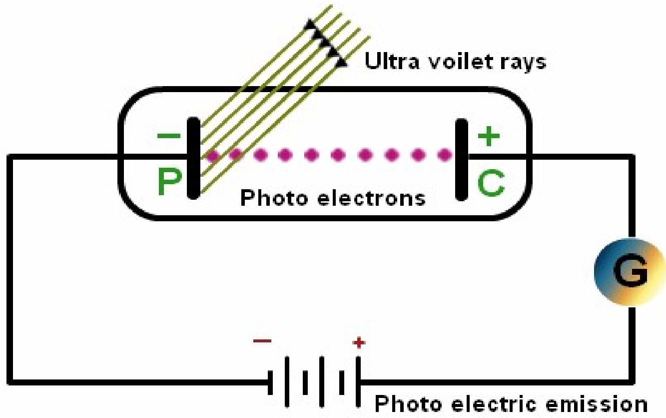
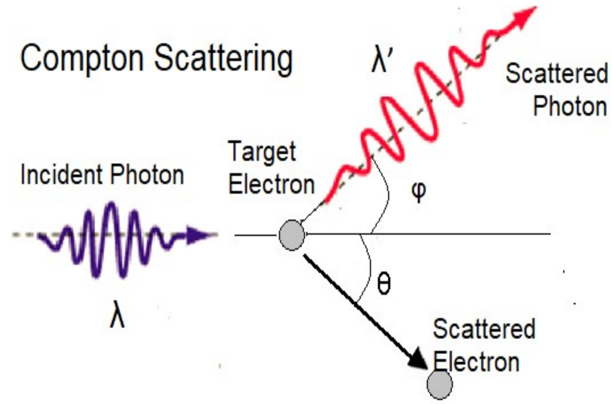
Wave Function Ψ and Schrödinger Wave Equation

Photoelectric Effect



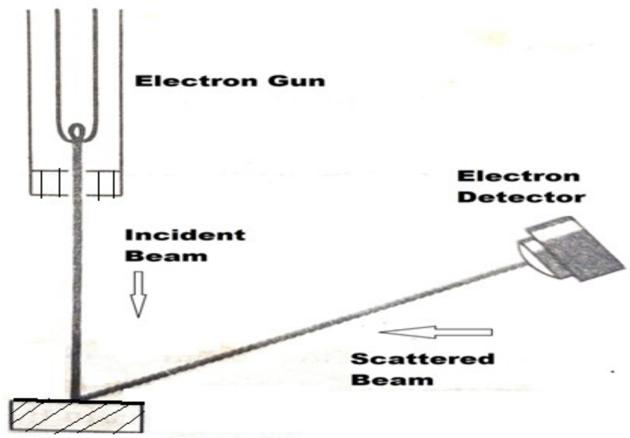
$$h\nu = h\nu_o + T_{max}$$

Compton Effect

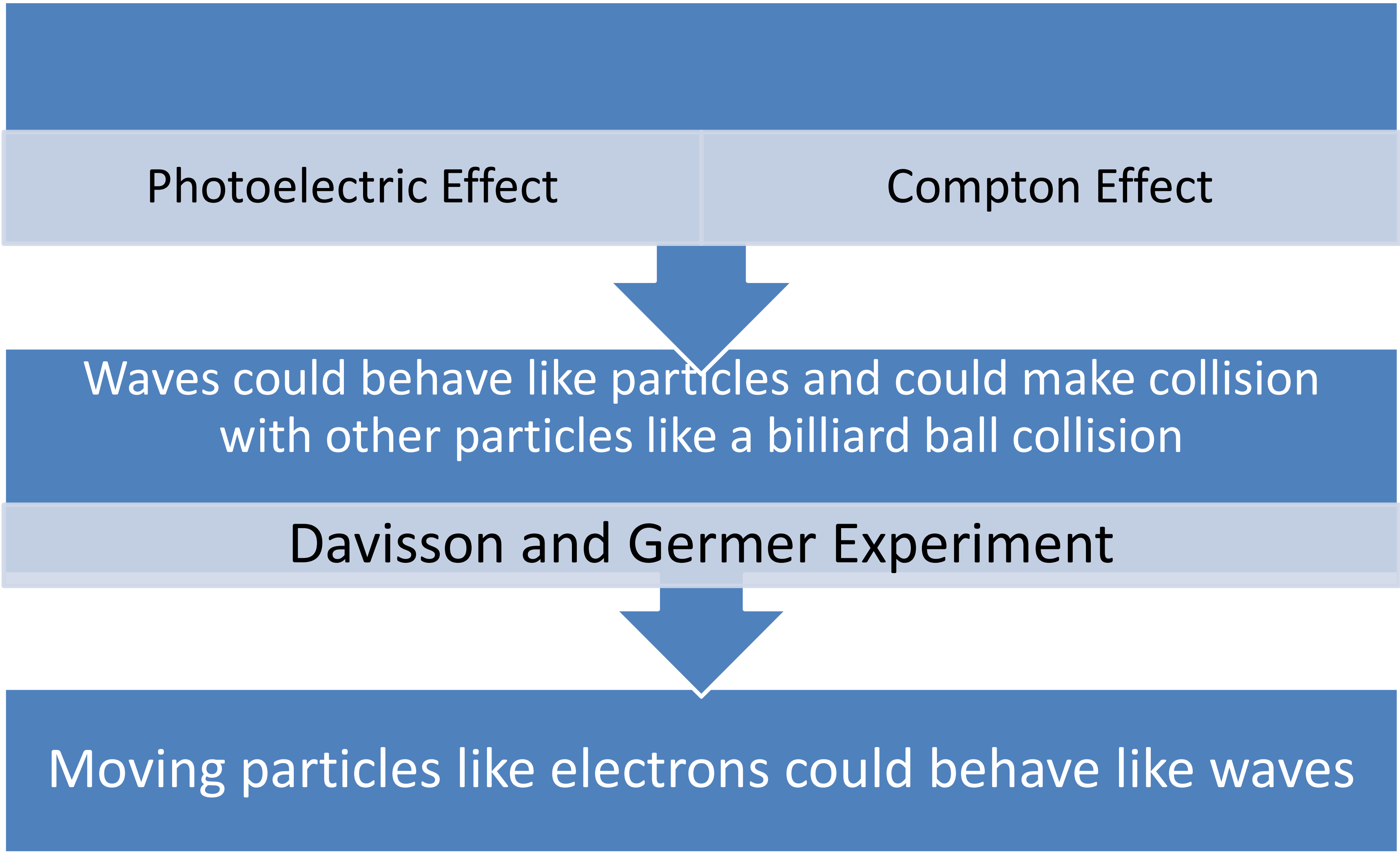


$$\lambda' - \lambda = \left(\frac{h}{m_0 c}\right)(1 - \cos\varphi)$$

Davisson and Germer Experiment



$$n\lambda = 2a\sin\theta$$


Photoelectric Effect
Compton Effect
Waves could behave like particles and could make collision with other particles like a billiard ball collision
Davisson and Germer Experiment
Moving particles like electrons could behave like waves

The energy of a photon is given by **$E = h\nu = hc/\lambda$**

The energy is also given by the formula $E = \sqrt{m_o^2 c^4 + p^2 c^2}$

Since photon doesn't have the rest mass **$E = pc$**

$hc / \lambda = pc$

$\lambda = h/p$

Wave function associated with de Broglie wave Ψ

Ψ is complex

$$\Psi = A + i B$$
$$\Psi^* = A - i B$$
$$|\Psi|^2 = A^2 + B^2$$

The probability density $|\psi|^2$ is given by the product $\psi^*\psi$

What is the speed of de Broglie wave?

