

**SOME STUDY MATERIALS
ON QUANTUM MECHANICS PART
OF PAPER C9T
(VU PHYSICS HONS. CBCS 4TH SEMESTER)**

DEBASISH AICH

VU CBCS Semester-IV 2019: Planck's quantum, Planck's constant and light as a collection of photons; Blackbody Radiation: Quantum theory of Light; Photo-electric effect and Compton scattering. De Broglie wavelength and matter waves; Davisson-Germer experiment. Wave description of particles by wave packets. Group and Phase velocities and relation between them. Two-Slit experiment with electrons. Probability. Wave amplitude and wave functions.

Historical Note

1. Situation towards the end of the 19th century and the beginning of the 20th century

1.1 Advancement in Physics:

- *Classical mechanics:*

Newtonian Mechanics (Principia 1687-1713-1726; Sir Isaac Newton, English, 1643-1727) > Lagrangian Formulation (1750s) (Joseph-Louis Lagrange, Italian-French, 1736-1813) > Hamiltonian Formulation (1833) (William Rowan Hamilton, Irish, 1805-1865)

- *Electrodynamics:*

Maxwell's (James Clerk Maxwell, Scottish, 1831-1879) Equations of Electromagnetic waves [1861]. [In present form by Oliver Heaviside (English), Josiah W Gibbs (American), Heinrich Hertz (German, 1857-1894) in 1884]

Lorentz (Dutch, 1853-1928) Force Equation [1861 Maxwell > 1881 J. J. Thomson¹ (English) > 1884 Heaviside > 1895 Lorentz]

- *Thermodynamics:*

Carnot Theorem (1824) [Nicolas Leonard Carnot, French 1796-1832], Maxwell-Boltzmann (Ludwig Eduard Boltzmann, German, 1844-1906) Statistics (1868).

1.2. Major unsolved Questions:

- Energy Distribution [$u(\nu)d\nu$ or $u(\lambda)d\lambda$] of Blackbody Radiation.
- Photo electric effect: Experiment by Hertz in 1887.
- Stability of Rutherford's (New Zealand-born British) atom (1911 Gold Foil Expt.).
- Existence of aether: Michelson (American) –Morley (American) Experiment (1887, at Western Reserve University, Ohio).
- Atomic Spectra: Balmer (Swiss Mathematician) series:

$$\text{Balmer formula (1885)} \quad \lambda = B \left(\frac{n^2}{n^2 - m^2} \right) = B \left(\frac{n^2}{n^2 - 2^2} \right)$$

$$\text{Rydberg (Swedish Physicist) Formula (1888)} \quad \bar{\nu} = \frac{1}{\lambda} = \frac{4}{B} \left(\frac{1}{2^2} - \frac{1}{n^2} \right) = R_H \left(\frac{1}{2^2} - \frac{1}{n^2} \right)$$

$$\text{With } R_H = 1.09737309 \times 10^7 \text{ m}^{-1}.$$

Anomalous Zeeman (Dutch) effect, Fine structures and other observation in atomic spectroscopy.

1.3 End of the era of triumph of classical physics.

1900 Planck (German) distribution formula of Blackbody Radiation > Assumption of **radiation quanta of energy $h\nu$** , where ν is the frequency of radiation and h is a constant determined by Planck to fit the experimental distribution curve and is called Planck constant.

¹ William Thomson is a different scientist having other name Lord Kelvin, Scots-Irish, 1824-1907.

1905 Einstein (German Jewish) > Photo electric effect > Particle nature of light/radiation > Photon.

1905 Einstein Special Theory of Relativity > Non existence of aether; dependence of mass, length and time on velocity.

1913 Niels Bohr (Danish) > Model of Hydrogen Atom > quantisation of angular momentum of atomic electron > explanation of atomic stability, Balmer formula, atomic spectroscopy.

1923 New observations: Compton (American) Effect > recoil of electron which scatters X-ray. X-ray photon has momentum $h\nu/c$ > Radiation has particle nature.

1923 de Broglie (French) hypothesis: Electron and all matter have wave nature.

1925 Heisenberg (German): Matrix Formulation.

1926 Schrodinger (German): Schrodinger Equation > Wave mechanics.

1927 Heisenberg: Uncertainty Relation (Earle Hesse Kennard in late 1927 & Hermann Wey in 1928 gave the formal relation involving standard deviations as uncertainties: $\sigma_x \sigma_p \geq \hbar/2$).

1923-27 Davisson (American) and Germer (American) experiment and explanation > Diffraction of electrons > Confirmation of wave nature of electrons i.e. de Broglie hypothesis.

1927 Max Born (German Jewish) probabilistic interpretation of wave mechanics > $P(x, t)dx = \int_{x_1}^{x_2} |\psi(x, t)|^2 dx$, where x_1 and x_2 are the limits within which the particle exists. In 3D $P(\vec{r}, t)dx = \iiint |\psi(\vec{r}, t)|^2 d\tau$, where the integration is over the region of space in which the particle exists.

