Wave Mechanics (TPH101)

By Dr. Vishal Chauhan

Contributions

- 17th Century

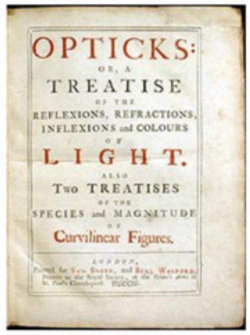
William Gilbert
Explained the dipping of the needle by the magnetic attraction of the earth

Johannes Kepler
The laws of the Rectilinear propagation of light

Issac Newton
Theory of light

Christiaan Huygens
Principle of wavefront

- 18th Century



OPTICKS:
OR, A
TREATISE
OF THE
REFLEXIONS, REFRACTIONS,
INFLEXIONS and COLOURS
OF
LIGHT.
ALSO
Two TREATISES
OF THE
SPECIES and MAGNITUDE
OF
Curvilinear Figures.
LONDON,

By Issac Newton

Benjamin Franklin
Kite experiment

Charles-Augustin de Coulomb

- 19th Century

Thomas Young

Alessandro Volta

Humphry Davy

Fraunhofer

Christian Ørsted

André-Marie Ampère

Michael Faraday

James Clerk Maxwell

Wave Particle Duality

Particle Nature of light:

An object has a definite position in space which cannot be simultaneously occupied by another particle and indentifiable by their distinct properties such as mass, momentum, kinetic engergy, spin and electric charge.

Examples: Photoelectric effect, emission and absroption of radiation by substances, black body radiation etc.

Wave Nature of light:

A wave means periodically repeated pattern in space which is specified by its wavelength, frequency, amplitude of disturbance, intensity, energy and momentum.

Examples: Interference, Diffraction, Polarization etc.

1900: Max Planck suggests that radiation is quantized (it comes in discrete amounts.)

1905: Albert Einstein, one of the few scientists to take Planck's ideas seriously, proposes a quantum of light (the photon) which behaves like a particle. Einstein's other theories explained the equivalence of mass and energy, the particle-wave duality of photons, the equivalence principle, and special relativity.

1913: Niels Bohr succeeds in constructing a theory of atomic structure based on quantum ideas.

1919: Ernest Rutherford finds the first evidence for a proton.

1921: James Chadwick and E.S. Bieler conclude that some strong force holds the nucleus together.

1923: Arthur Compton discovers the quantum (particle) nature of x rays, thus confirming photons as particles.

1924: Louis de Broglie proposes that matter has wave properties.

1925 (Jan): Wolfgang Pauli formulates the exclusion principle for electrons in an atom.

1926: Erwin Schroedinger develops wave mechanics, which describes the behavior of quantum systems for bosons. Max Born gives a probability interpretation of quantum mechanics. G.N. Lewis proposes the name "photon" for a light quantum.

1927: Werner Heisenberg formulates the uncertainty principle: the more you know about a particle's energy, the less you know about the time of the energy (and vice versa.) The same uncertainty applies to momenta and coordinates.

1928: Paul Dirac combines quantum mechanics and special relativity to describe the electron.

1930: Quantum mechanics and special relativity are well established. There are just three fundamental particles: protons, electrons, and photons.

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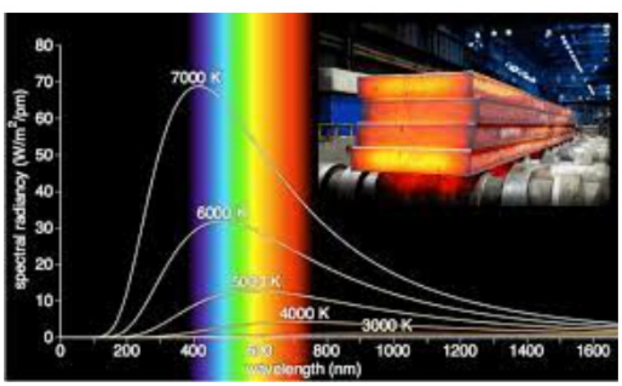
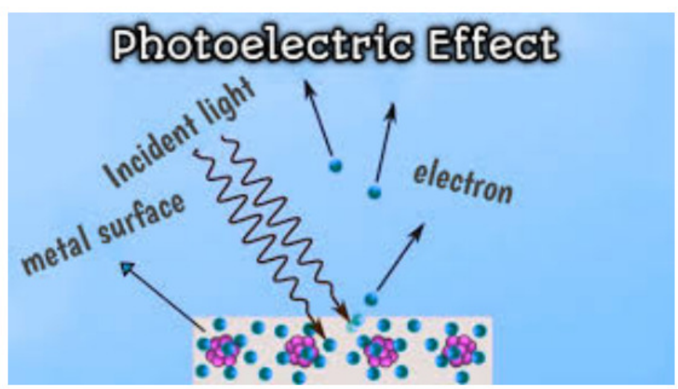
Three Unexplained Spectrums

