Classical Mechanics/ Newtonian /Hamiltonian Mechanics

Classical mechanics is a branch of physics that deals with the motion of bodies first enunciated by Sir Isaac Newton in his *Philosophiae Naturalis Principia Mathematica* (1687). Classical mechanics was the first branch of Physics to be discovered, and is the foundation upon which all other branches of Physics are built.

Importance of Classical Mechanics

- Classical mechanics has many important applications in other areas of science, such as Astronomy (*e.g.*, celestial mechanics), Chemistry (*e.g.*, the dynamics of molecular collisions), Geology (*e.g.*, the propagation of seismic waves, generated by earthquakes, through the Earth's crust), and Engineering (*e.g.*, the equilibrium and stability of structures).
- Classical mechanics--starting with the ground-breaking work of Copernicus, continuing with the researches of Galileo, Kepler, and Descartes, and culminating in the monumental achievements of Newton--involved the complete overthrow of the Aristotelian picture of the Universe.
- Classical mechanics support different types of motion:

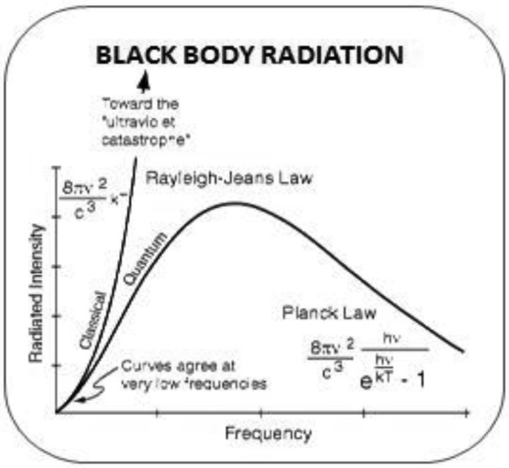
    - *Translational motion*--motion by which a body shifts from one point in space to another (*e.g.*, the motion of a bullet fired from a gun).
    - *Rotational motion*--motion by which an extended body changes orientation, with respect to other bodies in space, without changing position (*e.g.*, the motion of a spinning top).
    - *Oscillatory motion*--motion which continually repeats in time with a fixed period (*e.g.*, the motion of a pendulum in a grandfather clock).
    - *Circular motion*--motion by which a body executes a circular orbit about another fixed body [*e.g.*, the (approximate) motion of the Earth about the Sun].

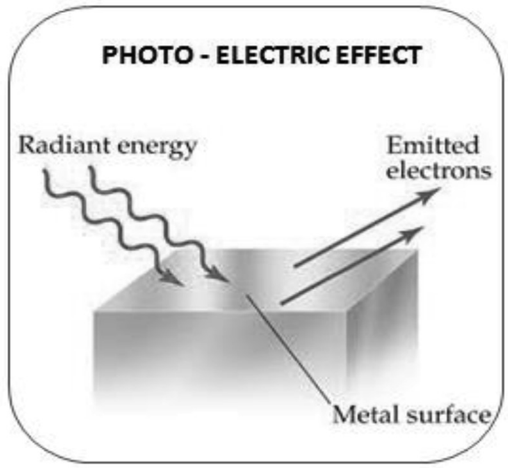
Example of event supported by classical mechanics

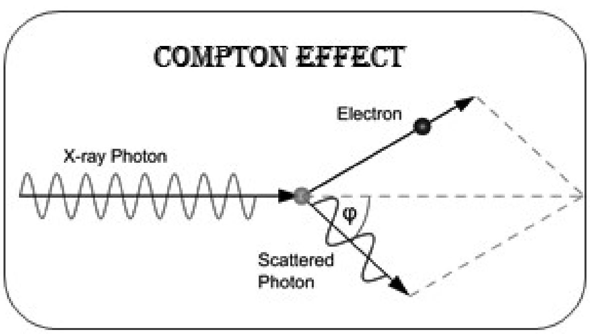
Classical mechanics describes the motion of macroscopic objects, from projectiles to parts of machinery, as well as astronomical objects, such as spacecraft, planets, stars, and galaxies. Besides this, many specializations within the subject deal with solids, liquids and gases and other specific sub-topics. Classical mechanics also 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.

