discrete energy (this became the basis for quantum theory).

## Bohr's theory in 1 page

$$\text{circular motion: } \frac{1}{4\pi\epsilon_0} \frac{e^2}{r^2} = \frac{mv^2}{r}$$

$$\text{quantization of angular momentum: } mv_n r_n = n\hbar$$

$$\text{total energy: } E_n = \frac{1}{2}mv_n^2 - \frac{1}{4\pi\epsilon_0} \frac{e^2}{r_n} = -\left(\frac{1}{4\pi\epsilon_0}\right)^2 \frac{me^4}{2\hbar^2} \frac{1}{n^2}$$

Quantum predictions must match classical results for large  $n$

$$\text{freq. of radiation at } n \gg 1: \quad h\nu = E_{n+1} - E_n \approx \left(\frac{1}{4\pi\epsilon_0}\right)^2 \frac{me^4}{n^3 \hbar^2}$$

$$\text{freq. of classical circular motion: } \nu = \frac{v_n}{2\pi r_n} = \left(\frac{1}{4\pi\epsilon_0}\right)^2 \frac{me^4}{n^3 2\pi \hbar^3}$$

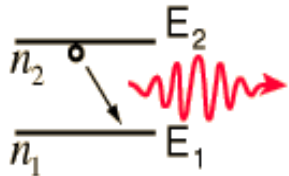
$$\hbar = \hbar / (2\pi)$$

$$mv_n r_n = \hbar / (2\pi) = \hbar$$



# Summary

## Electron Transitions



A downward transition involves emission of a photon of energy:

$$E_{\text{photon}} = h\nu = E_2 - E_1$$

Given the expression for the energies of the hydrogen electron states:

$$h\nu = \frac{2\pi^2 me^4}{h^2} \left[ \frac{1}{n_1^2} - \frac{1}{n_2^2} \right] = -13.6 \left[ \frac{1}{n_1^2} - \frac{1}{n_2^2} \right] \text{eV}$$

$$\frac{1}{\lambda} = R_H \left[ \frac{1}{n_1^2} - \frac{1}{n_2^2} \right] \text{ where } R_H = \frac{2\pi^2 me^4}{h^2} \text{ is called the Rydberg constant.}$$

$$R_H = 1.0973731 \times 10^7 \text{ m}^{-1}$$

## Failures of the Bohr Model

It fails to provide any understanding of why certain spectral lines are brighter than others. There is no mechanism for the calculation of transition probabilities.

The Bohr model treats the electron as if it were a miniature planet, with definite radius and momentum. This is in direct violation of the uncertainty principle which dictates that position and momentum cannot be simultaneously determined.

The Bohr model gives us a basic conceptual model of electrons orbits and energies. The precise details of spectra and charge distribution must be left to quantum mechanical calculations, as with the Schrödinger equation.

# de Broglie Wave

Prince de Broglie gets his Ph.D.

de Broglie matter wave hypothesis (1923):

All matter has a wave-like nature (wave-particle duality) and that the wavelength and momentum of a particle are related by a simple equation.



The Nobel Prize in Physics 1929

"for his discovery of the wave nature of electrons"



**Prince Louis-Victor Pierre Raymond de Broglie**

France

Sorbonne University, Institut Henri Poincaré  
Paris, France

b. 1892  
d. 1987

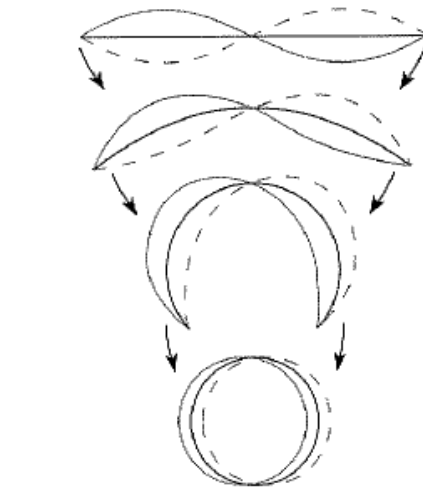
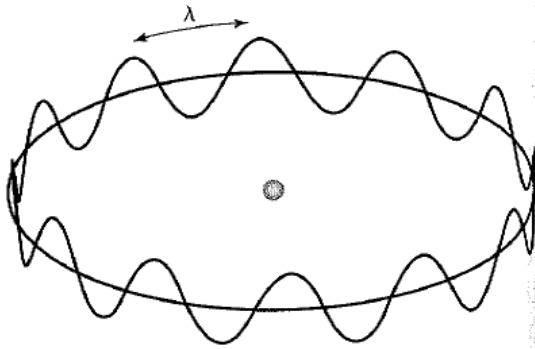
# de Broglie Wave

- Every particle or system of particles *can* be defined in quantum mechanical terms
  - and therefore have wave-like properties
- The quantum wavelength of an object is:
$$\lambda = h/p \quad (p \text{ is momentum})$$
  - called the de Broglie wavelength
- typical macroscopic objects
  - masses  $\sim$  kg; velocities  $\sim$  m/s  $\rightarrow p \approx 1$  kg·m/s
  - $\lambda \approx 10^{-34}$  meters (very small to even detect!!!!)
- typical “quantum” objects:
  - electron ( $10^{-30}$  kg) at thermal velocity ( $10^5$  m/s)  $\rightarrow \lambda \approx 10^{-8}$  m
  - so  $\lambda$  is 100 times larger than an atom: very relevant to an electron!

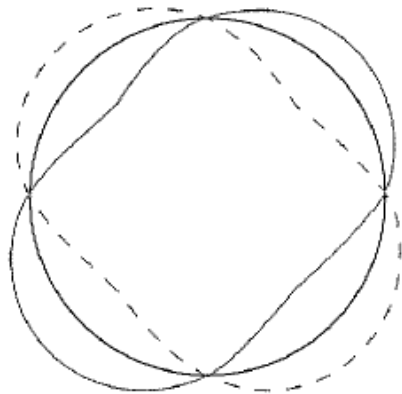
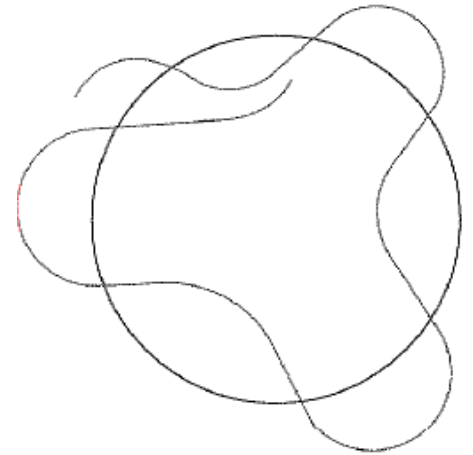
# de Broglie waves of electron

$$L = n\hbar$$

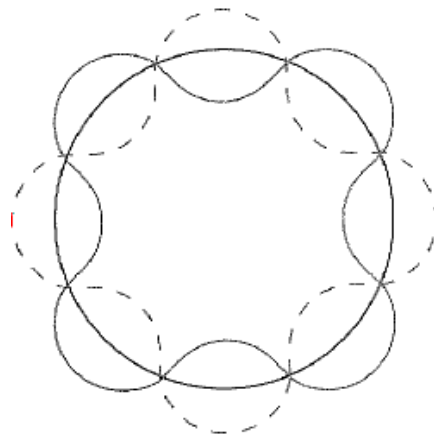
$$2\pi r = n\lambda$$



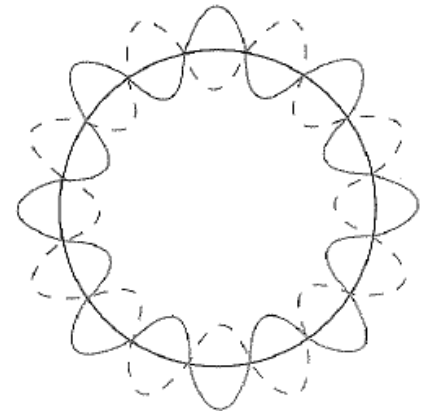
— Electron path  
- - - De Broglie electron wave