- Blackbody Spectrum
- Photoelectric Effect
- Bright Line Spectrum





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

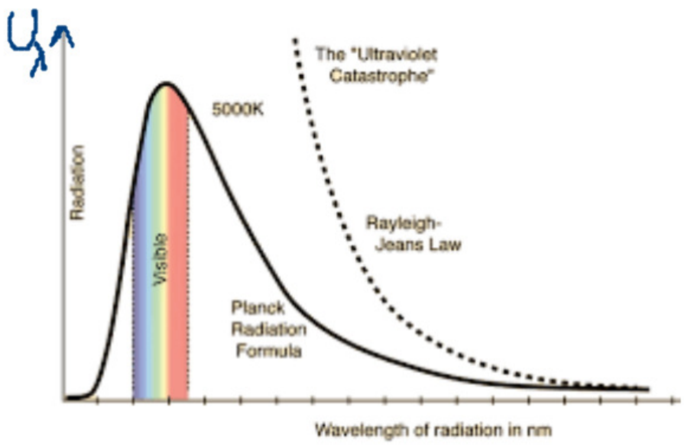
Rayleigh - Jeans law

$$U_\lambda = \frac{8\pi}{\lambda^4} kT$$

→ Good for larger wavelengths

→ Bad for smaller wavelengths

k = Boltzman Constant



Entry of Max Planck

* Max Planck made a big advancement in quantum theory when he put forward a model saying that energy of any oscillation can be absorbed or emitted only in units of a basic energy E which is proportional to the frequency of oscillation.

* In case of light, this means the energy of various modes of stationary waves in the enclosure can be E, 2E, 3E.......etc. with $E=h\nu = hc/\lambda$, h is a constant. Using this hypothesis he dervied the follwoing equation for spectral distribution;

$$U_\lambda = \frac{8\pi hc}{\lambda^5} \cdot \frac{1}{e^{hc/\lambda kT} - 1}$$

* This equation matches extremely well with experimental results in the entire range of wavelength, when the value of h is given 6.6×10^{-34} J.S

Planck's hypothesis was a great revolution and the constant h is rightly called 'Planck's Constant'.

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Equation of monochromatic light

$$\vec{E} = \vec{E}_0 \cos(kx - \omega t)$$

(i) light propagating in x-direction

(ii) $\lambda = \frac{2\pi}{k}$, $k = \frac{2\pi}{\lambda}$

k = propagation constant or wave factor

$$\boxed{\vec{k} = \frac{2\pi}{\lambda}\hat{e}}$$

(iii) frequency $(\nu) = \frac{\omega}{2\pi}$

$\omega = 2\pi\nu$ (Angular frequency)

If wave is a photon, then each photon has an energy (E)

or $E = h\nu$

$= h\nu \times \frac{2\pi}{2\pi}$

$= \frac{h}{2\pi} . 2\pi\nu$ $\quad \because \hbar = \frac{h}{2\pi}$

$\boxed{E = \hbar . \omega}$ $\quad$ & $\omega = 2\pi\nu$

For EM Radiation (No matter)

$c = \frac{\omega}{k}$ (Speed of light)

$\frac{\hbar\omega}{\hbar k} = c$, $c = \frac{E}{p}$ or $\boxed{E = pc}$

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Relation between momentum and wavelength

$$p = \frac{h}{\lambda} \quad \text{(Multiply \& Divide by } 2\pi\text{)}$$

$$= \frac{h}{\lambda} \times \frac{2\pi}{2\pi}$$

$$\text{or} = \frac{h}{2\pi} \times \frac{2\pi}{\lambda}$$

$$= \left(\frac{h}{2\pi}\right) \cdot \frac{2\pi}{\lambda} \quad , \text{ here } \frac{h}{2\pi} = \hbar$$

$$p = \hbar \cdot \frac{2\pi}{\lambda} \qquad \because k = \frac{2\pi}{\lambda}$$

$$\boxed{p = \hbar \cdot k} \qquad \hbar = 1.0545 \times 10^{-34}\ J.s$$

(Reduced Planck's Const.)

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When does quantum mechanics apply?