1928 Paul Dirac (English): Relativistic Quantum Mechanics > Prediction of Positron > Proof in 1932;

1939 bra ket notation by Dirac: Both Heisenberg's matrix formulation and Schrodinger's wave mechanics formulation can be handled with this.

1.3.1 Blackbody Radiation

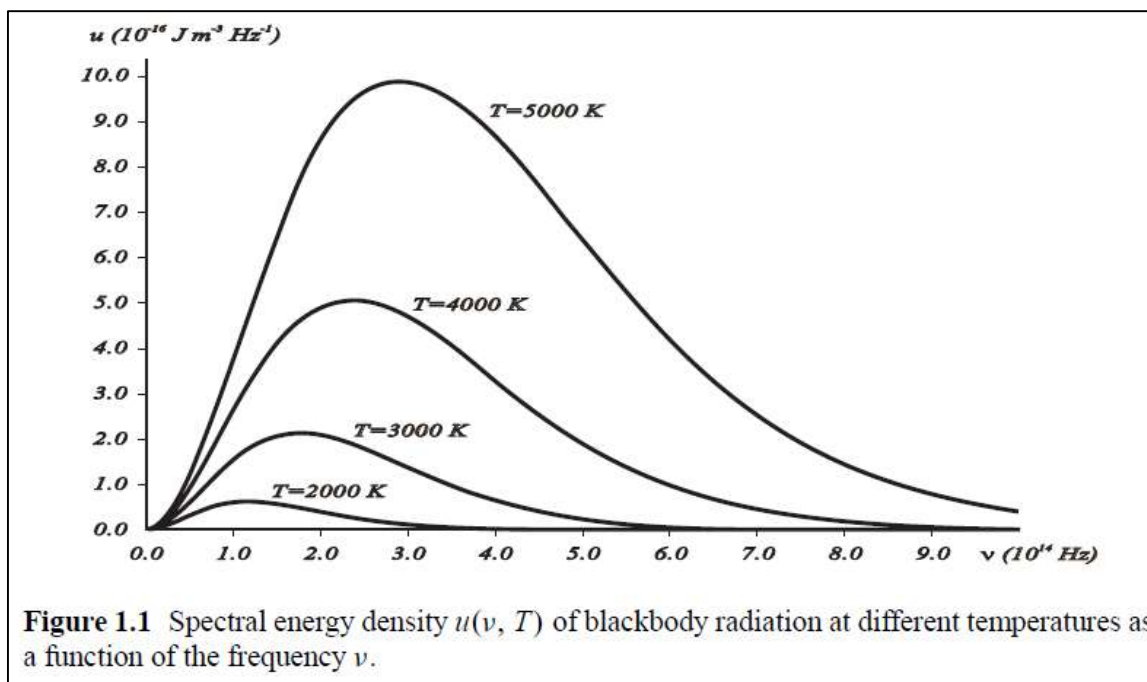


Figure 1.1 Spectral energy density $u(\nu, T)$ of blackbody radiation at different temperatures as a function of the frequency ν .

Quantum Mechanics Concepts and Applications - Nouredine Zettili

1879 J. Stefan (Carinthian Slovene) established from Tyndall's experimental results of IR emissions by platinum filament and its colour:

Per unit area of the surface of a radiating solid at absolute temperature T radiates normally (perpendicularly) a power (or energy per second)-

$$P = a\sigma T^4 \quad \dots\dots\dots (1)$$

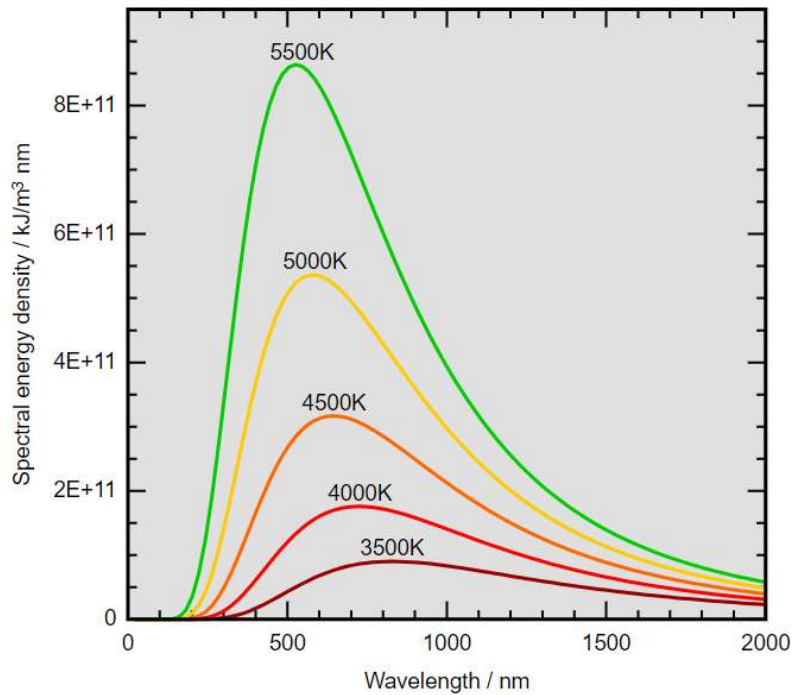
where $\sigma = 5.670367 \times 10^{-8} \text{ Wm}^2 \text{ K}^{-4}$ is called Stefan's constant; a is a coefficient ≤ 1 . For ideal blackbody $a = 1$. Equation (1) is called Stefan's law or Stefan-Boltzmann Law.