Circumference = 2 wavelengths



Circumference = 4 wavelengths



Circumference = 8 wavelengths

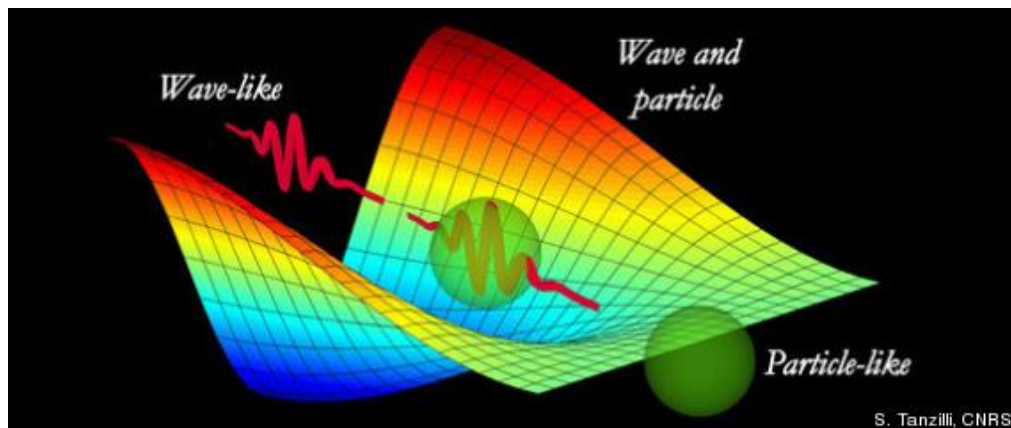
# Wave-Particle Duality

**Particle Nature of Light**



**Wave Nature of Light**

**Every Quantum Mechanical Particle (not just light or photon) behaves like a wave and a particle simultaneously**



**Interference, Diffraction, Polarization: Wave nature**

**Compton Effect, Photoelectric effect, Blackbody Radiation: Particle Nature**

Check this link for Particle-Wave Duality explanation

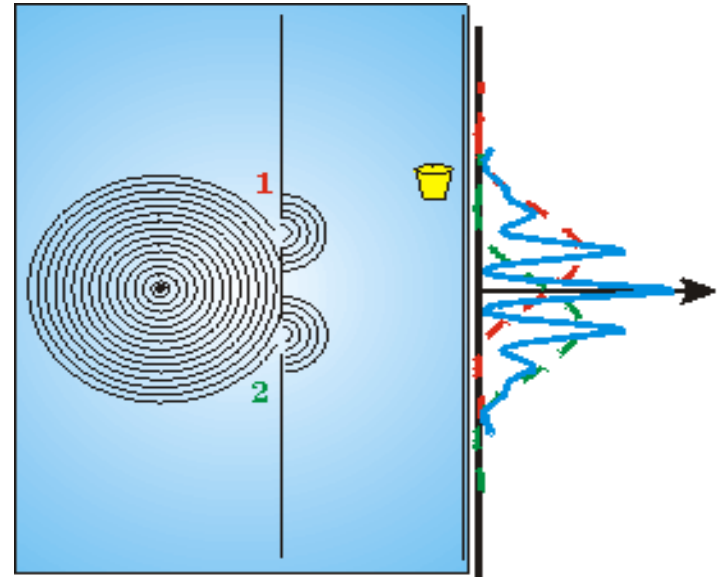
1. <http://www.youtube.com/watch?v=DfPeprQ7oGc>
2. <https://www.youtube.com/watch?v=Q1YqgPATzho>

# Wave-Particle Duality

Particle Nature



Wave Nature



# Heisenberg Uncertainty Principle

- The process of measurement involves interaction
  - this interaction necessarily “touches” the subject
  - by “touch,” we could mean by a photon of light
- The more precisely we want to know where something is, the “harder” we have to measure it
  - so we end up giving it a kick
- So we must unavoidably alter the velocity of the particle under study
  - thus changing its momentum
- If  $\Delta x$  is the position uncertainty, and  $\Delta p$  is the momentum uncertainty, then inevitably,

$$\Delta x \Delta p \geq h/2\pi$$

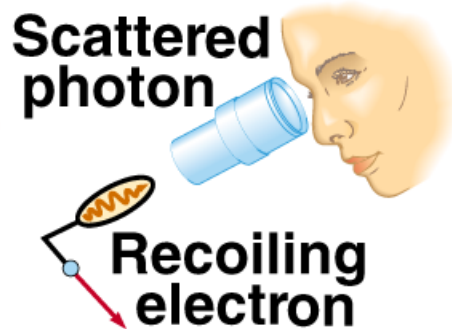
# Heisenberg Uncertainty Principle

Before  
collision

After  
collision

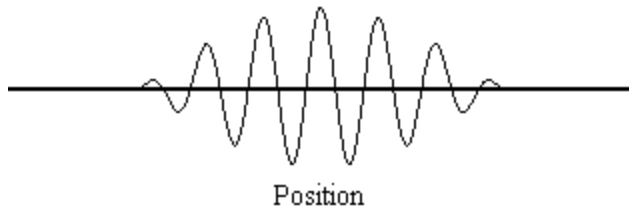
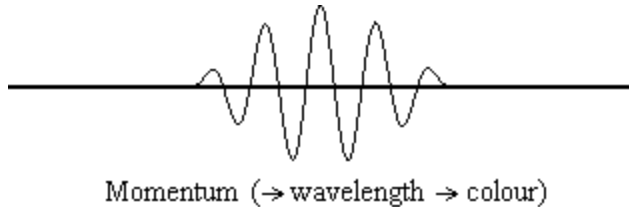
Incident  
photon

Scattered  
photon



$$\Delta E \Delta t \geq \hbar$$

Measurement disturbs the system





# Phase Velocity and Group Velocity

# Phase Velocity and Group Velocity

$$E = E_0 \cos k(x - ct)$$

$E_0$  = wave amplitude (related to the energy carried by the wave).

$$k = \frac{2\pi}{\lambda} = 2\pi \tilde{\nu} = \text{angular wavenumber}$$

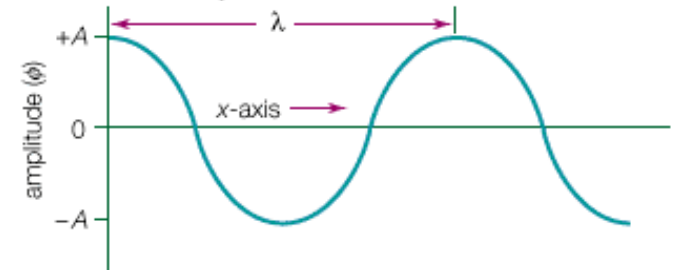
( $\lambda$  = wavelength;  $\tilde{\nu}$  = wavenumber =  $1/\lambda$ )

Alternatively:

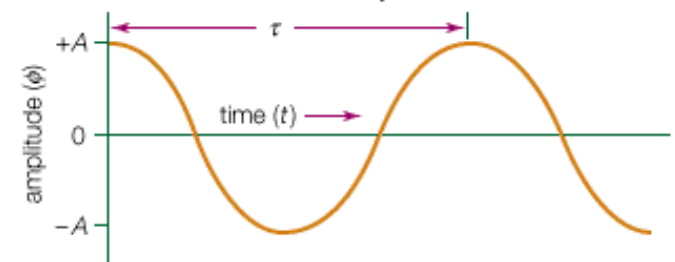
$$E = E_0 \cos(kx - \omega t)$$

Where  $\omega = kc = 2\pi c/\lambda = 2\pi f$  = angular frequency ( $f$  = frequency)