Since a de Broglie wave is associated with a moving body this wave should travel at the same speed as that of the body.

We may quote the usual formula as following:

$$\lambda = \frac{h}{mv}$$

$$E = h\nu = mc^2$$

$$\nu = \frac{mc^2}{h}$$

$$w = \nu\lambda = \frac{mc^2}{h}\frac{h}{mv} = \frac{c^2}{v}$$

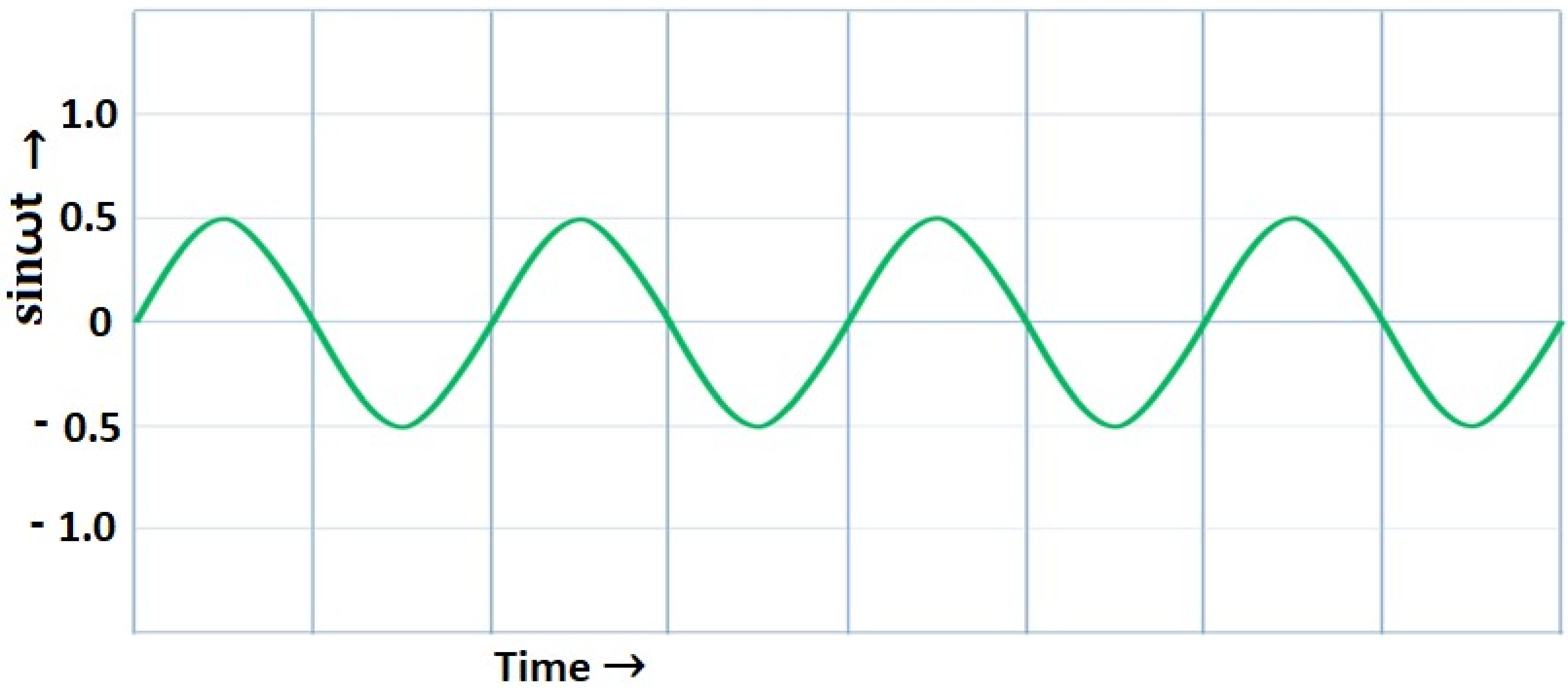
So, the de Broglie wave has speed greater than the speed of light in vacuum or the moving body !

Is it OK?

How to represent a wave associated with a moving particle?

Can the following equation of a plain progressive wave represent de Broglie wave associated with a moving particle?

$$y = A \sin(\omega t - kx)$$



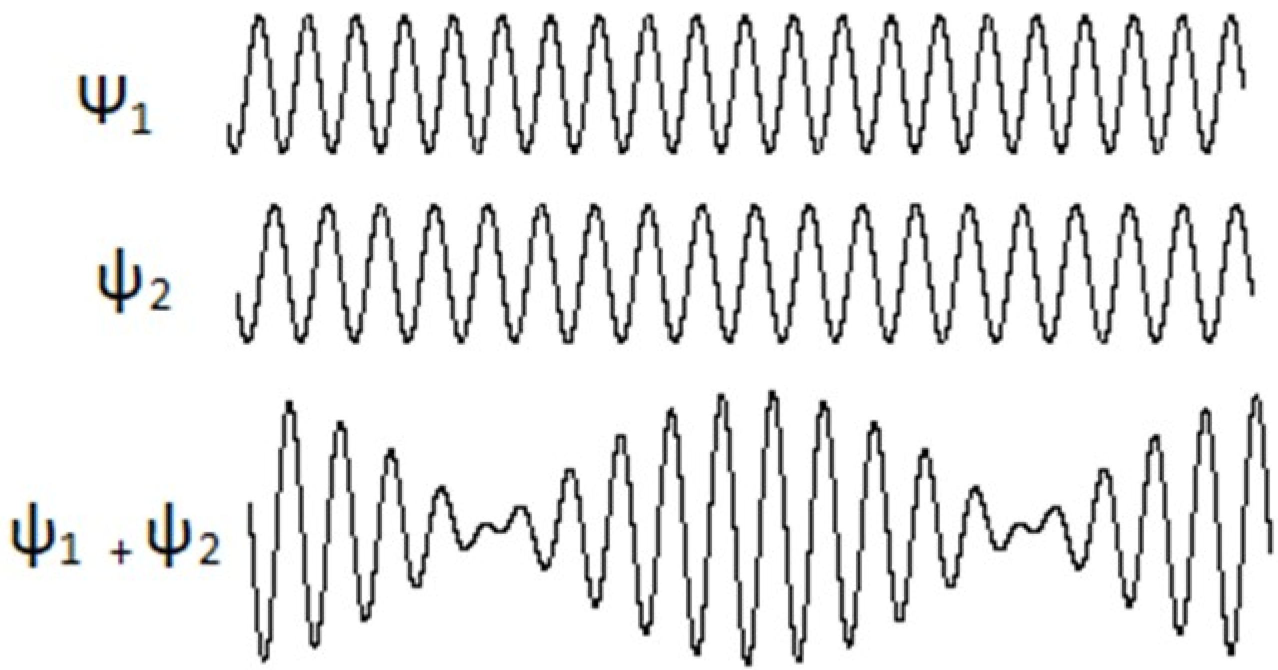
A **wave packet** (or **wave train**) is a small packet or short burst or envelope of localized wave action that travels as a unit.