In 1884 a theoretical derivation of the law was done by Boltzmann (German).

Up to a temperature 1535 K this law accurately matches experimental observations. But at higher temperature deviation from experimental results are observed.

1893 Wien (Wilhelm Wien, 1864-1928, German Physicist) displacement law:

$$\lambda_{max}T = \text{constant} \approx 2900 \mu\text{m} \cdot \text{K}$$



1894 Wien energy density distribution:

Wien proposed (from thermodynamic consideration) that, Stefan-Boltzmann law and Wien displacement law can be derived if the energy density of blackbody radiation at temperature T per unit wavelength at λ i.e. $u(\lambda, T)$ must be given by a relation:

$$u(\lambda, T)d\lambda = \frac{a}{\lambda^5} f(\lambda T)d\lambda, \text{ where } f(\lambda T) \text{ is any function of } \lambda T.$$

From some arbitrary assumptions regarding mechanisms of emission he proposed that $f(\lambda T) = ae^{-b/\lambda T}$ and so

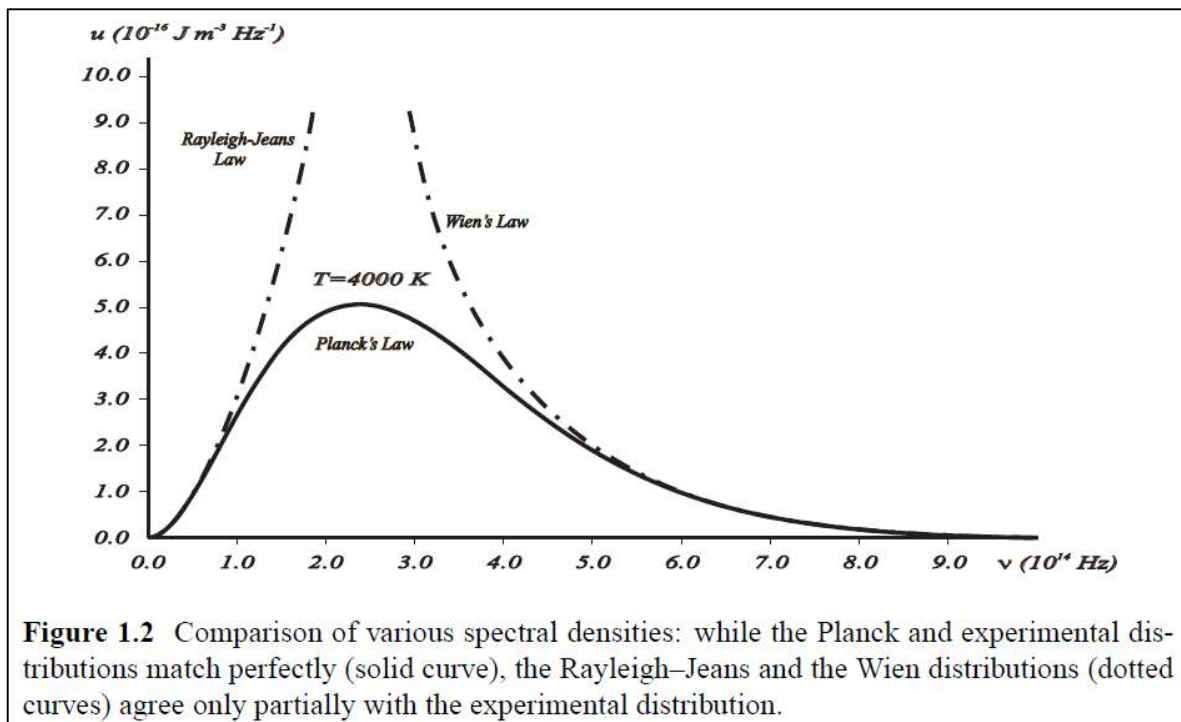
$$u(\lambda, T)d\lambda = \frac{a}{\lambda^5} e^{-b/\lambda T} d\lambda.$$

In terms of frequency $u(\nu, T)d\nu = A\nu^3 e^{-\beta\nu/T} d\nu$.

Unit of $u(\nu, T)$ is $\text{Jm}^{-3} \text{ Hz}^{-1}$ or $\text{Jm}^{-3} \text{ s}$ and unit of $u(\lambda, T)$ is Jm^{-4} .