Break down of classical theory

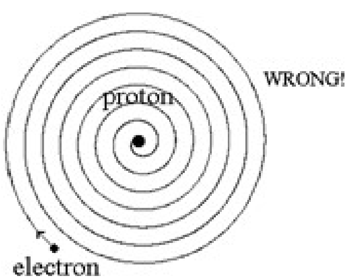
Classical theory ruled the Area of Physics till 18th century. In the year 1900, quantum theory starts with Planck's formula of black body radiation. In the year 1887, photo electric effect given by Hertz was also not able to explain based on classical theory. It also fails to explain the existence of spectral lines emitted by H_2, stability of atoms etc. Classical mechanics was not able to explain the new discoveries at that time like Zeeman Effect, Compton Effect, Stark effect etc.







Not explained by Classical Mechanics



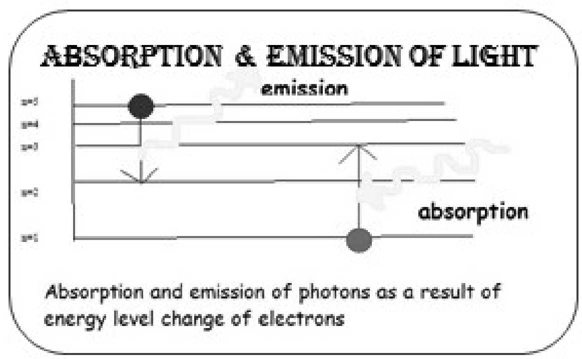
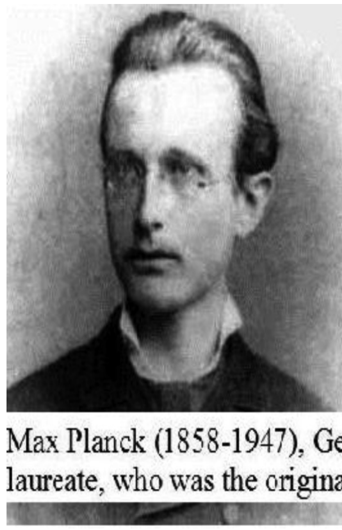


Figure 2 Event that was not supported by classical theory

Definition and development of quantum theory

Quantum theory is the theoretical basis of modern physics that explains the nature and behavior of matter and energy on the atomic and subatomic level. The nature and behavior of matter and energy at that level is sometimes referred to as quantum physics and quantum mechanics.



Max Planck (1858-1947), German physicist and Nobel laureate, who was the originator of the quantum theory.

In 1900, physicist Max Planck presented his quantum theory to the German Physical Society. Planck had sought to discover the reason that radiation from a glowing body changes in color from red, to orange, and, finally, to blue as its temperature rises. He found that by making the assumption that energy existed in individual units in the same way that matter does, rather than just as a constant electromagnetic wave - as had been formerly assumed - and was therefore *quantifiable*, he could find the answer to his question. The existence of these units became the first assumption of quantum theory.

Planck wrote a mathematical equation involving a figure to represent these individual units of energy, which he called *quanta*. The equation explained the phenomenon very well; Planck found that at certain discrete temperature levels (exact multiples of a basic minimum value), energy from a glowing body will occupy different areas of the color spectrum. Planck assumed there was a theory yet to emerge from the discovery of quanta, but, in fact, their very existence implied a completely new and fundamental understanding of the laws of nature. Planck won the Nobel Prize in Physics for his theory in 1918, but developments by various scientists over a thirty-year period all contributed to the modern understanding of quantum theory.

Planck's Quantum theory of radiation: Postulates

1. A Chamber that emits black body radiations are made up of large number of harmonic oscillators of molecular dimensions.

2. The oscillator vibrates in all possible frequency.
3. The oscillator emits radiation whose frequency is equivalent to the frequency of its vibration.
4. The oscillator emits discrete energy $E= nh\upsilon$ Where n= 0, 1, 2, 3……
5. The energy absorbed and emitted by the oscillator are in the order of $h\upsilon$.