A wave packet can be synthesized from, an infinite set of component sinusoidal waves of different wave numbers, with phases such that they interfere constructively only over a small region of space, and destructively elsewhere, resulting in the variation of amplitude that defines the group shape

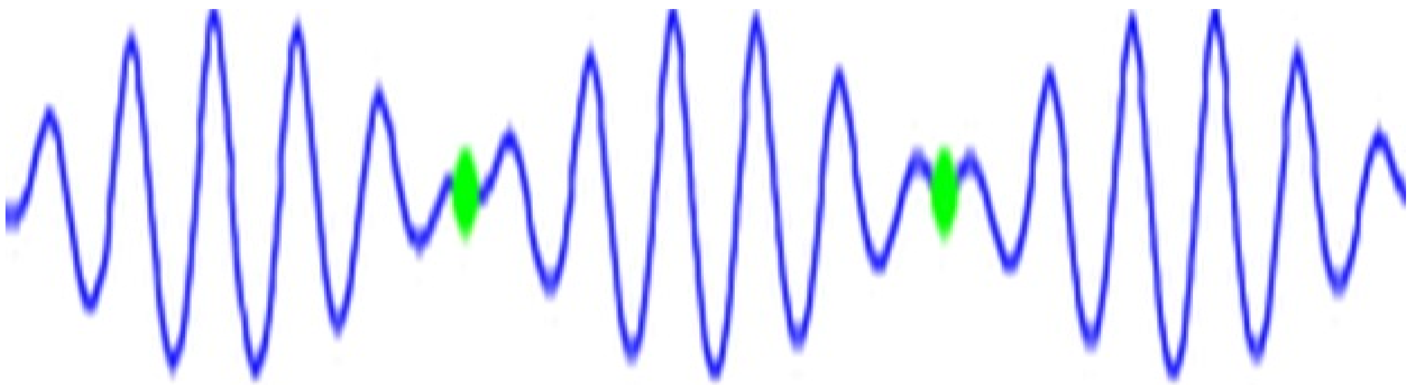
Each component wave function, and hence the wave packet, are solutions of the Schrödinger equation.

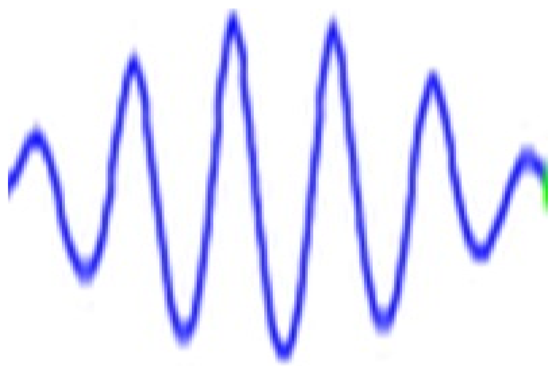
$\psi_1 = A\cos(\omega t - kx)$ $\psi_2 = A\cos[(\omega+d\omega)t - (k+dk)x]$

$\boldsymbol{\Psi = \psi_1 + \psi_2} = 2A\cos(\omega t - kx)\cos(d\omega/2 - dk/2)$



Phase or Wave velocity $w = \omega/k$; Group velocity $u = d\omega/dk$





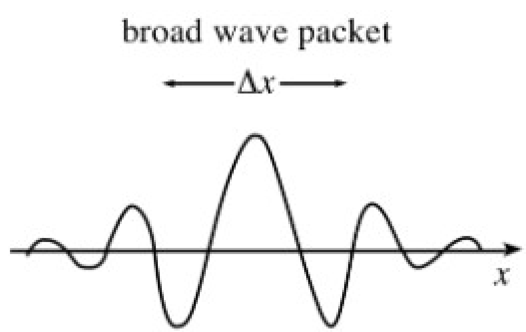
$$\omega = 2\pi\nu = \frac{2\pi mc^2}{h} = \frac{2\pi mc^2}{h\sqrt{1 - \frac{v^2}{c^2}}}$$

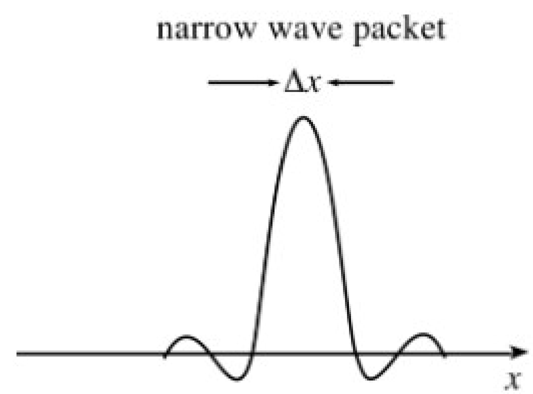
$$k = \frac{2\pi}{\lambda} = \frac{2\pi mv}{h} = \frac{2\pi m_o v}{h\sqrt{1 - \frac{v^2}{c^2}}}$$

$$w = \frac{\omega}{k} = \frac{c^2}{v}$$

$$u = \frac{d\omega}{dk} = \frac{d\omega}{dv} \Big/ \frac{dk}{dv} = v$$

The Uncertainty Principle





The Moving Wave Packet or de Broglie Wave

Propagation of a wave packet

https://en.wikipedia.org/wiki/Wave_packet#/media/File:Wave_packet_(no_dispersion).gif

Properties of Wave Function

$$\int_{+\infty}^{-\infty} |\Psi|^2 \, dx = 1$$

Ψ contains all the information about the particle.

Must be a solution of the Schrodinger equation.

Must be a continuous function of x.

The slope of the function in x must be continuous. Specifically $\partial\psi/\partial x$ must be continuous.

Mathematical Expression of the wave associated with a free particle

$$\Psi = A\, e^{-i\omega(t-x/v)}$$

$$\Psi = A\, e^{-2\pi i\,(\nu t-x/\lambda)}$$

$$E=h\nu=2\pi\hbar\nu$$

$$\lambda = h/p = 2\pi\hbar/p$$

$$\Psi = A\, e^{-\,i/\hbar\,(Et-px)}$$

The Wave Equation

The **wave equation** is an important second-order linear partial differential equation for the description of waves—as they occur in classical physics—such as mechanical waves like water waves or sound waves or electromagnetic waves.

Wave equation come up in fields like acoustics, electromagnetism, and fluid dynamics.

The wave equation for a stretched string

$$\frac{\partial^2 y}{\partial x^2} = \frac{\mu}{T}\frac{\partial^2 y}{\partial t^2}$$

The solution of this wave equation can be of many kinds that reflects the variety of possible wave types viz. a progressive wave plane, spherical or cylindrical), a train of waves of constant amplitude and wavelength, a standing wave, etc.

All solutions should be of the form $y = F(t \pm \sqrt{\frac{\mu}{T}}x)$

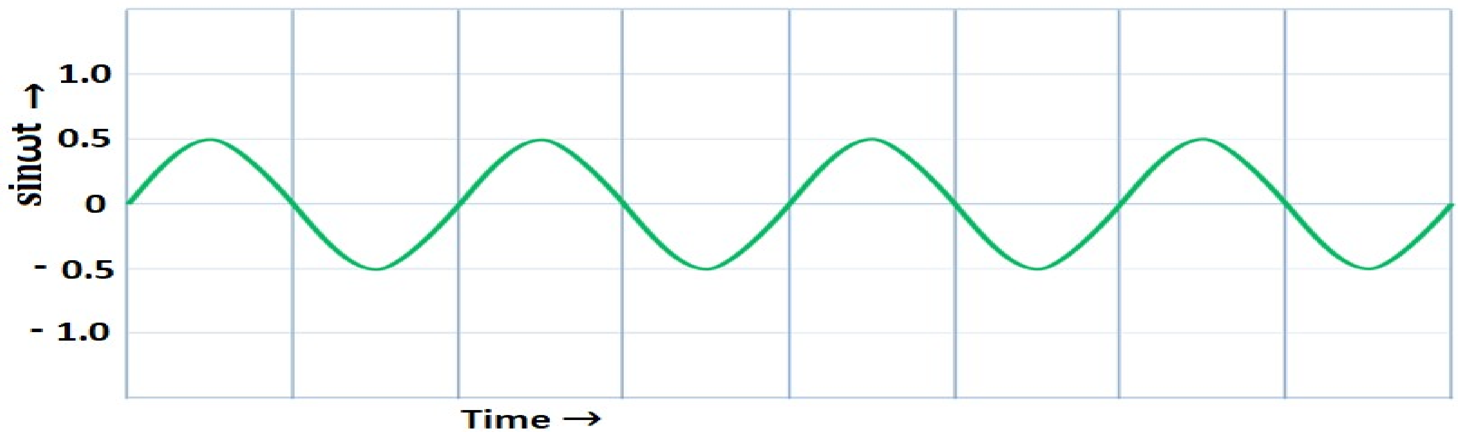
Here F is a differentiable function.