Constants a, b or A, β were determined to fit these equations to experimental curves.

Failure of Wien distribution: Wien's distribution satisfies experimental curve at lower wavelengths or higher frequencies but fails to explain them at higher wavelengths or lower frequencies. **[In those days producing radiation of higher frequencies or lower wavelengths was not easy.]** Thus Wien's distribution was insufficient to satisfy observations.



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1900 Rayleigh’s (Lord Rayleigh, 1842-1919, British physicist) energy density distribution:

Rayleigh assumed that in the cavity of a blackbody radiation exists in the form of electromagnetic standing waves with their nodes at the walls of the cavity. Density of states (or vibrational modes) of these standing waves i.e. number of states (or modes) per unit volume per frequency range of such standing waves is equal to $\frac{8\pi\nu^2}{c^3}$.

The electromagnetic standing waves are excited by the linear oscillation of the tiny electric dipoles of atomic or molecular dimension in the walls of the cavity. The energy of an oscillating dipole can have any value between 0 & ∞ i.e. the energy spectrum of an oscillator is continuous. At temperature T , the number of electric dipoles having energy E is given by M-B statistics, i.e. $N(E) = N_0 e^{-E/kT}$, where N_0 is the number of oscillators with zero energy and k ($= 1.38 JK^{-1}$) is Boltzmann constant. Then it can be shown that at temperature T , the average energy of the oscillators in the walls is $\langle E \rangle = kT$.

In equilibrium the energy distribution of the standing waves is same as the energy distribution of the oscillators over the frequency range. Therefore the average energy of the vibrational modes of the standing waves will also be $\langle E \rangle = kT$.

So, according to Rayleigh, the energy density distribution is given by:

$$u(\nu, T)d\nu = n(\nu, T)\langle E \rangle d\nu = \frac{8\pi\nu^2}{c^3} kT d\nu;$$

Or, in terms of wavelength $u(\lambda, T)d\lambda = \frac{8\pi}{\lambda^4} kT d\lambda$.

Density of states of vibrations in a cubical cavity of side L filled with a continuous elastic medium:

3D wave equation: $\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} = \frac{1}{c^2} \frac{\partial^2 \psi}{\partial t^2}$ (A)

Standing wave solution: $\psi(x, y, z, t) = A \sin\left(\frac{n_x \pi x}{L}\right) \sin\left(\frac{n_y \pi y}{L}\right) \sin\left(\frac{n_z \pi z}{L}\right) \cos(2\pi \nu t)$(B)

n_x, n_y, n_z are integers ≥ 1 . A vibrational mode is determined by the set of integers (n_x, n_y, n_z) .

What is the number of such modes within frequency range ν to $\nu + d\nu$?

Consider a coordinate system in which coordinates are the positive integers and zero. This is the first octant of the 3D integer space. Each point in this space will be at unit distance from its nearest neighbours; in other words each point will share unit volume of this space.

Substituting (B) in (A) and simplifying: $n_x^2 + n_y^2 + n_z^2 = \frac{4L^2\nu^2}{c^2} = R^2$ (say).

Above equation represents the portion of a sphere of radius $R = \frac{2L\nu}{c}$ in the first octant of the integer space. In this space a spherical shell between radii R and $R + dR$ corresponds to the frequency range ν to $\nu + d\nu$. Volume of such a shell in integer space is:

$$\frac{1}{8} \times 4\pi R^2 dR = \frac{1}{2} \pi R^2 dR = \frac{1}{2} \pi \times \frac{4L^2\nu^2}{c^2} \times \frac{2L}{c} d\nu = \frac{4\pi L^3\nu^2}{c^3} d\nu$$

The number of coordinate points (n_x, n_y, n_z) in this shell will also be $\frac{1}{2} \pi R^2 dR$, since each point shares unit volume in integer space. But this is equal to the number of vibrational modes in the frequency range ν to $\nu + d\nu$. Thus the number of modes in the frequency range ν to $\nu + d\nu$ per unit volume of the cavity will be

$$\frac{1}{L^3} \times \frac{4\pi L^3\nu^2}{c^3} d\nu = \frac{4\pi\nu^2}{c^3} d\nu$$

Now unpolarised electromagnetic waves contains two types of circularly polarised waves with the plane of polarisation rotating in clockwise and anticlockwise sense. Now two modes of the electromagnetic standing waves with plane of polarisation rotating in opposite sense but identical in all other respect will have same set of (n_x, n_y, n_z) , i.e. each point in the integer space represents two states. Therefore number of states per unit volume of the cavity in the frequency range ν to $\nu + d\nu$ will be

$$n(\nu)d\nu = 2 \times \frac{4\pi\nu^2}{c^3} d\nu = \frac{8\pi\nu^2}{c^3} d\nu.$$

$$n(\nu) = \frac{8\pi\nu^2}{c^3} \dots \dots \dots (C)$$

is called the density of states.