Variation with position at one time



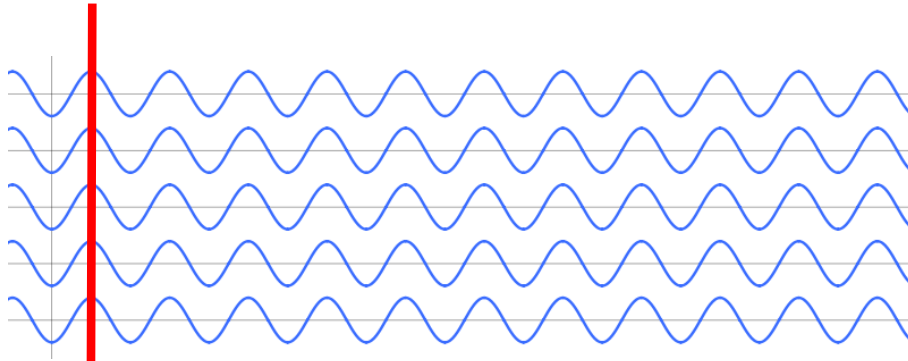
Variation with time at one place



# Phase Velocity and Group Velocity

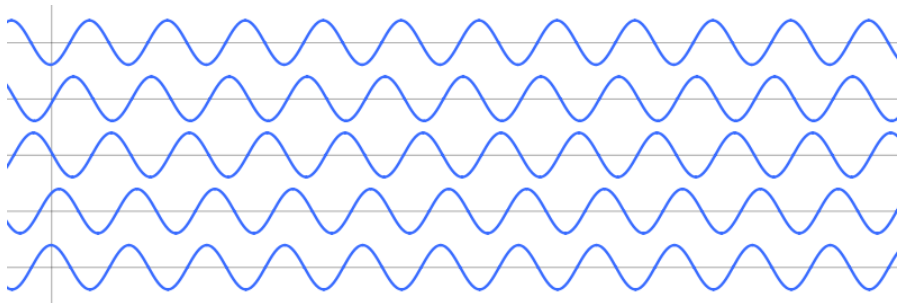
$$E = E_0 \cos k(x - ct); \quad \phi = k(x - ct)$$

The argument of the cosine function represents the *phase* of the wave,  $\phi$ , or the fraction of a complete cycle of the wave.



In-phase waves

Line of equal phase = wavefront = contours of maximum field

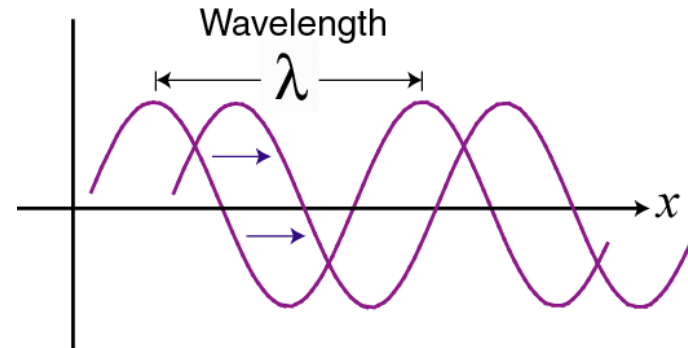


Out-of-phase  
waves

# The Phase Velocity

How fast is the wave traveling?

Velocity is a reference distance divided by a reference time.



The phase velocity is the wavelength / period:  $v = \lambda / \tau$

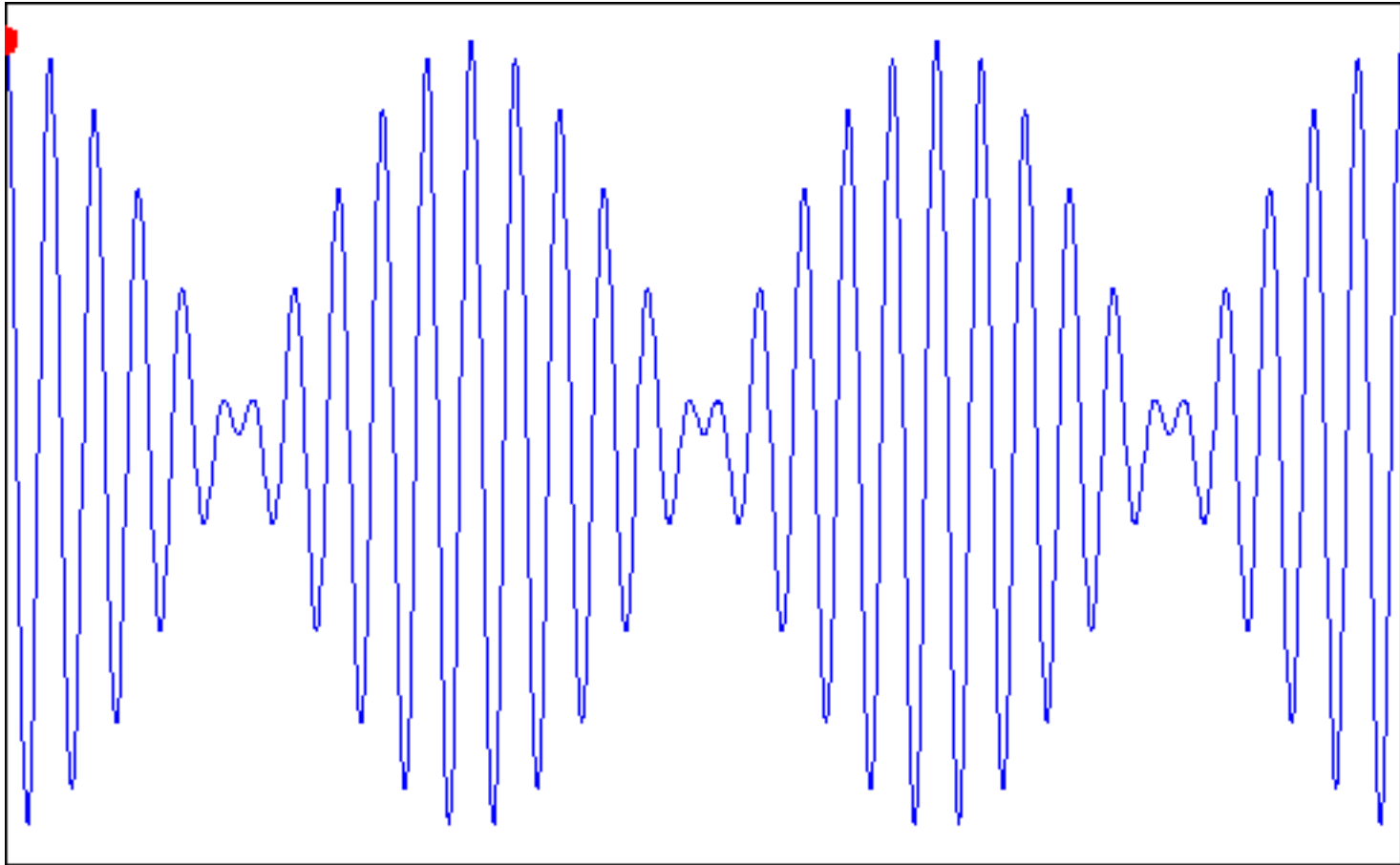
Since  $f = 1/\tau$ :

$$v = \lambda f$$

In terms of  $k$ ,  $k = 2\pi / \lambda$ , and the angular frequency,  $\omega = 2\pi / \tau$ , this is:

$$v = \omega / k$$

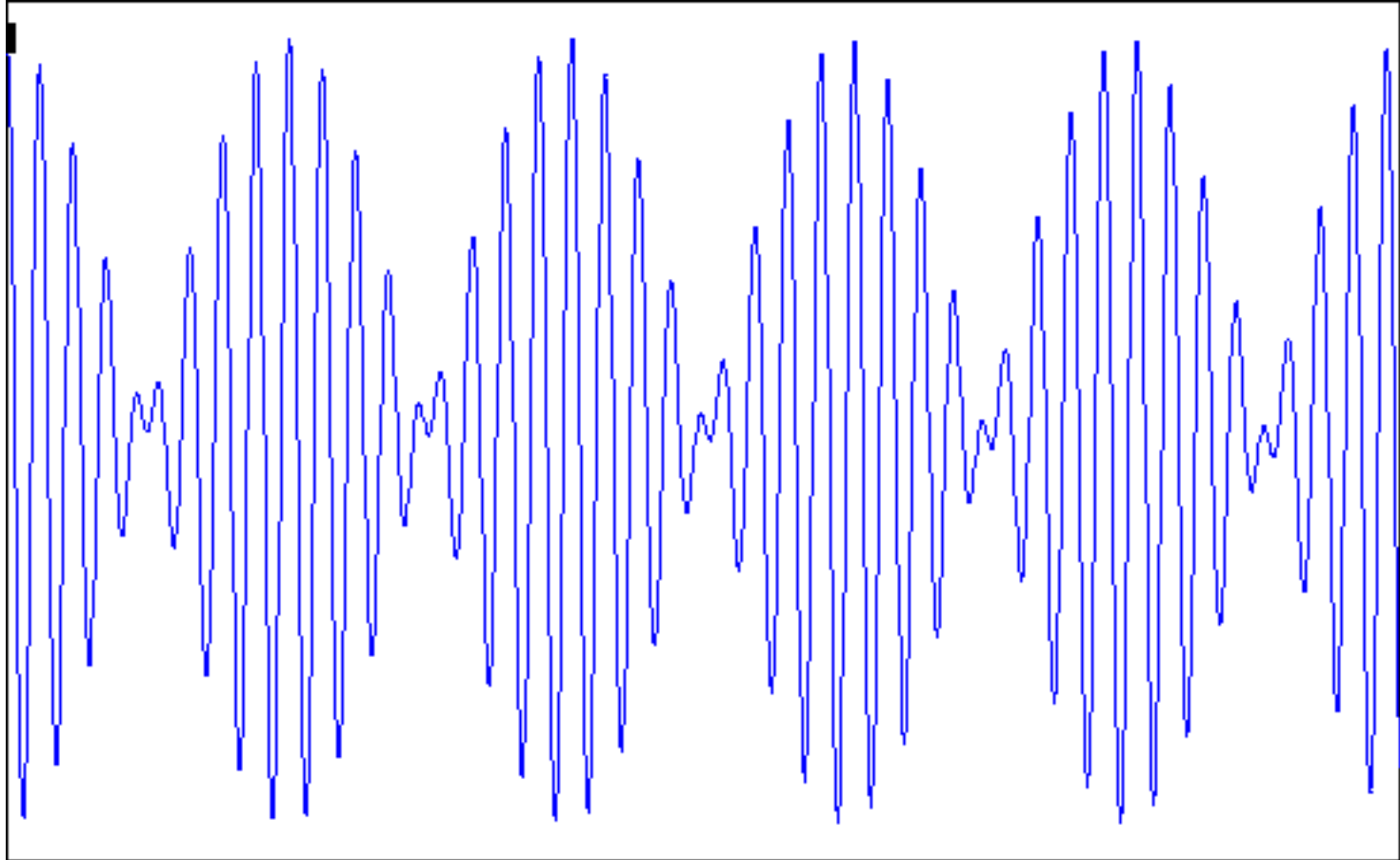
# The Group Velocity



This is the velocity at which the overall shape of the wave's amplitudes, or the wave 'envelope', propagates. (= *signal velocity*)

Here, phase velocity = group velocity (the medium is *non-dispersive*)

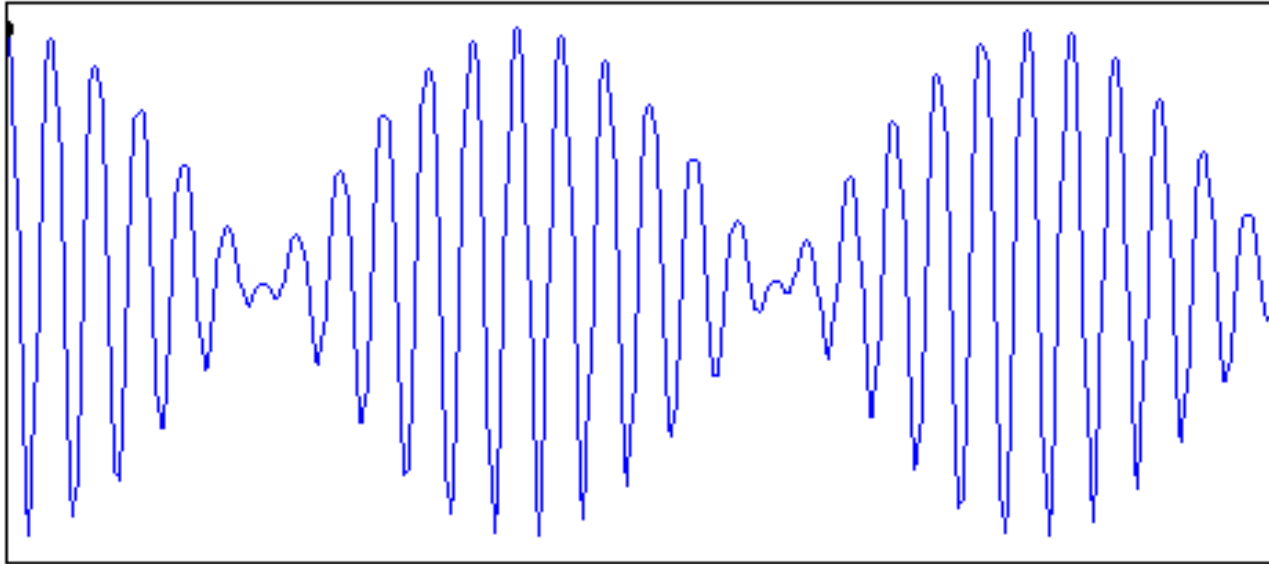
## Dispersion: phase/group velocity depends on frequency



Black dot moves at phase velocity. Red dot moves at group velocity.

This is *normal dispersion* (refractive index decreases with increasing  $\lambda$ )

## Dispersion: phase/group velocity depends on frequency



Black dot moves at group velocity. Red dot moves at phase velocity.

This is *anomalous dispersion* (refractive index *increases with increasing*  $\lambda$ )

# Phase Velocity and Group Velocity

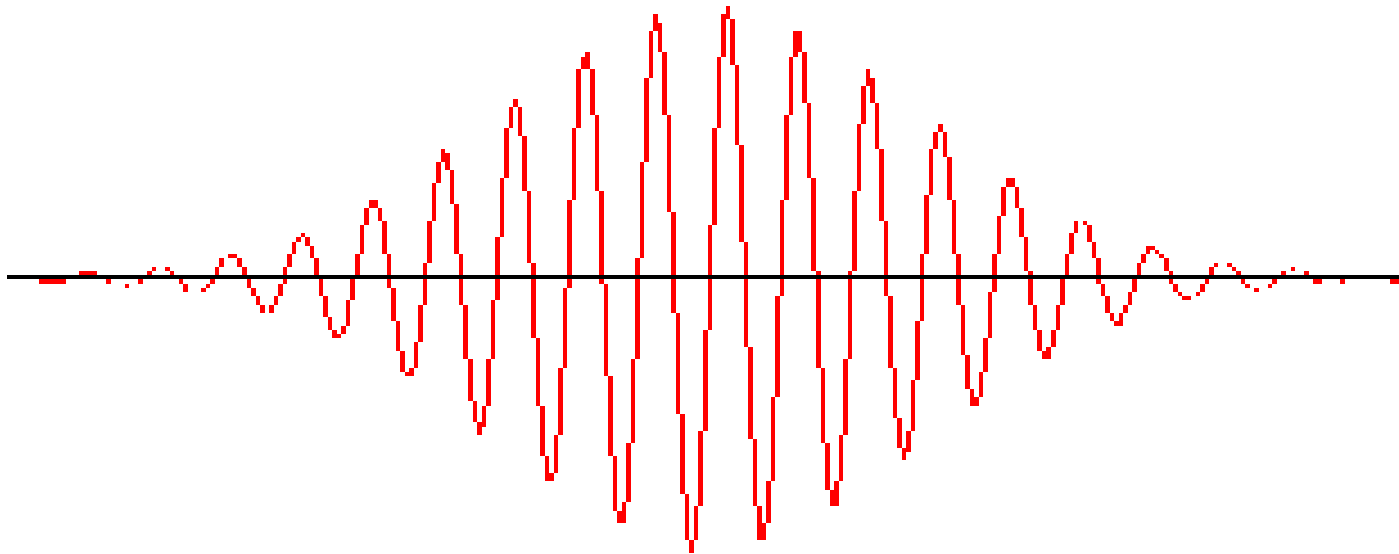
The **group velocity** is the velocity with which the envelope of the **wave packet**, propagates through space.