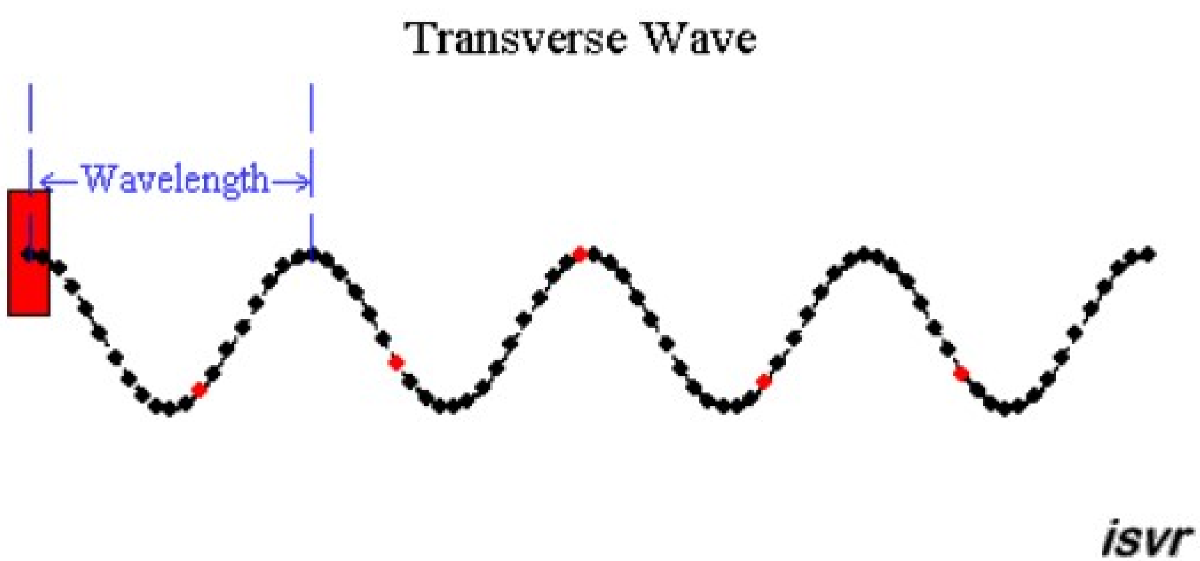
For a wave in a stretched string $\sqrt{\frac{T}{\mu}} = v$

So the wave equation for a stretched string becomes $\frac{\partial^2 y}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2 y}{\partial t^2}$

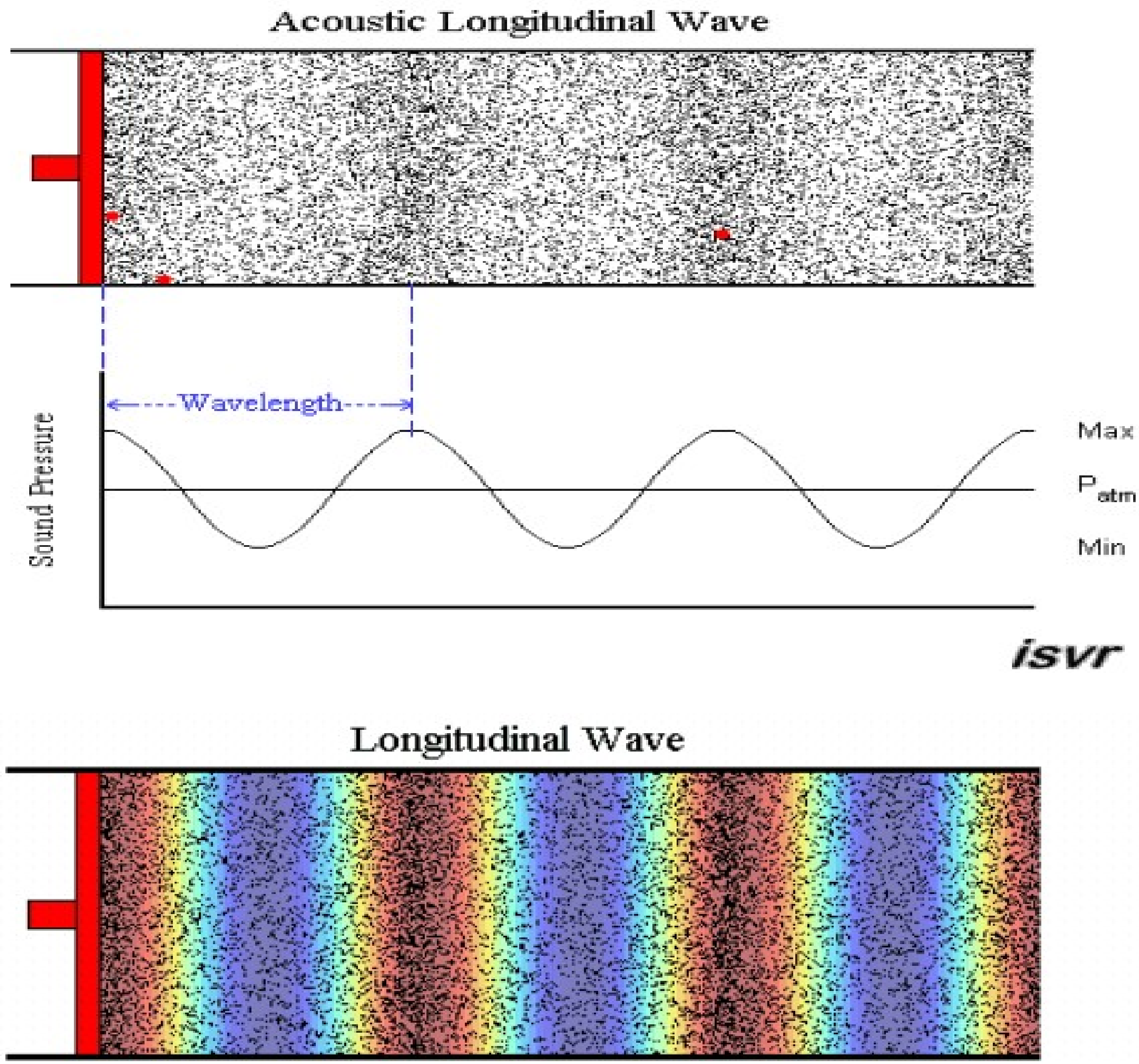
Solution $y = A \sin \omega (t \pm \frac{x}{v})$

y represents the displacement in the string.