The Development of Quantum Theory

- In 1900, Planck made the assumption that energy was made of individual units, or quanta.
- In 1905, Albert Einstein theorized that not just the energy, but the radiation itself was *quantized* in the same manner.
- In 1924, Louis de Broglie proposed that there is no fundamental difference in the makeup and behavior of energy and matter; on the atomic and subatomic level either may behave as if made of either particles or waves. This theory became known as the *principle of wave-particle duality*: elementary particles of both energy and matter behave, depending on the conditions, like either particles or waves.
- In 1927, Werner Heisenberg proposed that precise, simultaneous measurement of two complementary values - such as the position and momentum of a subatomic particle - is impossible. Contrary to the principles of classical physics, their simultaneous measurement is inescapably flawed; the more precisely one value is measured, the more flawed will be the measurement of the other value. This theory became known as the uncertainty principle, which prompted Albert Einstein's famous comment, "God does not play dice."

Quantum mechanics support of the event

- Black body radiation
- Photoelectric effect
- Atomic and molecular spectra
- Molar heat capacity at constant volume
- Stark Effect
- Zeeman Effect

- Compton Effect
- Absorption and Emission of light etc.

Comparison between classical and quantum Mechanics

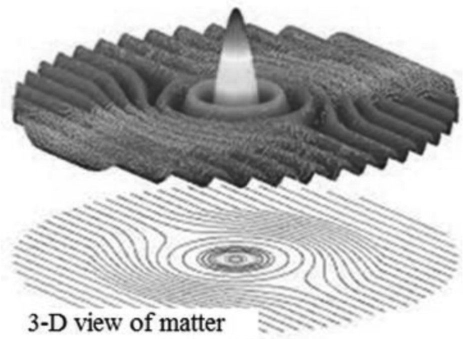
Classical Mechanics	Quantum Mechanics
(i) It deals with macroscopic particles.	(i) It deals with microscopic particles.
(ii)It is based upon Newton's laws of motion	(ii) It takes into account Heisenberg's uncertainty principle and de Broglie concept of dual nature of matter (particle nature and wave nature)
(iii) It is based on Maxwell's electromagnetic wave theory according to which any amount of energy may be emitted or absorbed continuously.	(iii) It is based on Planck's quantum theory according to which only discrete values of energy are emitted or absorbed.
(iv) The state of a system is defined by specifying all the forces acting on the particles as well as their positions and velocities (moment). The future state then can be predicted with certainty.	(iv) It gives probabilities of finding the particles at various locations in space.

Dual nature of matter- de Broglie wavelength

Definition of matter: Anything that occupies space and has mass. Dual nature of matter: In 1924, Lewis de-Broglie proposed that matter has dual characteristic just like radiation. The whole universe is composed of matter and electromagnetic radiations. Since both are forms of energy so can be transformed into each other.

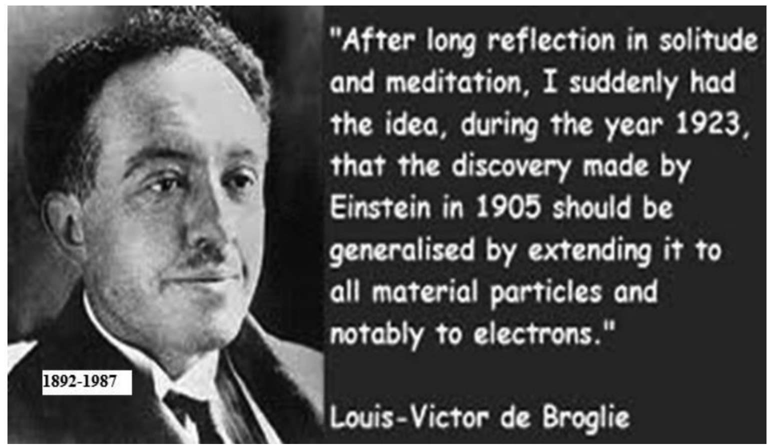
The matter loves symmetry. As the radiation has dual nature, matter should also possess dual character. According to the de Broglie concept of matter waves, the matter has dual nature. It means when the matter is moving it shows the wave properties (like interference, diffraction etc.) are associated with it and when it is in the state of rest then it shows particle properties. Thus the matter has dual nature. The waves associated with moving particles are matter waves or de-Broglie waves.