Though for simplicity here we derive this result for a cubical medium, it is applicable to any shape.

Average energy per vibrational mode:

According to M-B statics the number of oscillators (or vibrational states in this case) having energy E at temperature T is $N_E = N_0 e^{-E/kT}$, where N_0 is the number of oscillators in the state of zero energy (ground state) and k is Boltzmann constant ($k = 1.38 \times 10^{-23} \text{JK}^{-1}$). Therefore for a continuous energy distribution:

$$\langle E \rangle = \frac{\int_0^\infty E N_0 e^{-E/kT} dE}{\int_0^\infty N_0 e^{-E/kT} dE} = \frac{(kT)^2 \int_0^\infty (E/kT) e^{-E/kT} d(E/kT)}{(kT) \int_0^\infty e^{-E/kT} d(E/kT)} = kT \frac{\Gamma(2)}{\Gamma(1)} = kT \dots \dots (D).$$

Rayleigh formula satisfies experimental curves at higher wavelengths or lower frequencies but deviates badly from the experimental curves towards lower wavelengths or higher frequencies i.e. towards ultraviolet region of the spectrum. This failure is known as ultraviolet catastrophe.

Particle nature of wave

1905 Planck blackbody radiation formula:

Planck's quantisation rule / Planck's quantum hypothesis / Planck's postulate: According to classical mechanics, a harmonic oscillator of frequency ν can have any amount of energy $E [= 4\pi^2 m a^2 \nu^2]$, which is proportional to the square of its amplitude a . And it can have any energy between 0 & ∞ . But to explain blackbody radiation Planck made the following revolutionary assumptions:

- i) An oscillator frequency ν in the wall of the blackbody can have only discrete energies given by $\epsilon_n = nh\nu$, where $n = 0, 1, 2, \dots$ and h is a constant, which was determined by him to fit his formula with the experimental distribution curves of blackbody radiation.
- ii) *When an oscillator of frequency ν absorbs or emits energy in the form of radiation its energy can change only in the steps of $h\nu$. Since the radiation absorbed or emitted by an oscillator have same frequency as that of the oscillator therefore it follows from Planck assumptions that an oscillator of frequency ν can absorb or emit radiation of frequency ν and this emitted or absorbed radiation can have only an amount of energy $h\nu$, no less no more.*

Regarding the nature and density of states of the radiation inside the cavity of blackbody, Planck's assumption was same as that of Rayleigh.

Average energy of the oscillators of frequency ν in the walls of the blackbody:

Oscillators of frequency ν have discrete energies $\epsilon_n = nh\nu$, $n = 0, 1, 2, \dots$. According to M-B statics the number of such oscillators at temperature T is $N_n = N_0 e^{-\epsilon_n/kT} = N_0 e^{-nh\nu/k}$. Therefore the average energy of the oscillators of frequency ν will be:

$$\langle \epsilon_\nu \rangle = \frac{\sum_{n=0}^{\infty} \epsilon_n N_0 e^{-\epsilon_n/kT}}{\sum_{n=0}^{\infty} N_0 e^{-\epsilon_n/kT}} = \frac{\sum_{n=0}^{\infty} \epsilon_n e^{-\epsilon_n/kT}}{\sum_{n=0}^{\infty} e^{-\epsilon_n/kT}}.$$

Note that the integrations of equation (D) have been replaced here by summations since in this case discrete energies are assumed for the oscillators in place of continuous energies of the oscillators in Rayleigh theory.

Now

$$\begin{aligned} \langle \epsilon_\nu \rangle &= \frac{\sum_{n=0}^{\infty} \epsilon_n e^{-\epsilon_n/kT}}{\sum_{n=0}^{\infty} e^{-\epsilon_n/kT}} = \frac{\sum_{n=0}^{\infty} nh\nu e^{-nh\nu/k}}{\sum_{n=0}^{\infty} e^{-nh\nu/k}} = \frac{h\nu e^{-h\nu/kT} + 2h\nu e^{-2h\nu/kT} + 3h\nu e^{-3h\nu/kT} + \dots}{1 + e^{-h\nu/kT} + e^{-2h\nu/kT} + e^{-3h\nu/kT} + \dots} \\ &= \frac{h\nu x(1 + 2x + 3x^2 + 4x^3 \dots)}{1 + x + x^2 + x^3 \dots} \quad (\text{where } x = e^{-h\nu/kT}) \\ &= h\nu x \frac{(1-x)^{-2}}{(1-x)^{-1}} = h\nu x \frac{1}{1-x} = \frac{h\nu}{\frac{1}{x} - 1} = \frac{h\nu}{e^{h\nu/kT} - 1}. \end{aligned}$$

Since the radiation in the cavity of the blackbody is in equilibrium with the oscillators in the wall so this above expression will also give the average energy of the vibrational modes of the standing waves in the cavity.