Courtesy: ISVR, University of Southampton



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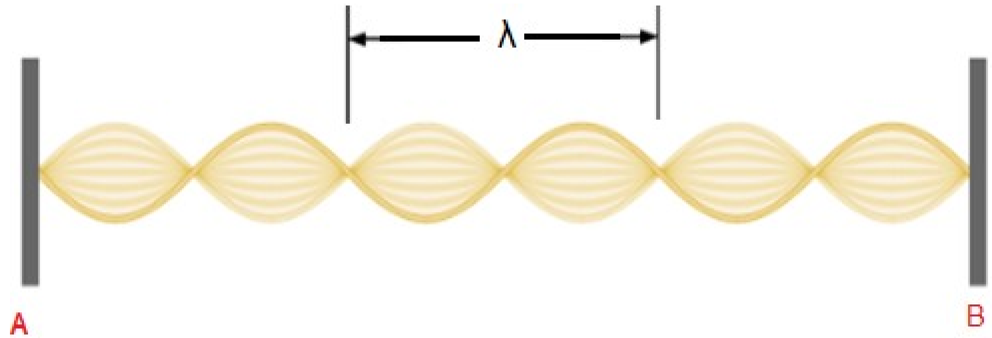

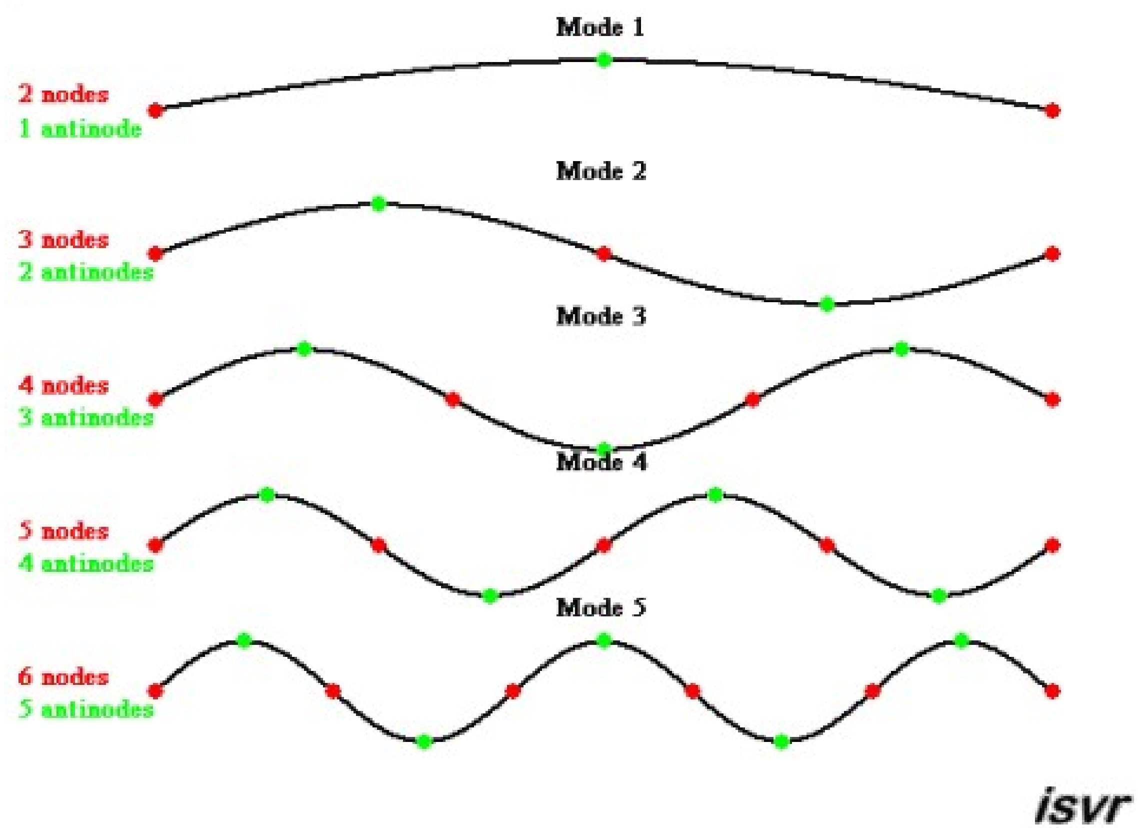

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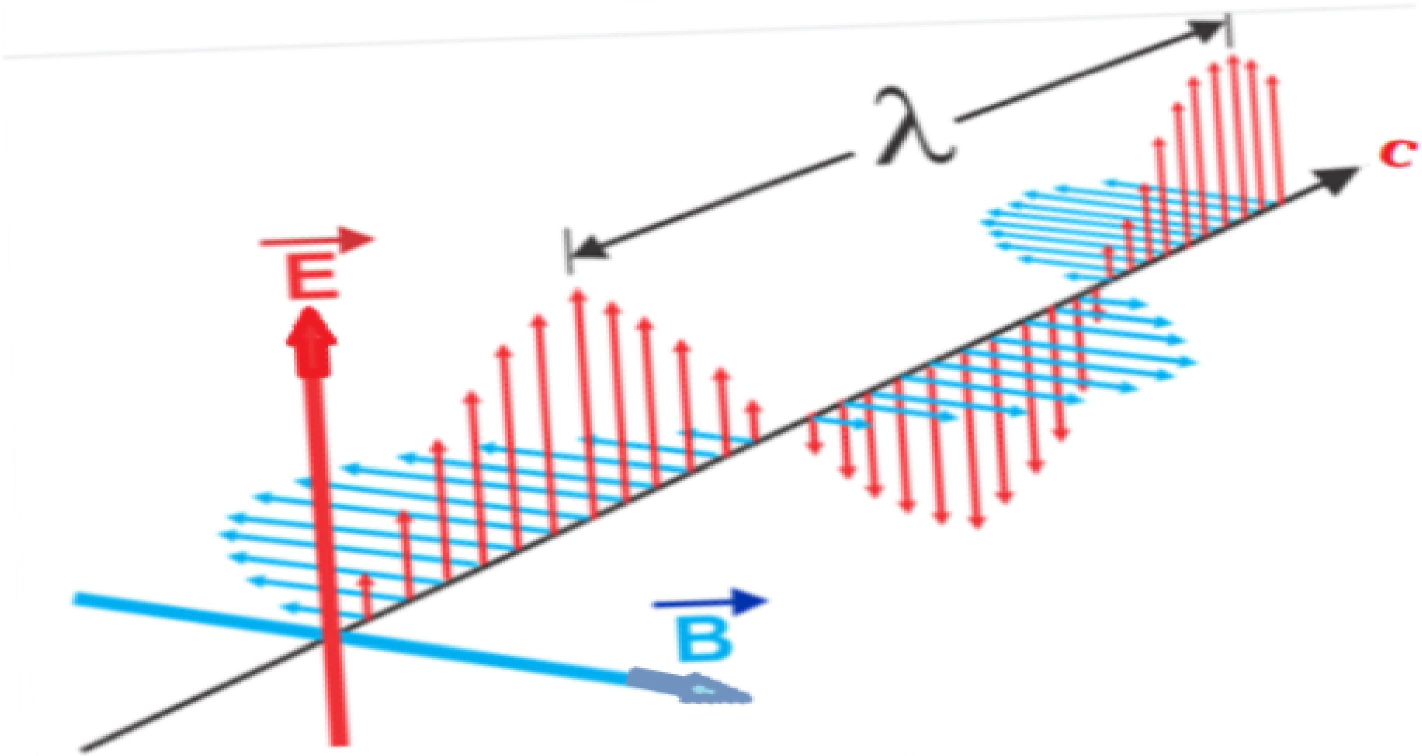
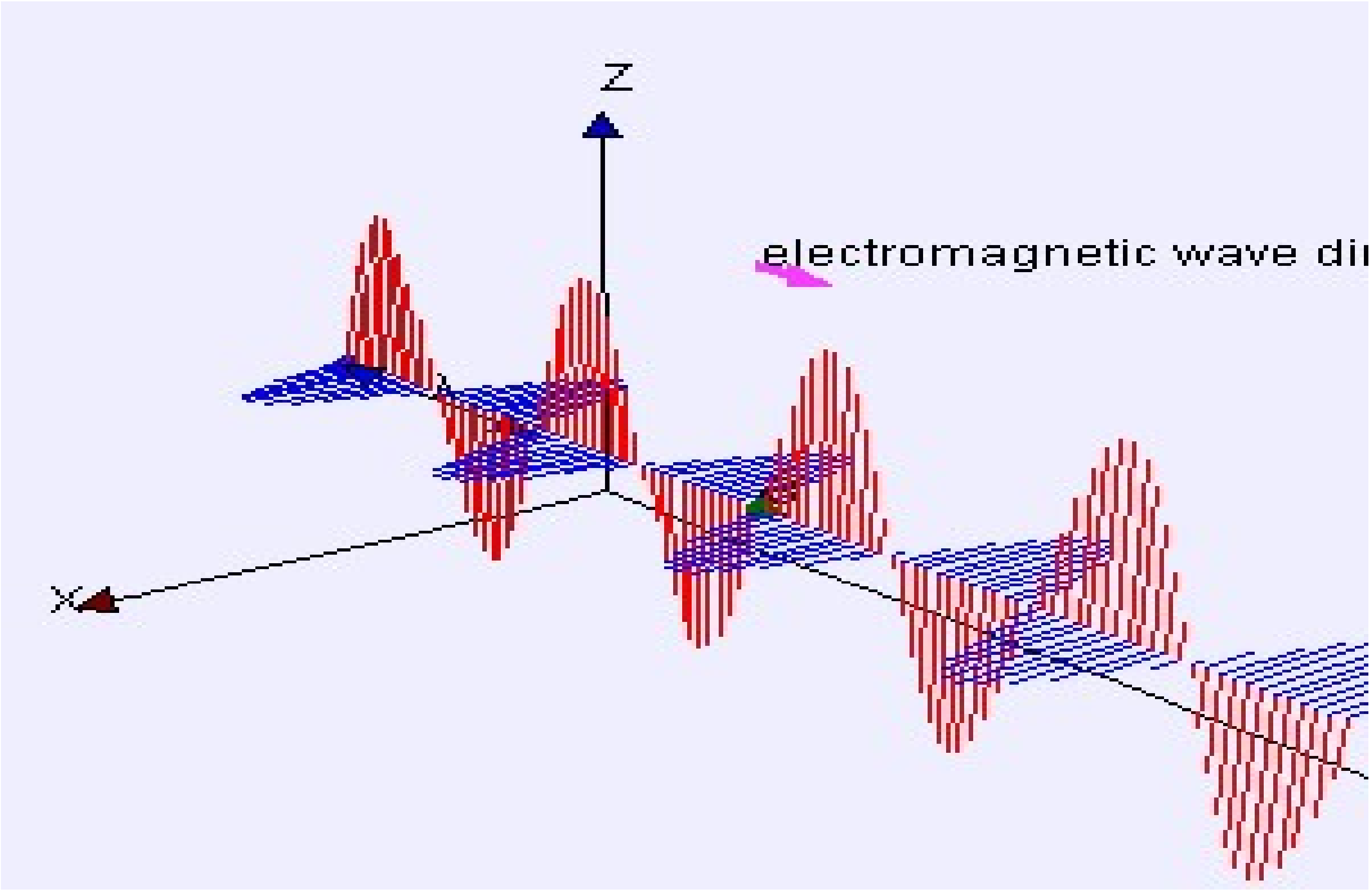
An Electromagnetic Wave Equation