The phenomena of interference, diffraction and polarization of light could be explained on the wave nature of light. But certain phenomena like photo electric effect, Compton effect etc. can

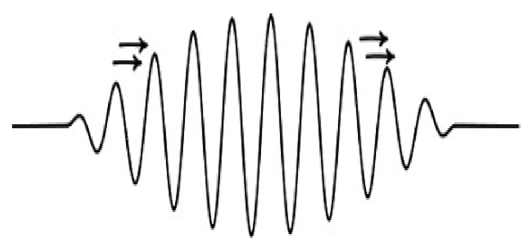


be explained only by corpuscular nature of radiation. Thus light exhibit dual nature that of particle and wave nature can be associated with wave.

Louis de Broglie hypothesis:



1. Nature loves symmetry- Nature manifest itself in two forms matter and radiation. Radiation possess a dual nature hence it undergo interference, diffraction and polarization also photo electric effect, Compton Effect etc.
2. Parallelism between mechanics and optics – The principle of least action of particles choosing shortest distance in mechanics is also followed in Fermat's principle in optics which states wave chooses a path of shortest distance.
3. Bohr's theory of atomic structure: Distribution of electron in the energy states are governed by "integer rules". The phenomena involving integers in Physics are those interference and mode of vibration of stretched string in wave motion.



Matter waves: Waves associated with a particle are called matter wave. The amplitude of the wave is high where the probability of finding the particle high.

Matter waves- De Broglie wavelength

- Wave associated with a particle are called matter wave
- Matter wave are wave like behavior exhibited by matter
- This concept was proposed by de-Broglie in his hypothesis.
- Matter waves are a central part of the theory of quantum mechanics.
- Matter waves are often referred to as de-Broglie waves.

Consider a photon whose energy is given by E= hυ= hc/λ −− (1)

If a photon possesses mass (rest mass is zero), then according to the theory of relatively, its energy is given by

$E= mc^2$ −− (2)

From (1) and (2),

Mass of photon m= h/cλ, Therefore Momentum of photon

P=mc=h c / c λ = h/λ −− (3) Or λ = h/p

If instead of a photon, we consider a material particle of mass m moving with velocity v, then the momentum of the particle, p=mv. Therefore, the wavelength of the wave associated with this moving particle is given by: h/mv

Or $\boxed{\lambda = h/p \ (p = mv) \quad \ldots\ldots. (4)}$

This wavelength is called de-Broglie wavelength.

De- Broglie wavelength from particle nature:

Let a particle be pictured as a standing wave system in a space occupied by a particle that has wave function ψ at instant of time t_0 at some point x_0 is given by:

$$\psi = \psi_0 \sin 2\pi \upsilon_0 t_0 \ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (1)$$

Where ψ_0 - amplitude

υ_0 - frequency for an observer at rest

Wave equation in classical mechanics: $Y = A \sin \omega t$ ………………… (2)

If the particle is moving with velocity v along x axis, the value of ψ at any instant t is given by:

$$\psi = \psi_0 \sin 2\pi \upsilon_0 t \ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (3)$$

Using Lorentz transformation equation for time dilation:

$$t_0 = \frac{t - \frac{vx}{c^2}}{\sqrt{1 - \frac{v^2}{c^2}}} \quad \text{……………………………………. (4)}$$

Substituting (4) in (1)

$$\psi = \psi_0 \sin 2\pi\upsilon_0 \frac{t - \frac{vx}{c^2}}{\sqrt{1 - \frac{v^2}{c^2}}} \quad \text{………………………….. (5)}$$

This equation can be compared with the standard equation of wave motion

$$y = A\sin\left\{\frac{2\pi}{T}(t - \frac{x}{u}\right\} \quad \text{……………………………….. (6)}$$

Where A- Amplitude, T- periodic time, u- wave velocity

Comparing equation 5 & 6 we get,

$$\frac{1}{T} = \upsilon = \frac{\upsilon_0}{\sqrt{1 - \frac{v^2}{c^2}}}, \quad \text{and } u = \frac{c^2}{v} \quad \text{………………… (7)}$$

From Einstein mass- energy equation

$$h\upsilon_0 = m_0 c^2 \text{ or } \upsilon_0 = \frac{m_0 c^2}{h} \quad \text{………………………….. (8)}$$

$$\therefore \upsilon = \frac{m_0 c^2}{h\sqrt{1 - \frac{v^2}{c^2}}} = \frac{m}{h}c^2 \quad \text{………………………………….. (9)}$$

Wavelength of matter wave} = λ= velocity/ frequency

$$\lambda = \frac{u}{\upsilon} = \frac{h}{mv} \quad \text{……………………………………………………….. (10)}$$