Not a simple question

But

* when angular momentum $\sim \hbar$
* when uncertainties $\Delta p \Delta x \sim \hbar$
* " " $\Delta E \Delta t \sim \hbar$
* when any action $S \sim \hbar$

$$\hbar = 1.0545 7148 \times 10^{-34}\ \text{kg m}^2/\text{s}$$

Electron in hydrogen atom	Speck of dust
energy $= 10\text{eV} = \frac{p^2}{2m}$	mass $\sim 10^{-6}$ kg
$\Delta p = 1.7 \times 10^{-24}$ kg·m/s	velocity ~ 1 m/s
Size of atom $\sim 10^{-10}$ m (Δx)	Size $\sim 10^{-5}$ m
$\Delta p \Delta x \sim 1.7 \times 10^{-34}$ kg m²/s	momentum $p = 10^{-6}$ kg m/s
$\simeq \hbar$	$\Delta p = 10^{-8}$ kg m/s
Quantum domain	position uncertainty $\Delta x \sim 10^{-6}$ m
	$\Delta p \Delta x = 10^{-14}$ kg m²/s $\sim 10^{20}\hbar$
	Classical Domain

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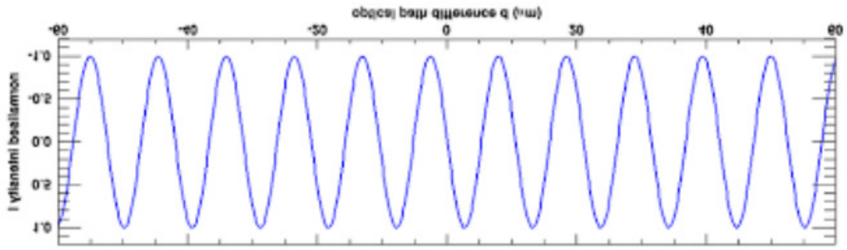

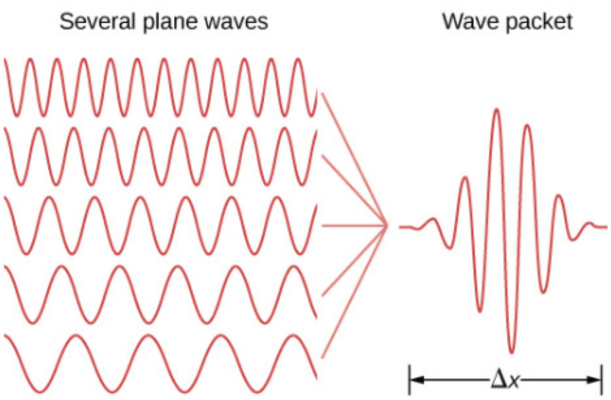

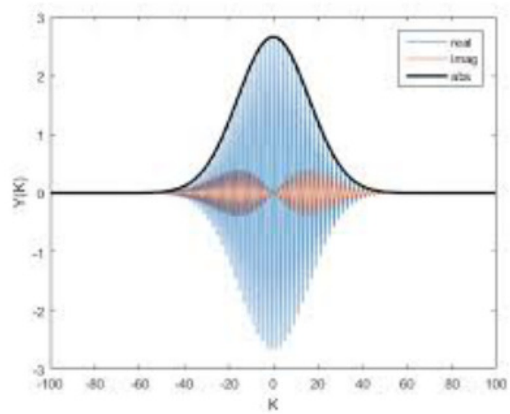

Many waves in a wave packet can be defined by a single differential equation.

The general wave equation

$$\boxed{\frac{\partial^2 y}{\partial x^2} = \frac{1}{v^2} \cdot \frac{\partial^2 y}{\partial t^2}}$$?

In this equation velocity (v) is considered constant but it is not practical in case of material waves therefore Schrodinger provided a solution for it which is known as Schrodinger wave equation.

$$\boxed{-\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V(x)\Psi = i\hbar\frac{\partial \Psi}{\partial t}}$$?

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Let a common wave is defined as

$$y = Af(x - vt)$$

wave propagating in x-direction with v-velocity
v (fixed) = Const.

$$\frac{dy}{dx} = A\frac{df}{d(x-vt)} \cdot \frac{d}{dx}(x-vt)$$

① First differentiate w.r.to x, t-fixed

$$\frac{\partial y}{\partial x} = Af'$$

$$\frac{\partial^2 y}{\partial x^2} = A\frac{df'}{d(x-vt)} \cdot \frac{d}{dx}(x-vt)$$

$$\boxed{\frac{\partial^2 y}{\partial x^2} = Af''}$$

Now differentiate w.r.to t, x-fixed

$$\frac{\partial y}{\partial t} = Af' \cdot \frac{d}{dt}(x - vt)$$
$$= Af' \cdot (-v)$$

$$\frac{\partial^2 y}{\partial t^2} = Af''(-v)(-v)$$
$$= Af'' v^2$$

$$\frac{\partial^2 y}{\partial t^2} = v^2 (Af'') \qquad \because Af'' = \frac{\partial^2 y}{\partial x^2}$$

$$\therefore \quad \frac{\partial^2 y}{\partial t^2} = v^2 \frac{\partial^2 y}{\partial x^2} \quad \text{or} \quad \boxed{\frac{\partial^2 y}{\partial x^2} = \frac{1}{v^2} \cdot \frac{\partial^2 y}{\partial t^2}}$$