$$\frac{\partial^2 E}{\partial x^2} = \frac{1}{c^2}\frac{\partial^2 E}{\partial t^2}$$

The solution

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





https://commons.wikimedia.org/wiki/File:Electromagneticwave3D.gif

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In quantum mechanics wave function Ψ corresponds to displacement y of waves motion in a string or the oscillating electric or magnetic vector in an electromagnetic wave. However, the wave function associated with a moving particle Ψ is complex and not measurable.

Wave function ψ represents the probability of locating a particle in space at point (x, y, z) at the instant of time t.

ψ is a complex function. It can be positive or negative. However, probability can neither be complex nor negative.

Hence, the probability density $|\psi|^2$ is defined so that this quantity is always positive whether ψ is complex or negative.

A **wave function** in quantum physics is a mathematical description of the quantum state of an isolated quantum system.

According to the superposition principle of quantum mechanics, wave functions can be added together and multiplied by complex numbers to form new wave functions and form a Hilbert space.

A wave function behaves qualitatively like other waves, such as water waves or waves on a string, because the Schrödinger equation is mathematically a type of wave equation. This explains the name "wave function", and gives rise to wave–particle duality.

Since the wave function is complex valued, only its relative phase and relative magnitude can be measured—its value does not, in isolation, tell anything about the magnitudes or directions of measurable observables; one has to apply quantum operators, whose eigenvalues correspond to sets of possible results of measurements, to the wave function ψ and calculate the statistical distributions for measurable quantities.

The mathematical expression of the wave equivalent of a free particle of total energy E and momentum p moving along x-axis.

$$\psi = A\, e^{\left(-i/\hbar\right)(Et-px)}$$

For a particles subjected to some forces a second order differential equation is proposed and formulated which is then applied to special cases.

Differentiate the free particle expression twice with respect to x and once with respect to t.

$$\frac{\partial^2\psi}{\partial x^2} = -\frac{p^2}{\hbar^2}\psi \qquad \frac{\partial\psi}{\partial t} = -\frac{iE}{\hbar}\psi$$

Apply it to the non relativistic case having the total energy **E** of the particle is written as

$$E = \frac{p^2}{2m} + V$$

Multiply by ψ on both sides of the total energy expression

$$E\psi = \frac{p^2}{2m}\psi + V\psi$$

$$E\psi = -\frac{\hbar}{i}\frac{\partial\psi}{\partial t} \qquad p^2\psi = -\hbar^2\frac{\partial^2\psi}{\partial x^2}$$

$$\frac{\hbar}{i}\frac{\partial\psi}{\partial t} = \frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} - V\psi$$

This is time dependent Schrodinger equation.

In 3-dimensions the Schrödinger equation may be written as

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

Here particles' potential V is some function of x, y, z and t.

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

$$\frac{\hbar}{i}\frac{\partial\psi}{\partial t} = \frac{\hbar^2}{2m}\nabla^2\psi - V\psi$$

This holds in all coordinate systems.

A problem with this derivation of Schrödinger equation

We obtained the equation starting from the special case of a wave function of a freely moving particle and then established a general equation !

Is this is plausible?

We have no way to prove that this method of establishing the equation is correct or wrong.

What we have in our hand is to straight away postulate Schrödinger's equation, solve it for different variants of physical conditions and compare the results of the calculations with the results of experiments.

If they agree the postulate embodied in Schrödinger equation is valid.

If they disagree the postulate must be discarded and some other approach would have to be explored.

Schrödinger's equation cannot be derived from the first principle but represents a first principle itself.

The equation is a postulate in the same sense as the postulate of special relativity, or the laws of thermodynamics. None of these postulates can be derived from some other principle. Each principle is a fundamental generalization, equally valid as the empirical data it is based upon.

Form of Schrödinger equation depends on the physical situation. The most general form is the time-dependent Schrödinger equation, which gives a description of a system evolving with time

Time-dependent Schrödinger equation *(single non-relativistic particle)*

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t) = \left[\frac{-\hbar^2}{2\mu}\nabla^2 + V(\mathbf{r},t)\right]\Psi(\mathbf{r},t)$$

$$i\hbar\frac{\partial}{\partial t}\Psi = \hat{H}\Psi$$

The general equation is indeed quite general, used throughout quantum mechanics, for everything from the Dirac equation to quantum field theory, by plugging in various complicated expressions for the Hamiltonian. The specific non-relativistic version is a simplified approximation to reality, which is quite accurate in many situations, but very inaccurate in others

Time-independent Schrödinger equation is the equation describing stationary states

$$E\Psi(\mathbf{r}) = \left[\frac{-\hbar^2}{2\mu}\nabla^2 + V(\mathbf{r})\right]\Psi(\mathbf{r})$$

$$E\Psi = \hat{H}\Psi$$

When the Hamiltonian operator acts on a certain wave function Ψ, and the result is proportional to the same wave function Ψ, then Ψ is a stationary state, and the proportionality constant, E, is the energy of the state Ψ.