Characteristics of de Broglie matter wave:

1. The amplitude of the wave is high where the probability of finding the particle high.

2. Two different velocities are associated with the material particle in motion:
   v- velocity of particle & u- velocity of wave
3. If $v<c$, $u>c$ that is velocity of matter wave is greater than velocity of light

Special Cases:

1. de-Broglie wavelength for material particle:

If E is the kinetic energy of the material particle of mass m moving with velocity v, then

$E=1/2\ mv^2=1/2\ m^2v^2=p^2/2m$

Or $\qquad p=\sqrt{2mE}$

Therefore the by putting above equation in equation (4), we get de-Broglie wavelength equation for material particle as:

$\lambda = h/\sqrt{2mE} \quad --(5)$

This is the dE-Broglie wavelength for particle in gaseous state

2. dE-Broglie wavelength for an accelerated electron:

Suppose an electron accelerates through a potential difference of V volt. The work done by electric field on the electron appears as the gain in its kinetic energy

That is $E = eV$

Also $E = p^2/2m$

Where e is the charge on the electron, m is the mass of electron and v is the velocity of electron, then comparing the above two equations, we get:

$eV= p^2/2m$, or $p = \sqrt{2meV}$

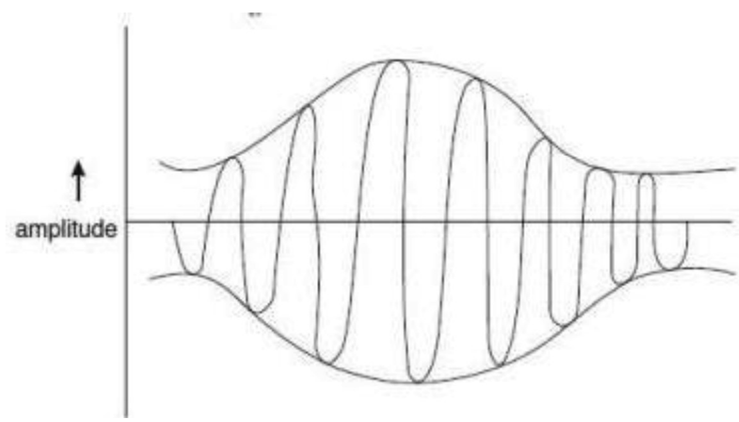
Thus by putting this equation in equation (4), we get the the de-Broglie wavelength of the electron as

$\lambda = h/\sqrt{2meV}\ \ 6.63 \times 10^{-34}/\sqrt{2} \times 9.1 \times 10\text{-}^{31} \times 1.6 \times 10^{-19}\ V$

$$\lambda = \frac{12.27}{\sqrt{V}} \mathring{A}$$

This is the de-Broglie wavelength for electron moving in a potential difference of V volt.

Wave packet



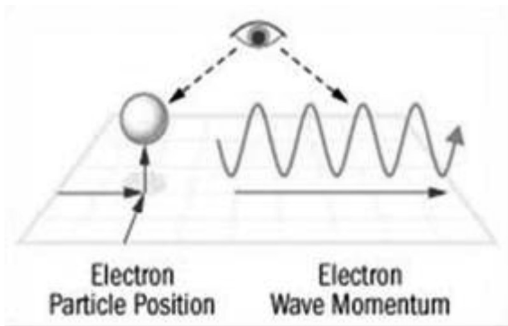
It is an addition of matter waves with a small range of momenta. The resulting packet occupies a range of positions in space and is associated with a range of momenta. A wave packet is a group of several wavs of slightly different velocity and wavelength. It is the resultant wave represented obtained by the superposition of component waves of different velocity and different wavelength

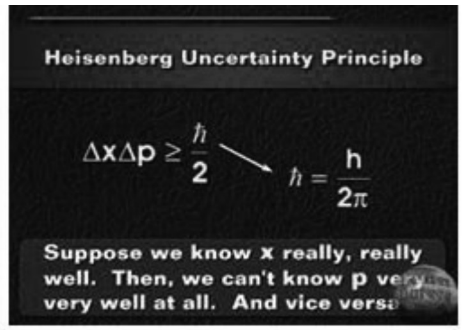
Heisenberg uncertainty principle

An early incarnation of the uncertainty principle appeared in a 1927 paper by Heisenberg, a German physicist who was working at Niels Bohr's institute in Copenhagen at the time, titled "On the Perceptual Content of Quantum Theoretical Kinematics and Mechanics". The more familiar form of the equation came a few years later when he had further refined his thoughts in subsequent lectures and papers.