The **phase velocity** is the velocity at which the phase of any one frequency component of the wave will propagate. You could pick one particular phase of the wave (for example the crest) and it would appear to travel at the phase velocity.



# A “Wave Packet”

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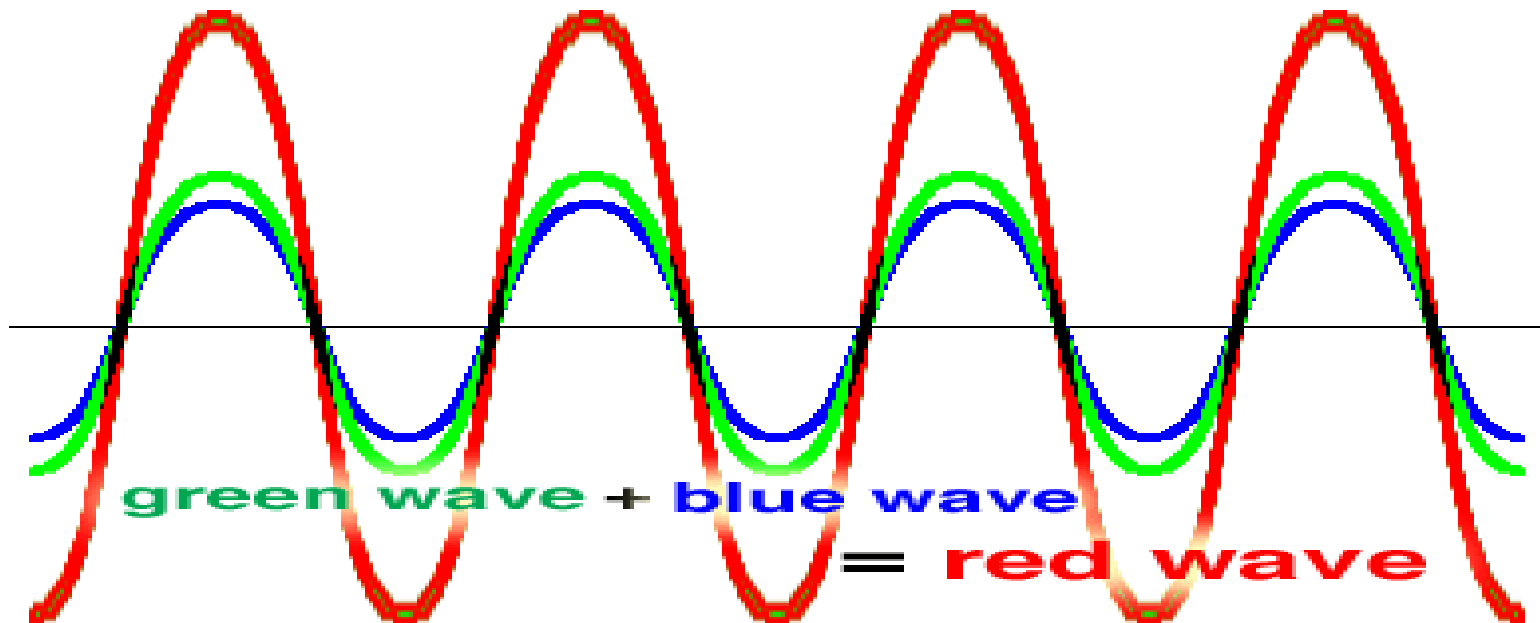


How do you construct a wave packet?

# What happens when you add up waves?

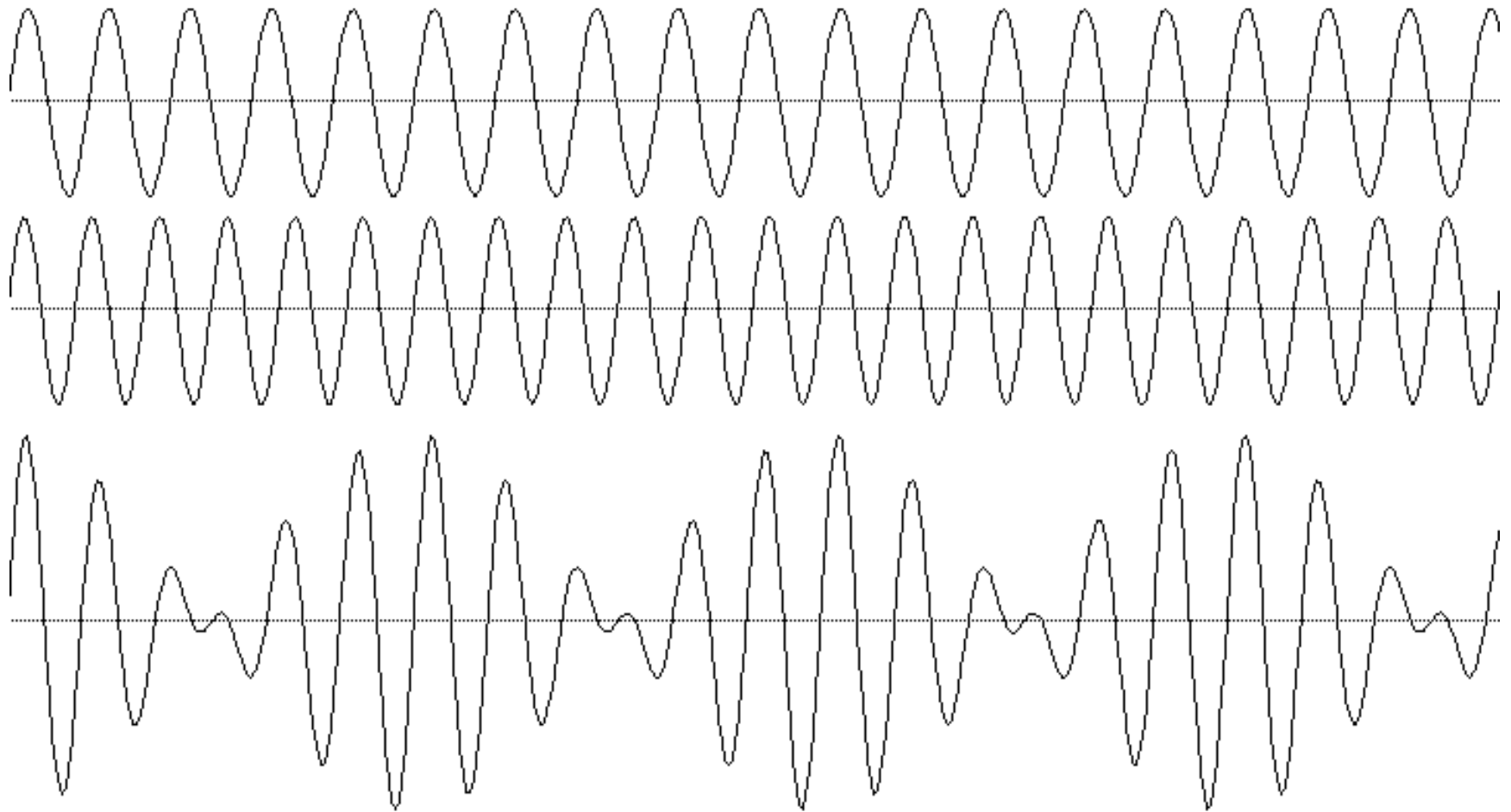
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## The Superposition principle



## Adding up waves of different frequencies.....

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# Group velocity

Group velocity of a wave is the velocity with which the variations in the shape of the wave's amplitude (known as the **modulation** or **envelope** of the wave) propagate through space.