In large number of cases the potential energy V is not a function of time but of position only. For such cases any reference to time is excluded.

$$\psi = A\, e^{\left(-i/\hbar\right)(Et-px)}$$

$$\psi = A\, e^{\left(-i/\hbar\right)(Et-px)} = Ae^{\frac{-iEt}{\hbar}}\, e^{\frac{ipx}{\hbar}} = \psi\, e^{\frac{-iEt}{\hbar}}$$

Thus **ψ** is a function of position dependent function ψ a time dependent function. Substitute this ψ in the time dependent Schrödinger equation to get

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2m}{\hbar^2}(E - V)\psi = 0$$

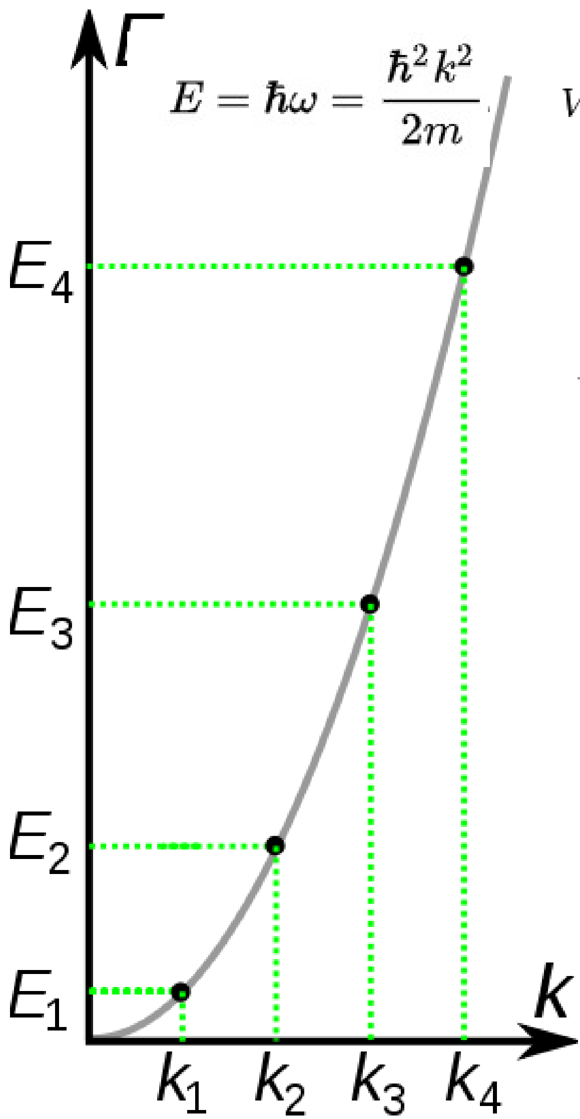
In quantum mechanics, the analogue of Newton's law is Schrödinger's equation.

Schrödinger’s equation has turned out to be completely accurate in predicting the results of experiments. To be sure we must keep in mind that the equation can be used only for non-relativistic problems.

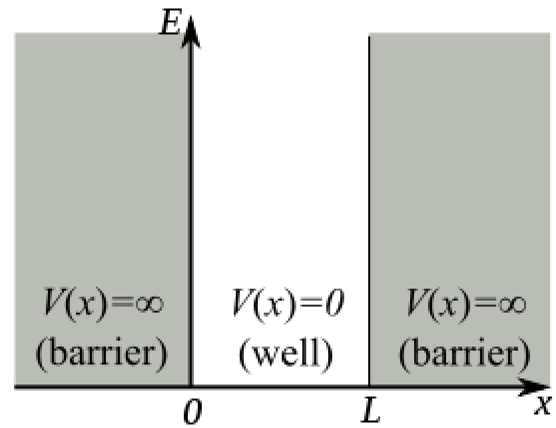
The wave function is the most complete description that can be given of a physical system. Solutions to Schrödinger's equation describe not only molecular, atomic, and subatomic systems, but also macroscopic systems, possibly even the whole universe.

Particle in a box

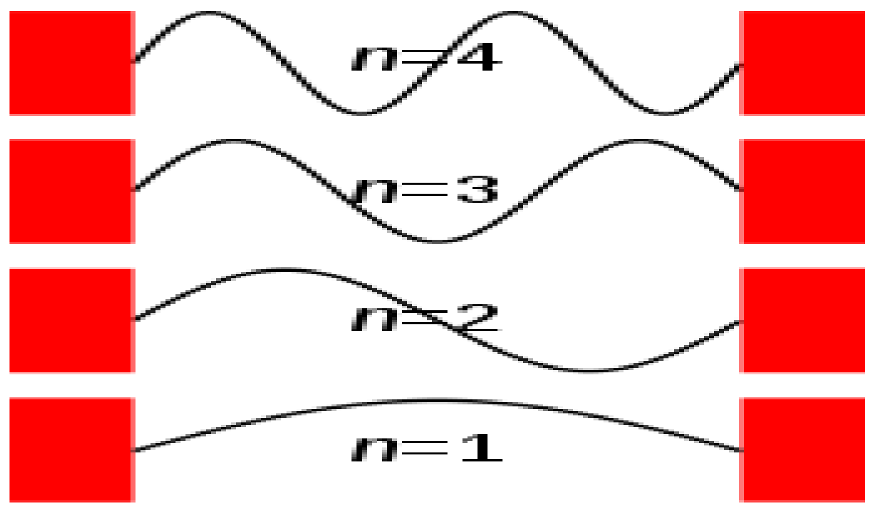
$$E_n = \hbar\omega_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

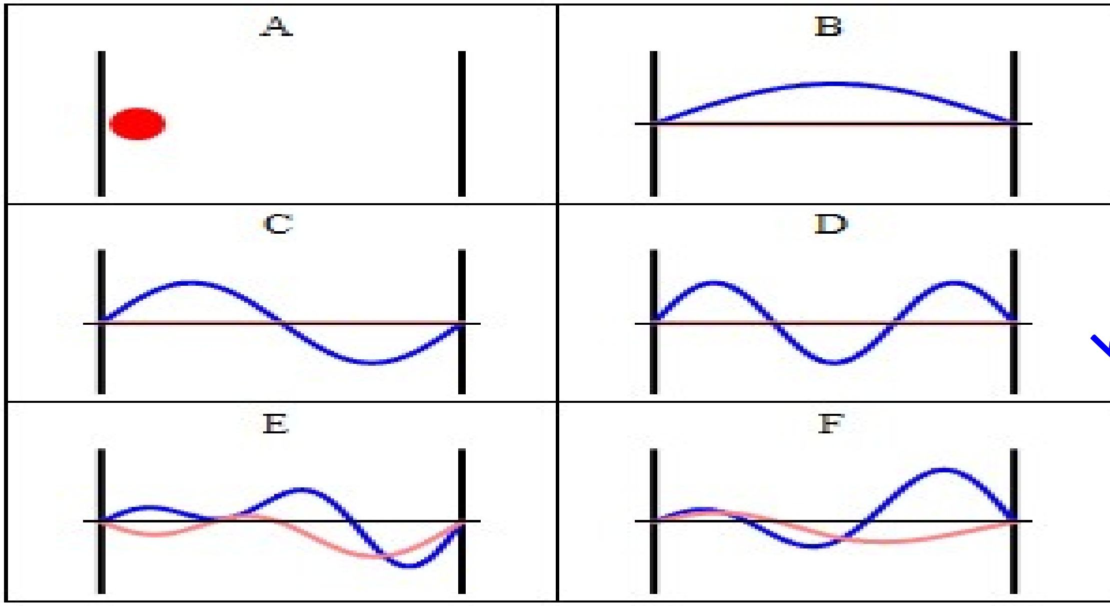


$$V(x) = \begin{cases} 0, & 0 < x < L, \\ \infty, & \text{otherwise}, \end{cases}$$



$$\psi_n(x,t) = \begin{cases} \sqrt{\frac{2}{L}}\sin\left(k_n x - \frac{n\pi x0}{L}\right)e^{-i\omega_n t}, & x_0 < x < x_0 + L, \\ 0, & \text{otherwise}, \end{cases}$$