The Heisenberg Uncertainty Principle states that you can never simultaneously know the exact position and the exact speed of an object. As everything in universe behaves like both a particle and a wave at the same moment.

The position and momentum of a particle cannot be simultaneously measured with arbitrarily high precision. There is a minimum for the product of the uncertainties of these two measurements. There is likewise a minimum for the product of the uncertainties of the energy and time.





$$\Delta p\, \Delta x\ \geq \frac{1}{2}\,\hbar$$

$$\Delta E\, \Delta t\ \geq \frac{1}{2}\,\hbar$$

Postulates of wave mechanics

Definition: The matter wave describing a given microscopic situation is called wave function.

A **wave function** in quantum mechanics describes the quantum state of an isolated system of one or more particles. There is *one* wave function containing all the information about the entire system, not a separate wave function for each particle in the system. The most common symbols for a wave function are the Greek letters ψ or Ψ (lower-case and capital psi).

Postulates of wave mechanics: All the properties of microscopic particle in a quantum system can be studied with a set of rules called the postulates of wave mechanics.

1. Any parameter associated with the motion of a particle is linked with an operator

Observable		Operator	
Name	Symbol	Symbol	Operation
Position	$\mathbf{r}$	$\hat{\mathbf{r}}$	Multiply by $\mathbf{r}$
Momentum	$\mathbf{p}$	$\hat{\mathbf{p}}$	$-i\hbar\left(\hat{i}\frac{\partial}{\partial x}+\hat{j}\frac{\partial}{\partial y}+\hat{k}\frac{\partial}{\partial z}\right)$
Kinetic energy	T	$\hat{T}$	$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)$
Potential energy	$V(\mathbf{r})$	$\hat{V}(\mathbf{r})$	Multiply by $V(\mathbf{r})$
Total energy	E	$\hat{H}$	$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)+V(\mathbf{r})$
Angular momentum	l_x	$\hat{l}_x$	$-i\hbar\left(y\frac{\partial}{\partial z}-z\frac{\partial}{\partial y}\right)$
	l_y	$\hat{l}_y$	$-i\hbar\left(z\frac{\partial}{\partial x}-x\frac{\partial}{\partial z}\right)$
	l_z	$\hat{l}_z$	$-i\hbar\left(x\frac{\partial}{\partial y}-y\frac{\partial}{\partial x}\right)$

2. The wave function is also represented by a linear Eigen value equation linked with each operator.

$$i\hbar\frac{\partial\psi}{\partial t}=E\psi \ , \quad H\psi=E\psi$$

Here ψ is the Eigen function, E is the total energy Eigen value and H is the operator.

3. Measurement of a dynamical quantity p is made in a particle for which the wave function is ψ. Different values are got at different trials as uncertainty principle. Hence the most probable value total energy of a particle is given by <p>

$$<p>=\int \varphi*(-i\frac{h}{2\pi}\frac{\partial}{\partial t})\varphi dx\, dy\, dz$$

$$\langle\hat{A}\rangle=\frac{\int\psi^*\hat{A}\psi\,d\tau}{\int\psi^*\psi\,d\tau} \qquad \text{if } \psi \text{ is not normalized.}$$

$$=\int\psi^*\hat{A}\psi\,d\tau \qquad \text{if } \psi \text{ is normalized,}$$

since then by definition $\int\psi^*\psi\,d\tau=1$

Schrodinger time dependent and independent equation

In quantum mechanics, the **Schrödinger equation** is a partial differential equation that describes how the quantum state of a physical system changes with time. It was formulated by Erwin Schrödinger.

Schrodinger time dependent equation

Erwin Schrödinger in extension to deBroglie's hypothesis introduced a differential wave equation of second order to explain the wave nature of matter and particle associated to wave. This equation is analogous to the equation for waves in optics, which assumes that the particle behaves as wave and yields solution in terms of a function called the wave function. When this equation is solved, it gives two things; namely the wave function Ψ and the energy E, of the particle under consideration. Once the wave function Ψ is known, then everything about the particle is known or can be deduced from the wave function.