The group velocity is defined by the equation

$$v_g \equiv \frac{\partial \omega}{\partial k},$$

where:

$v_g$  is the group velocity;

$\omega$  is the wave's angular frequency;

$k$  is the wave number.

The function  $\omega(k)$ , which gives  $\omega$  as a function of  $k$ , is known as the dispersion relation.

# Birth of QM

- The necessity for quantum mechanics was thrust upon us by a series of observations.
- The theory of QM developed over a period of 30 years, culminating in 1925-27 with a set of postulates.
- QM cannot be deduced from pure mathematical or logical reasoning.
- QM is not intuitive, because we don't live in the world of electrons and atoms.
- QM is based on observation. Like all science, it is subject to change if inconsistencies with further observation are revealed.

# The wave function, $\Psi$

- De Broglie waves can be represented by a simple quantity  $\Psi$ , called a wave function, which is a complex function of time and position
- A particle is completely described in quantum mechanics by the wave function
- A specific wave function for an electron is called an orbital
- The wave function can be used to determine the energy levels of an atomic system
- <https://www.youtube.com/watch?v=vShpwplJyXk>

# First Postulate of Quantum Mechanics

Every physically-realizable state of the system is described in quantum mechanics by a state function  $\psi$  that contains all accessible physical information about the system in that state.

<https://www.youtube.com/watch?v=EmNQuK-E0kl>

<https://www.youtube.com/watch?v=KKr91v7yLcM>

# First Postulate of Quantum Mechanics

- ❑ Physically realizable states  $\rightarrow$  states that can be studied in laboratory
- ❑ Accessible information  $\rightarrow$  the information we can extract from the wave function
- ❑ State function  $\rightarrow$  function of position, momentum, energy that is spatially localized.



# First Postulate of Quantum Mechanics

If  $\psi_1$  and  $\psi_2$  represent two physically-realizable states of the system, then the linear combination

$$\Psi = c_1\psi_1 + c_2\psi_2$$

where  $c_1$  and  $c_2$  are arbitrary complex constants, represents a third physically realizable state of the system.

**Note:**

Wave function  $\psi(x,t) \rightarrow$  position and time probability amplitude

Quantum mechanics describes the outcome of an ensemble of measurements, where an ensemble of measurements consists of a very large number of identical experiments performed on identical non-interacting systems, all of which have been identically prepared so as to be in the same state.

# Second Postulate of Quantum Mechanics

If a system is in a quantum state represented by a wave function  $\psi$ , then

$$P dV = |\psi|^2 dV$$

is the probability that in a position measurement at time  $t$  the particle will be detected in the infinitesimal volume  $dV$ .

$|\psi(x, t)|^2 \rightarrow$  position and time probability density

The importance of normalization follows from the Born interpretation of the state function as a position probability amplitude. According to the second postulate of quantum mechanics, the integrated probability density can be interpreted as a probability that in a position measurement at time  $t$ , we will find the particle anywhere in space.

# Second Postulate of Quantum Mechanics

Therefore, the normalization condition for the wave function is:

$$\int P dV = \int |\psi(x, y, z)|^2 dV = \int \psi^*(x, y, z) \psi(x, y, z) dV = 1$$

**Probability of finding the quantum mechanical particle at a particular region of space at a particular time.**

Limitations on the wave function:

- ☐ Only normalized functions can represent a quantum state and these are called physically admissible functions.
- ☐ State function must be continuous and single valued function.
- ☐ State function must be a smoothly-varying function (continuous derivative).

# Third Postulate of Quantum Mechanics

Every observable in quantum mechanics is represented by an operator which is used to obtain physical information about the observable from the state function. For an observable that is represented in classical physics by a function  $Q(x,p)$ , the corresponding operator is  $Q(\hat{x}, \hat{p})$ .

Observable	Operator
Position	$\hat{x}$
Momentum	$\hat{p} = \frac{\hbar}{i} \frac{\partial}{\partial x}$
Energy	$E = \frac{\hat{p}^2}{2m} + V(\hat{x}) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x)$

# Fourth Postulate of Quantum Mechanics

1926 Erwin Schrödinger proposed an equation that describes the evolution of a quantum-mechanical system → SWE which represents quantum equations of motion, and is of the form:

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(x)\psi(x,t) = \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] \psi(x,t) = i\hbar \frac{\partial \psi}{\partial t}$$

This work of Schrödinger was stimulated by a 1925 paper by Einstein on the quantum theory of ideal gas, and the de Broglie theory of matter waves.

Note:

Examining the time-dependent SWE, one can also define the following operator for the total energy:

$$\hat{E} = i\hbar \frac{\partial}{\partial t}$$

# Fourth Postulate of Quantum Mechanics

## Fourth (Fundamental) postulate of Quantum mechanics:

The time development of the state functions of an isolated quantum system is governed by the time-dependent SWE  $\hat{H}\psi = i\hbar\partial\psi / \partial t$ , where  $\hat{H} = \hat{T} + \hat{V}$  is the Hamiltonian of the system.

### Note on isolated system:

The TDSWE describes the evolution of a state provided that no observations are made. An observation alters the state of the observed system, and as it is, the TDSWE can not describe such changes.

# Non-Relativistic Schrödinger Equation

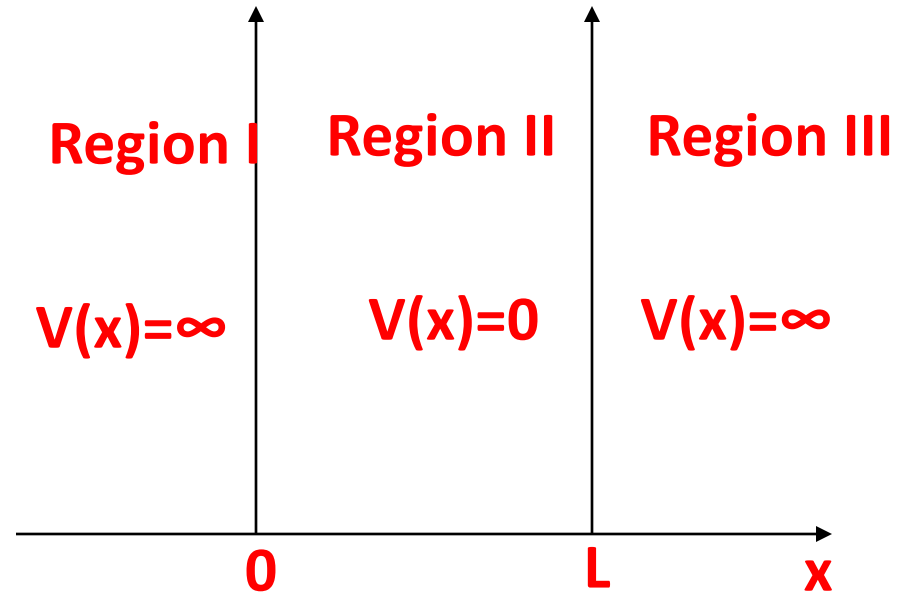
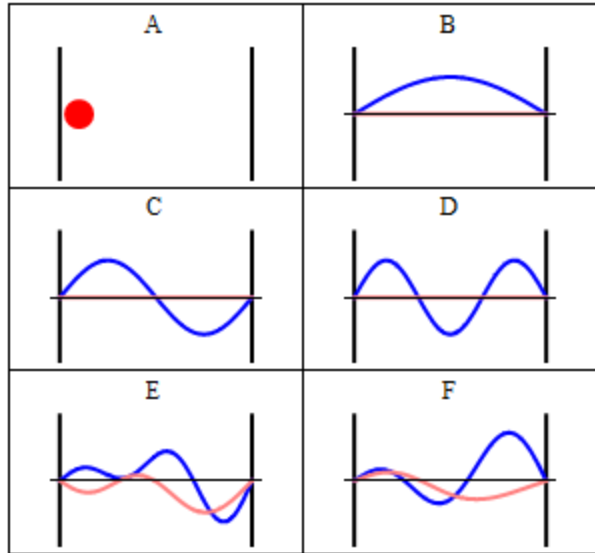
$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}) + V(\mathbf{r})\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

Time independent,  $E$  is a constant, Hamiltonian ( $\hat{H}$ ) is independent of time. Same as eigenvalue equation of  $\hat{H}$ , where  $E$  is the Eigenvalue of  $\hat{H}$

$$i\hbar\frac{\partial\psi(\mathbf{r},t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r},t) + V(\mathbf{r})\psi(\mathbf{r},t)$$

Time dependent, Hamiltonian ( $\hat{H}$ ) is a function of time. It gives up time evolution of wave function.