The number of vibrational modes or states per unit volume of the cavity in the frequency range ν to $\nu + d\nu$ can be determined as before and is given by:

$$n(\nu)d\nu = \frac{8\pi\nu^2}{c^3} d\nu.$$

Thus the energy distribution of the radiation is given by: $u(\nu)d\nu = \langle \epsilon_\nu \rangle n(\nu)d\nu = \frac{8\pi\nu^2}{c^3} \cdot \frac{h\nu}{e^{h\nu/kT} - 1} d\nu$.

$$u(\nu)d\nu = \frac{8\pi h\nu^3}{c^3} \cdot \frac{1}{e^{h\nu/kT} - 1} d\nu \dots \dots \dots (1)$$

In terms of wavelength:

$$u(\lambda)d\lambda = \frac{8\pi hc}{\lambda^5} \cdot \frac{1}{e^{hc/\lambda kT} - 1} d\lambda \dots \dots \dots (2)$$

Note that the discreteness of vibrational modes indexed by (n_x, n_y, n_z) arises here from purely classical considerations. But the discreteness of possible energies of an oscillator is due to the assumptions of a new type, called Planck's quantum conditions.

Fitting his equation with experimental curves Planck determined the value of h . Its value is $6.626 \times 10^{-34} \text{ J.s}$ and it is a universal constant of immense importance as was revealed later years with the advancement of quantum mechanics.

Derivations from Planck's law:

Stefan-Boltzmann law: Total energy (in all wavelength range) per unit volume of the cavity of a black body is

$$\begin{aligned}
 u &= \int_0^{\infty} u(\nu) d\nu = \frac{8\pi h}{c^3} \int_0^{\infty} \frac{\nu^3}{e^{h\nu/kT} - 1} d\nu = \frac{8\pi h}{c^3} \left(\frac{kT}{h}\right)^4 \int_0^{\infty} \frac{x^3}{e^x - 1} dx \quad [\text{where } x = h\nu/kT] \\
 &= \frac{8\pi h}{c^3} \left(\frac{kT}{h}\right)^4 \int_0^{\infty} x^3 e^{-x} (1 - e^{-x})^{-1} dx = \frac{8\pi h}{c^3} \left(\frac{kT}{h}\right)^4 \int_0^{\infty} x^3 e^{-x} (1 + e^{-x} + e^{-2x} + e^{-3x} + \dots) dx \\
 &= \frac{8\pi h}{c^3} \left(\frac{kT}{h}\right)^4 \int_0^{\infty} x^3 (e^{-x} + e^{-2x} + e^{-3x} + e^{-4x} + \dots) dx = \frac{8\pi h}{c^3} \left(\frac{kT}{h}\right)^4 \sum_{p=1}^{\infty} \int_0^{\infty} x^3 e^{-px} dx \\
 &= \frac{8\pi h}{c^3} \left(\frac{kT}{h}\right)^4 \sum_{p=1}^{\infty} \frac{1}{p^4} \int_0^{\infty} (px)^{4-1} e^{-px} d(px) = \frac{8\pi h}{c^3} \left(\frac{kT}{h}\right)^4 \sum_{p=1}^{\infty} \frac{1}{p^4} \Gamma(4) = \frac{8\pi h}{c^3} \left(\frac{kT}{h}\right)^4 \sum_{p=1}^{\infty} \frac{3!}{p^4} \\
 &= \frac{48\pi h}{c^3} \left(\frac{kT}{h}\right)^4 \frac{\pi^4}{90} = \frac{8\pi^5 k^4}{15c^3 h^3} T^4
 \end{aligned}$$

It can be shown that the energy radiated normally per unit area from a blackbody is $E = u \frac{c}{4}$. Thus

$$E = \frac{8\pi^5 k^4}{15c^3 h^3} \cdot \frac{c}{4} T^4 = \left(\frac{2\pi^5 k^4}{15 \cdot 2h^3}\right) T^4 \text{ or } E \propto T^4.$$

Wien displacement law:

$$u(\lambda) = \frac{8\pi hc}{\lambda^5} \cdot \frac{1}{e^{hc/\lambda kT} - 1} = \frac{8\pi hc}{z(\lambda)}, \text{ say. Where } z(\lambda) = \lambda^5 (e^{hc/\lambda kT} - 1).$$

The value of λ for which $u(\lambda)$ is maximum is obtained from the condition:

$$\left. \frac{\partial u(\lambda)}{\partial \lambda} \right|_{\lambda=\lambda_{max}} = 0$$

This is equivalent to:

$$\left. \frac{\partial z(\lambda)}{\partial \lambda} \right|_{\lambda=\lambda_{max}} = 0$$

$$\text{Or, } 5\lambda_{max}^4 \cdot (e^{hc/\lambda_{max} kT} - 1) - \lambda_{max}^5 \cdot \frac{hc}{\lambda_{max}^2 kT} e^{hc/\lambda_{max} kT} = 0;$$

$$\text{Or, } 1 - e^{-hc/\lambda_{max} kT} = \frac{hc}{5\lambda_{max} kT};$$

$$\text{Or, with } \frac{hc}{\lambda_{max} kT} = x, \text{ this equation can be written as: } 1 - e^{-x} = \frac{x}{5}$$