The wave function Ψ defined in a x- direction is given by

$$\psi = Ae^{i\omega(t-\frac{x}{v})} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (1)$$

Substituting ω = 2πυ and v= υλ in equation (1)

$$\psi = Ae^{-2\pi i\left(\upsilon t-\frac{x}{\lambda}\right)} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (2)$$

Let total energy E = hυ and momentum of the particle p=mv of the particle. Substituting the factor in equation (2)

$$\psi = Ae^{-\left(2\pi i/h\right)[Et-px]} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (3)$$

This is the wave equivalent of an unrestricted particle of total energy E and momentum p moving in +x direction.

Differentiating equation (3) twice with respect to" x" we get:

$$\frac{\partial^2 \psi}{\partial x^2} = -\frac{4\pi^2}{h^2} p^2 \psi \quad \text{...} (4)$$

Differentiating equation (3) with respect to” t” we get:

$$\frac{\partial \psi}{\partial t} = -\frac{2\pi i}{h} E\psi \quad \text{...} (5)$$

As the speed of the particle is less than that of light, Equation of total energy E is given by:

$$E = \frac{p^2}{2m} + V \quad \text{...} (6)$$

Multiply by Ψ throughout the equation (6) we get:

$$E\psi = \frac{p^2}{2m}\psi + V\psi \quad \text{..} (7)$$

From equation (4) and (5) we get

$$E\psi = -\frac{h}{2\pi i}\frac{\partial \psi}{\partial t} \quad \text{..} (8)$$

$$p^2\psi = -\frac{h^2}{4\pi^2}\frac{\partial^2 \psi}{\partial x^2} \quad \text{...} (9)$$

Substituting equation (8) and (9) in equation (7) we get:

$$i\hbar\frac{\partial \psi}{\partial t} = -\frac{h^2}{8\pi^2 m}\left[\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2}\right] + V\psi \quad \text{.................} (10)$$

The above is the three dimensions equation of time dependent form of Schrodinger’s equation.

Schrodinger time independent equation

In many situations the potential energy of a particle does not dependent upon time explicitly. The forces that act upon the particle in negligible hence V vary with only the position of the particle. Schrodinger’s equation may be simplified by removing all reference to “t”. The one dimensional wave function of an unrestricted particle may be written of the form:

$$\psi = Ae^{-\left(2\pi i/h\right)[Et-px]} \text{ .... (1)}$$

$$\psi = Ae^{\frac{-2\pi iEt}{h}}.e^{\frac{2\pi ipx}{h}} \text{ .... (2)}$$

Define a wave equation ψ_0 so that

$$\psi_0 = Ae^{\frac{2\pi ipx}{h}} \text{ .... (3)}$$

Substituting equation (3) in (2) we get:

$$\psi = \psi_0 e \frac{-2\pi iEt}{h} \text{ .... (4)}$$

So Ψ is the product of position dependent function Ψ_0 and a time dependent function $e\frac{-2\pi iEt}{h}$

Differentiating equation (4) with respect to" t" we get:

$$\frac{\partial\psi}{\partial t} = -\frac{2\pi i}{h}E\psi_0 e^{\frac{-2\pi iEt}{h}} \text{ .... (5)}$$

Differentiating equation (4) twice with respect to" x" we get:

$$\frac{\partial^2\psi}{\partial x^2} = \frac{\partial^2\psi_0}{\partial x^2}e^{\frac{-2\pi iEt}{h}} \text{ .... (6)}$$

Equation (5) and (6) can be substituted in in Schrodinger time dependent equation:

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{h^2}{8\pi^2 m}\left[\frac{\partial^2\psi}{\partial x^2}\right] + V\psi \text{ .... (7)}$$

$$E\psi_0 e^{\frac{-2\pi iEt}{h}} = \frac{-h^2}{8\pi^2 m}\frac{\partial^2\psi_0}{\partial x^2}e^{\frac{-2\pi iEt}{h}} + V\psi_0 e^{\frac{-2\pi iEt}{h}} \text{ .... (8)}$$