# Particle in a box



The Particle does not exist outside the box or the wave function ( $\psi=0$ ) is zero.

$$\begin{aligned} V(x) &= 0 & \text{for } L > x > 0 \\ V(x) &= \infty & \text{for } x \geq L, x \leq 0 \end{aligned}$$

Time independent Schrödinger equation,

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + V(x)\psi = E\psi$$



# Particle in a box

Schrödinger equation of the particle inside the box,

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi = -k^2\psi$$

Where,

$$k = \sqrt{2mE / \hbar^2}$$



$$\psi(x) = A \sin kx + B \cos kx$$

A & B are constants

Boundary conditions of the potential dictate that the wave function must be zero at  $x = 0$  and  $x = L$ .

$$B=0 \text{ and } kL = n\pi$$

Therefore, the wave function becomes,

$$\psi_n(x) = A \sin\left(\frac{n\pi x}{L}\right)$$

# Particle in a box

After normalizing the wave function inside the box,

$$\int_{-\infty}^{\infty} \psi_n^*(x) \psi_n(x) dx = 1$$



$$A^2 \int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx = 1$$

Therefore,

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

$$|A|^2 \left[ \frac{x}{2} - \frac{\sin 2kx}{4k} \right]_0^L = 1$$

$$|A|^2 \left( \frac{L}{2} \right) = 1 \quad |A| = \sqrt{\frac{2}{L}}$$

# Quantized Energy

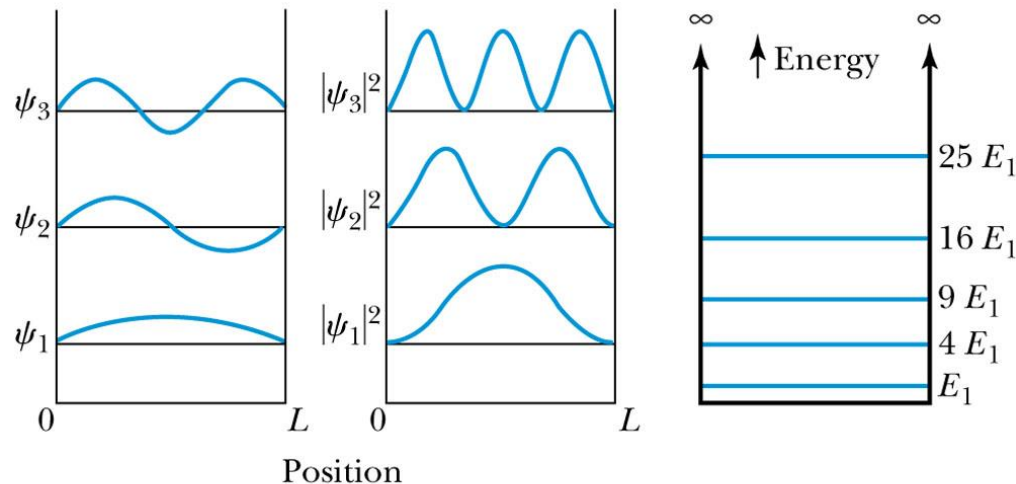
- The quantized wave number now becomes
- Solving for the energy yields

$$k_n = \frac{n\pi}{L} = \sqrt{\frac{2mE_n}{\hbar^2}}$$

$$E_n = n^2 \frac{\pi^2 \hbar^2}{2mL^2} \quad (n = 1, 2, 3, \dots)$$

- Note that the energy depends on the integer values of  $n$ . Hence the energy is quantized and nonzero.
- The special case of  $n = 0$  is called the ground state energy.

$$E_1 = \frac{\pi^2 \hbar^2}{2mL^2}$$



# Quantum Tunnelling

- Quantum tunneling, also known as tunneling (in USA) is a quantum mechanical phenomenon whereby a wave function can propagate through a potential barrier.
- The transmission through the barrier can be finite and depends exponentially on the barrier height and barrier width. The wave function may disappear on one side and reappear on the other side. The wave function and its first derivative are continuous. Tunneling occurs with barriers of thickness around 1–3 nm and smaller.