This equation can not be solved analytically, but can be solved numerically. Or by writing as a pair of equation: $y = 1 - e^{-x}$; and $y = \frac{x}{5}$ it can also be solved graphically. The curves represented by these equations intersect for $x \approx 4.965$.

$$\text{Thus } \frac{hc}{\lambda_{max} kT} \approx 4.965; \lambda_{max} T = \frac{hc}{4.965k} = \frac{6.626 \times 10^{-34} \times 3 \times 10^8}{4.965 \times 1.38 \times 10^{-23}} \approx 0.0029 \text{ m.K} = \text{constant}$$

Wien and Rayleigh-Jeans distribution law:

Planck's law: $u(\nu)d\nu = \frac{8\pi h\nu^3}{c^3} \cdot \frac{1}{e^{h\nu/kT}-1} d\nu$

At high frequencies $e^{h\nu/kT} - 1 \approx e^{h\nu/kT}$

So $u(\nu)d\nu = \frac{8\pi h\nu^3}{c^3} \cdot e^{-h\nu/kT} d\nu = A\nu^3 e^{-\beta\nu/T} d\nu$ where $A = \frac{8\pi h}{c^3}$ and $\beta = h/k$ are constants.

[Wien's distribution law.]

At low frequencies $e^{h\nu/kT} - 1 = (1 + h\nu/kT + \frac{(h\nu/kT)^2}{2!} + \frac{(h\nu/kT)^3}{3!} \dots) - 1 \approx h\nu/kT$

So $u(\nu)d\nu = \frac{8\pi h\nu^3}{c^3} \cdot \frac{1}{h\nu/kT} d\nu = \frac{8\pi\nu^2 kT}{c^3} d\nu$ [Rayleigh-Jeans law].

Problems:

JAM 2017

Q.23 In the radiation emitted by a black body, the ratio of the spectral densities at frequencies 2ν and ν will vary with ν as:

- (A) $[e^{h\nu/k_B T} - 1]^{-1}$ (C) $[e^{h\nu/k_B T} - 1]$
 (B) $[e^{h\nu/k_B T} + 1]^{-1}$ (D) $[e^{h\nu/k_B T} + 1]$

Ans.: $u(\nu) = \frac{8\pi h\nu^3}{c^3} \cdot \frac{1}{e^{h\nu/kT}-1}$

$$\frac{u(2\nu)}{u(\nu)} = \frac{8\pi h(2\nu)^3}{c^3} \cdot \frac{1}{e^{2h\nu/kT}-1} \cdot \frac{c^3}{8\pi h\nu^3} \cdot \frac{e^{h\nu/kT}-1}{1} = 8 \cdot \frac{e^{h\nu/kT}-1}{e^{2h\nu/kT}-1} = 8 \cdot \frac{e^{h\nu/kT}-1}{(e^{h\nu/kT}-1)(e^{h\nu/kT}+1)}$$

$$= 8 \cdot \frac{1}{e^{h\nu/kT}+1} = 8 \cdot (e^{h\nu/kT} + 1)^{-1}$$

$$\frac{u(2\nu)}{u(\nu)} \propto (e^{h\nu/kT} + 1)^{-1} \Rightarrow (B).$$

JAM 2014

Q.42 According to Wien's theory of black body radiation, the spectral energy density in a blackbody cavity at temperature T is given as

$$u_T(\lambda) d\lambda = \frac{\alpha}{c^3 \lambda^5} e^{-\beta/\lambda T} d\lambda$$

where α and β are constants and c is the speed of light. Further, the intensity of radiation coming out of the cavity is $\frac{u_T c}{4}$, where $u_T = \int_0^\infty u_T(\lambda) d\lambda$ is the total energy density of radiation. Given that Stefan-Boltzmann constant $\sigma = 5.67 \times 10^{-8} \text{ Wm}^{-2}\text{K}^{-4}$ and $\lambda_{\max} T = 2.90 \times 10^{-3} \text{ m.K}$, find the values of α and β . The value of integral $\int_0^\infty x^3 e^{-x} dx = 6$.