General wave equation

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Time Dependent Schrodinger wave equation

In general wave equation velocity (v) is considered constant but it is not practical in case of material waves threfore Schrodinger provided a solution for it which is known as Schrodinger wave equation.

Consider a case of free particle which is not interacting and no force is applied.

particle nature → E (energy)
p (momentum)

wave nature → k (wave factor)
ω (Angular freq.)

Total energy ⇒ $E = K.E. = \frac{1}{2}mv^2$

or $E = \frac{p^2}{2m}$

& $E = \frac{p^2}{2m}$, $E = h\nu$, $p = \hbar k$ (wave associated with free particle)

As we know → $y = A\cos(kx - \omega t)$

It is the real part of

$$e^{i(kx-\omega t)} = \cos(kx-\omega t) + i\sin(kx-\omega t)$$

or $$e^{ix} = \cos x + i\sin(x)$$

or $$\boxed{\psi = A e^{[i(kx-\omega t)]}}$$ $(i = \sqrt{-1}$ or $i^2 = -1)$

General wave equation

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$$\because \psi = A e^{[i(kx-\omega t)]} \quad \text{——— (1)}$$

$$\& \quad k = \frac{p}{\hbar}, \quad \omega = \frac{E}{\hbar}$$

$$\therefore \quad \psi = A e^{i\left(\frac{p}{\hbar}x - \frac{E}{\hbar}t\right)}$$

$$\boxed{\psi = A e^{i/\hbar\,(px - Et)}} \quad \text{——— (2)}$$

1. Now differentiate equation (2) w. r. to (x) two times.

2. Then differentiate equation (2) w. r. to (t) two times

① Diff. (2) w.r. to $x \rightarrow$

$$\frac{\partial \psi}{\partial x} = A e^{i/\hbar(px - Et)} \cdot \frac{\partial}{\partial x}\left[\frac{i}{\hbar}(px - Et)\right]$$

$$= A e^{i/\hbar(px - Et)} \cdot \frac{i}{\hbar}\frac{\partial}{\partial x}(px - Et)$$

$$= \psi \cdot \frac{i}{\hbar} p$$

$$\frac{\partial \psi}{\partial x} = \frac{i}{\hbar} p\psi \Rightarrow \boxed{p\psi = \frac{\hbar}{i}\frac{\partial \psi}{\partial x}}$$

or

$$\boxed{p\psi = -i\hbar\frac{\partial \psi}{\partial x}}$$

$$\frac{\partial^2 \psi}{\partial x^2} = A\left(\frac{i}{\hbar}p\right)\left(\frac{i}{\hbar}p\right) e^{i/\hbar(px-Et)}$$

$$= -A\frac{p^2}{\hbar^2} e^{i/\hbar(px-Et)}$$

$$= -\frac{p^2}{\hbar^2}\left[A e^{i/\hbar(px-Et)}\right]$$

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

$$\boxed{p^2\psi = -\hbar^2 \cdot \frac{\partial^2 \psi}{\partial x^2}}$$

(2) Now diff. w.r.t. t →

$$\frac{\partial \psi}{\partial t} = \left[A e^{i/\hbar(px-Et)}\right]\left(-\frac{i}{\hbar}E\right)$$

$$= [\psi]\left(-\frac{i}{\hbar}E\right)$$

$$\frac{\partial \psi}{\partial t} = -\frac{i}{\hbar}E\psi$$

$$E\psi = \frac{-\hbar}{i}\frac{\partial \psi}{\partial t}$$

$$\boxed{E\psi = i\hbar\frac{\partial \psi}{\partial t}}$$

For free particle

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

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

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

or

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

if particle is not free
inclusion of potential energy

then $E = K.E + P.E.$

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

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

$$\boxed{-\frac{\hbar^2}{2m}\cdot\frac{\partial^2\psi}{\partial x^2} + V(x)\psi = i\hbar\frac{\partial\psi}{\partial t}}$$

This is final time dependent Schrodinger wave equation