<https://www.youtube.com/watch?v=RF7dDt3tVml>



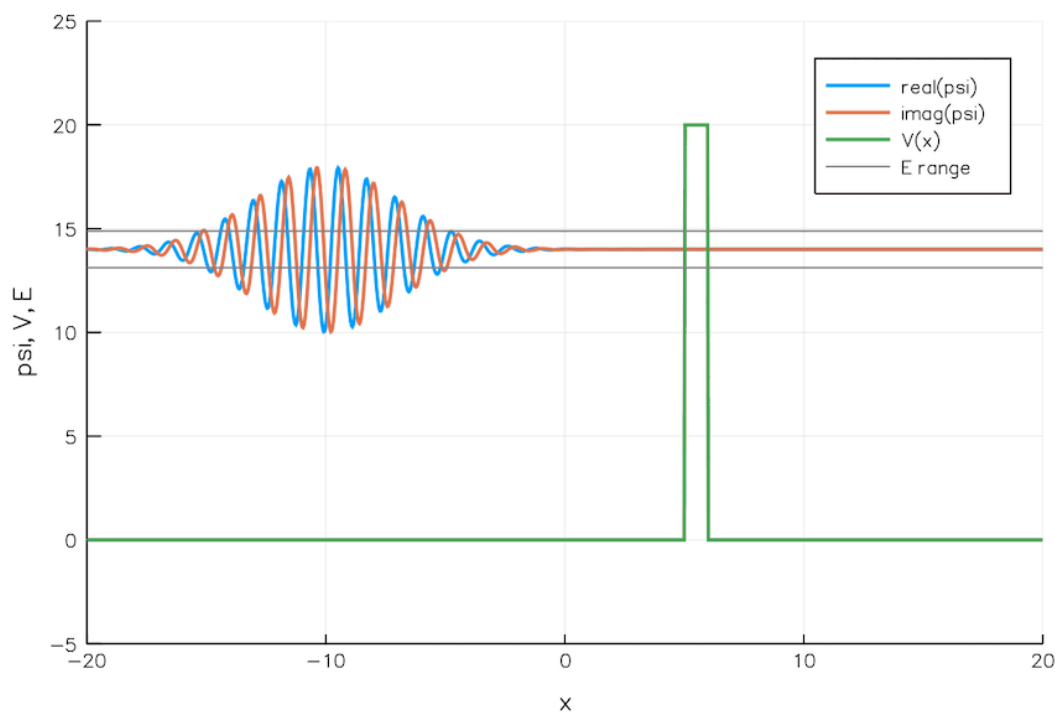
Classical Mechanics



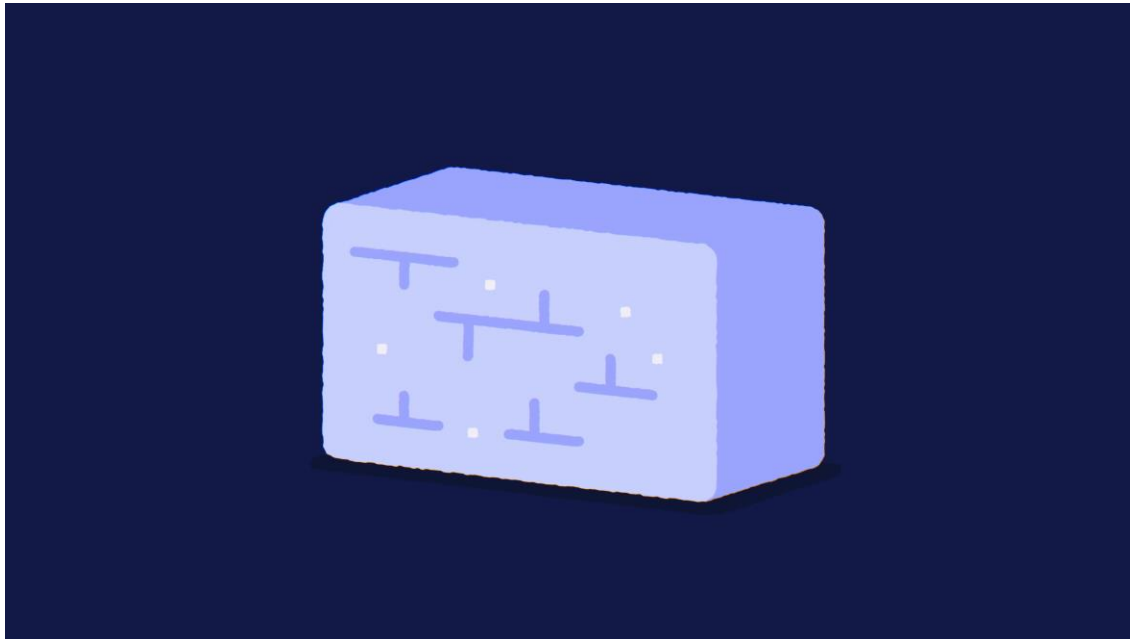
Quantum Mechanics

## TUNNEL EFFECT

All the animations and explanations on  
[www.toutestquantique.fr](http://www.toutestquantique.fr)



**A simulation of a wave packet incident on a potential barrier. In relative units, the barrier energy is 20, greater than the mean wave packet energy of 14. A portion of the wave packet passes through the barrier.**



# Applications of Quantum Tunnelling

- **Scanning Tunnelling Microscope.**
- **Nuclear Fusion:** Quantum tunnelling is a crucial part of nuclear fusion. The average temperature of a star's core is usually not sufficient for atomic nuclei to overcome the Coulomb barrier and kick start thermonuclear fusion. The tunnelling increases the chances of infiltrating this barrier. Though the probability is still low, the huge number of nuclei in the stellar core is enough to drive a steady fusion reaction.
- **Electronics:** Tunneling is a frequent source of current leakage in very-large-scale integration (VLSI) electronics. The VLSI electronics experience substantial power loss and heating effects that cripple such devices. It is usually considered the lower threshold on how microelectronic device elements can be created. Tunnelling is also a basic technique employed to set the floating gates in flash memory. Cold emission, tunnel junction, quantum-dot cellular automata, tunnel diode, and tunnel field-effect transistors are some of the main electronic processes or devices that use quantum tunneling.

# Applications of Quantum Tunnelling

- **Quantum Biology:** Quantum tunnelling is one of the core quantum phenomena in quantum biology. It is essential for both proton tunnelling and electron tunnelling. Electron tunnelling is a critical factor in numerous biochemical redox reactions (cellular respiration, photosynthesis) and enzymatic catalysis. Proton tunnelling also has a key role in spontaneous DNA mutation.



# Quantum Computing

- Quantum computing is a rapidly-emerging technology that harnesses the laws of quantum mechanics to solve problems too complex for classical computers/conventional computers.
- When scientists and engineers encounter difficult problems, they turn to supercomputers. These are very large classical computers, often with thousands of classical CPU and GPU cores. However, even supercomputers struggle to solve certain kinds of problems.
- If a supercomputer gets stumped, that's probably because the big classical machine was asked to solve a problem with a high degree of complexity. When classical computers fail, it's often due to complexity.

- **Quantum computing is an area of computer science that uses the principles of quantum theory.**
- **Quantum computing uses subatomic particles, such as electrons or photons. Quantum bits, or qubits, allow these particles to exist in more than one state (i.e., 1 and 0) at the same time.**
- **Theoretically, linked qubits can "exploit the interference between their wave-like quantum states to perform calculations that might otherwise take millions of years."**
- **Classical computers today employ a stream of electrical impulses (1 and 0) in a binary manner to encode information in bits. This restricts their processing ability, compared to quantum computing.**

- Unlike a normal computer bit, which can be either 0 or 1, a qubit can exist in a multidimensional state.
- The power of quantum computers grows exponentially with more qubits.
- Classical computers store information as bits with either 0s or 1s, quantum computers use qubits. Qubits carry information in a quantum state that engages 0 and 1 in a multidimensional way.

## **Features of Quantum Computing**

**Superposition and entanglement are two features of quantum physics on which quantum computing is based. They empower quantum computers to handle operations at speeds exponentially higher than conventional computers and with much less energy consumption.**

# **Qubit**

- In quantum computing, a qubit or quantum bit is a basic unit of quantum information—the quantum version of the classic binary bit physically realized with a two-state device.
- A qubit is a two-state (or two-level) quantum-mechanical system.
- Examples include the spin of the electron in which the two levels can be taken as spin up and spin down; or the polarization of a single photon in which the two states can be taken to be the vertical polarization and the horizontal polarization.
- In a classical system, a bit would have to be in one state or the other. However, quantum mechanics allows the qubit to be in a coherent superposition of both states simultaneously, a property that is fundamental to quantum mechanics and quantum computing.

# **Qubit**

**In quantum mechanics, the general quantum state of a qubit can be represented by a linear superposition of its two orthonormal basis states (or basis vectors). These vectors are usually denoted as,  $|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$  and  $|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ . They are written in conventional “Bra-Ket” notation. The notation  $|0\rangle$  and  $|1\rangle$  are represented as ‘ket 0’ and ‘ket 1’ respectively. These two orthonormal basis states,  $\{|0\rangle, |1\rangle\}$ , together called the computational basis, are said to span the two-dimensional linear vector (Hilbert) space of the qubit.**

**Qubit basis states can also be combined to form product basis states. A set of qubits taken together is called a quantum register. For example, two qubits could be represented in a four-dimensional linear vector space spanned by the following product basis states:**

# **Qubit**

**$(00)=(1\ 0\ 0\ 0)$ ,  $(0,1)=(0\ 1\ 0\ 0)$ ,  $(10)=(0\ 0\ 1\ 0)$  and  $(11)=(0\ 0\ 0\ 1)$ . In general,  $n$  qubits are represented by a superposition state vector in  $2^n$  dimensional Hilbert space.**

**A pure qubit state is a coherent superposition of the basis states. This means that a single qubit can be described by a linear combination of  $(0)$  and  $(1)$ ,  $\psi=\alpha(0) + \beta(1)$ , where  $\alpha$  and  $\beta$  are probability amplitude.**

# **Superposition**

**It's what a qubit can do rather than what it is that's remarkable. A qubit places the quantum information that it contains into a state of superposition. This refers to a combination of all possible configurations of the qubit. "Groups of qubits in superposition can create complex, multidimensional computational spaces. Complex problems can be represented in new ways in these spaces."**

# **Entanglement**

**Entanglement is integral to quantum computing power. Pairs of qubits can be made to become entangled. This means that the two qubits then exist in a single state. In such a state, changing one qubit directly affects the other in a manner that's predictable.**

**Quantum algorithms are designed to take advantage of this relationship to solve complex problems. While doubling the number of bits in a classical computer doubles its processing power, adding qubits results in an exponential upswing in computing power and ability.**

## **De-coherence**

**De-coherence occurs when the quantum behavior of qubits decays. The quantum state can be disturbed instantly by vibrations or temperature changes. This can cause qubits to fall out of superposition and cause errors to appear in computing. It's important that qubits be protected from such interference by, for instance, supercooled-refridgerators, insulation, and vacuum chambers.**