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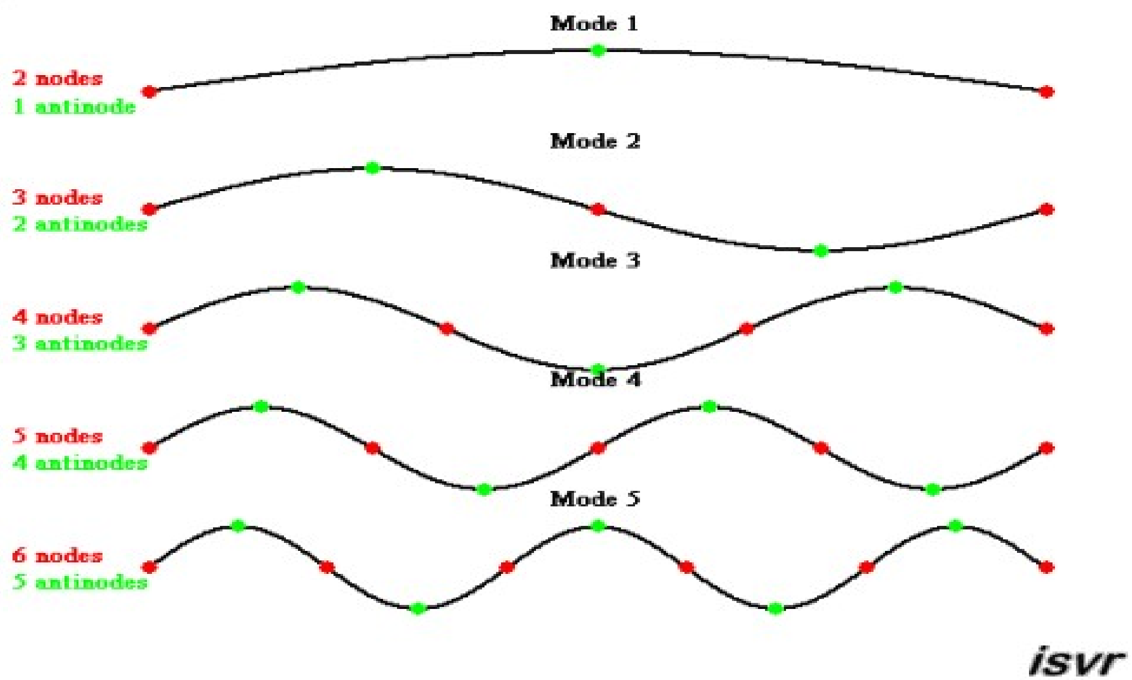
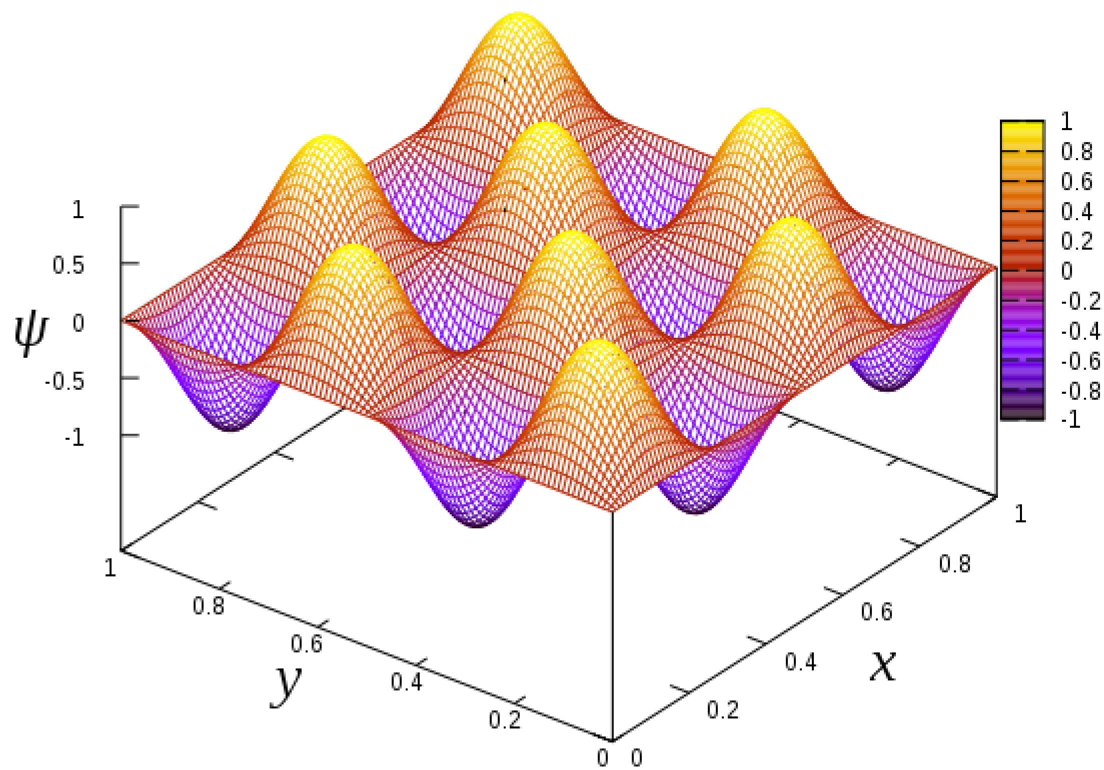


Courtesy: ISVR, University of Southampton

Two-dimensional box

$$\psi_{n_x,n_y} = \sqrt{\frac{4}{L_x L_y}} \sin\left(k_{n_x} x\right) \sin\left(k_{n_y} y\right)$$

$$E_{n_x,n_y} = \frac{\hbar^2 k_{n_x,n_y}^2}{2m}$$



Review

- Newtonian Mechanics versus Quantum Mechanic
- Ψ is complex, $|\psi|^2$ represents the probability density
- Just the way we have y and E for displacement and electromagnetic waves, ψ is the wave function of the wave associated with a moving body
- Speed of de Broglie wave is same as the speed of the body

- Ψ is formed by superposition of infinite number of sinusoidal waves differing from each other by $\Delta\omega$ and Δk
- A wave called the matter wave or de Broglie wave is associated with a moving particle leading to uncertainty in the position of the particle
- Ψ is the solution of the Schrodinger equation
- Schrodinger equation is in itself a postulate like the theory of special relativity of the laws of thermodynamics

NICLE OF HIGHER EDUCATION

MISCHA RICHTER AND HARALD BA

"Basically, I came here as an undergraduate to look for girls, accidentally got hooked on quantum physics, and have been here ever since."

Thanks for your kind attention

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Prof. Narendra Kumar Pandey
Department of Physics
University of Lucknow
Lucknow-226007
Email: profnarendrapandey137@gmail.com