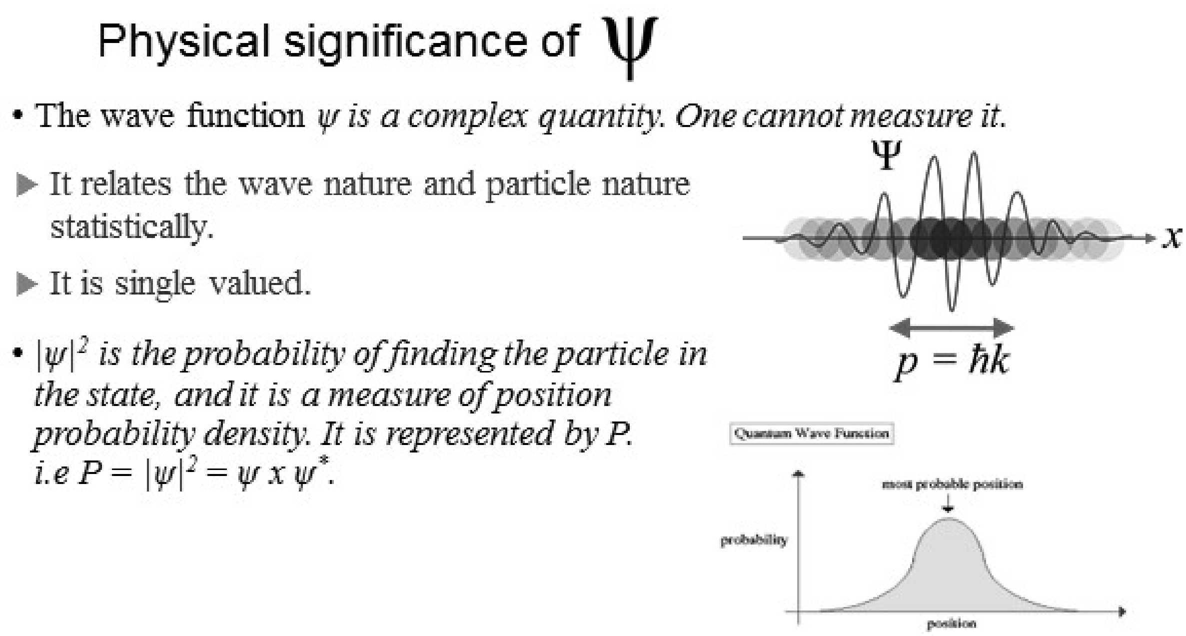
Simplifying the above equation we get:

$$\frac{h^2}{8\pi^2 m}\frac{\partial^2\psi_0}{\partial x^2}+(E-V)\psi_0=0 \quad \text{………………………………………….. (9)}$$

Equation (9) is the steady state form of Schrodinger's equation. In 3 dimensional general form of the above equation can be written as:

$$\nabla^2\psi+\frac{8\pi^2 m(E-V)}{h^2}\psi=0 \quad \text{……………………………………………… (10)}$$

Physical significance of ψ



$$\boxed{\Psi(x,t)=0 \quad as\ x\rightarrow\pm\infty}$$

- ψ contains all the measurable information about the particle
- ψ $\psi^*\psi$ summed over all space = 1 (if the particle exists, the probability of finding it somewhere must be one)
- ψ is continuous
- ψ allows energy calculations via the Schrodinger equation
- ψ establishes the probability distribution in three dimensions
- ψ permits calculation of the effective average value (expectation value) of a given variable
- ψ for a free particle is a sine wave, implying a precisely determined momentum and a totally uncertain position (uncertainty principle)

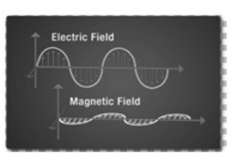
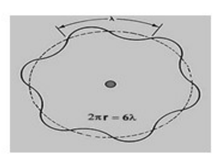
Wave function should be normalized

$\int \psi\psi^* dv = 1$ or $|\psi^2| = 1$

Wave function should be orthogonal

$\int \psi_1(x)\psi_2^*(x)dx = 0$ where $\psi_1(x)$ is the real part of wave function $\psi_1$and ψ_2^* is the complex conjugate of wave function ψ_2.

Difference between electromagnetic waves and matter waves

• Associated with electric and magnetic fields	• Not associated with these fields
	
• Can be radiated into space.	• Cannot be radiated in space.
	
• Travel with same velocity	• Travel with different velocities