Ans.: $\left[\frac{\partial}{\partial \lambda} (u_T(\lambda)) \right]_{\lambda_{\max}} = 0$

So, from $u_T(\lambda) = \frac{\alpha}{c^3 \lambda^5} e^{-\beta/\lambda T}$, we have $\left[-\frac{5\alpha}{c^3 \lambda^6} e^{-\beta/\lambda T} + \frac{\alpha\beta}{c^3 \lambda^7 T} e^{-\beta/\lambda T} \right]_{\lambda_{\max}} = 0$

$$\Rightarrow -5 + \frac{\beta}{\lambda_{\max} T} = 0 \quad \Rightarrow \beta = 5\lambda_{\max} T = 5 \times 2.9 \times 10^{-3} = \mathbf{0.0145 \text{ m.K}}$$

$$\sigma T^4 = E$$

$$= \frac{u_T c}{4} = \frac{c}{4} \int_0^\infty u_T(\lambda) d\lambda = \frac{c}{4} \frac{\alpha}{c^3} \int_0^\infty \frac{1}{\lambda^5} e^{-\beta/\lambda T} d\lambda$$

$$\text{Let } \beta/\lambda T = x. \text{ Then } dx = -(\beta/\lambda^2 T) d\lambda \Rightarrow d\lambda = -\frac{\lambda^2 T}{\beta} dx.$$

$$\sigma T^4 = E = -\frac{T c \alpha}{\beta^4 c^3} \int_\infty^0 \frac{1}{\lambda^3} e^{-x} dx = \left(\frac{T}{\beta}\right)^4 \frac{c \alpha}{4 c^3} \int_0^\infty \left(\frac{\beta}{\lambda T}\right)^3 e^{-x} dx = \left(\frac{T}{\beta}\right)^4 \frac{c \alpha}{4 c^3} \int_0^\infty x^3 e^{-x} dx$$

$$= \left(\frac{T}{\beta}\right)^4 \frac{c \alpha}{4 c^3} \cdot 6 = \frac{3}{2} \left(\frac{T}{\beta}\right)^4 \frac{\alpha}{c^2}$$

$$\Rightarrow \frac{3}{2} \left(\frac{T}{\beta}\right)^4 \frac{\alpha}{c^2} = \sigma T^4 \Rightarrow \frac{3}{2} \frac{\alpha}{c^2 \beta^4} = \sigma \Rightarrow \alpha = \frac{2c^2 \sigma \beta^4}{3}$$

$$\Rightarrow \alpha = \frac{2 \times (3 \times 10^8)^2 \times 5.67 \times 10^{-8} \times (0.0145)^4}{3} = \frac{2 \times 9 \times 5.67 \times (1.45)^4}{3} = 150.3856.$$

JAM 2013

Q.6 A blackbody at temperature T emits radiation at a peak wavelength λ . If the temperature of the blackbody becomes $4T$, the new peak wavelength is

- (A) $\frac{1}{256} \lambda$ (B) $\frac{1}{64} \lambda$ (C) $\frac{1}{16} \lambda$ (D) $\frac{1}{4} \lambda$

$$\text{Ans.: } \lambda_{max} T = \text{constant} \Rightarrow (\lambda_{max})_2 T_2 = (\lambda_{max})_1 T_1 \Rightarrow (\lambda_{max})_2 = \frac{(\lambda_{max})_1 T_1}{T_2} = \frac{\lambda T}{4T} = \frac{\lambda}{4} \Rightarrow (D).$$

JAM 2012

Q.8 When the temperature of a blackbody is doubled, the maximum value of its spectral energy density, with respect to that at initial temperature, would become

- (A) $\frac{1}{16}$ times (B) 8 times (C) 16 times (D) 32 times

$$\text{Ans.: } u(\lambda) = \frac{8\pi h c}{\lambda^5} \cdot \frac{1}{e^{hc/\lambda k T} - 1} = \frac{8\pi h}{\lambda^5} \cdot \frac{1}{e^{hc/k \lambda T} - 1}$$

$$\text{For } \lambda = \lambda_{max} \text{ we have } u(\lambda_{max}) = \frac{8\pi h c}{\lambda_{max}^5} \cdot \frac{1}{e^{hc/k \lambda_{max} T} - 1}.$$

$$\text{Also } \lambda_{max} T = \text{constant} \Rightarrow [\lambda_{max}]_2 T_2 = [\lambda_{max}]_1 T_1 \Rightarrow \frac{[\lambda_{max}]_1}{[\lambda_{max}]_2} = \frac{T_2}{T_1}$$

$$\frac{u([\lambda_{max}]_2)}{u([\lambda_{max}]_1)} = \frac{8\pi h c}{[\lambda_{max}]_2^5} \cdot \frac{1}{e^{hc/k[\lambda_{max}]_2 T_2} - 1} \cdot \frac{[\lambda_{max}]_1^5}{8\pi h c} \cdot \frac{e^{hc/k[\lambda_{max}]_1 T_1} - 1}{1} = \left(\frac{[\lambda_{max}]_1}{[\lambda_{max}]_2}\right)^5 = \left(\frac{T_2}{T_1}\right)^5$$

$$= 2^5 = 32 \Rightarrow (D).$$

JAM 2007:

7. The black body spectrum of an object O_1 is such that its radiant intensity (i.e., intensity per unit wavelength interval) is maximum at a wavelength of 200 nm. Another object O_2 has the maximum radiant intensity at 600 nm. The ratio of power emitted per unit area by O_1 to that of O_2 is

- (A) $\frac{1}{81}$ (C) 9
 (B) $\frac{1}{9}$ (D) 81

Ans.: Clearly the temperatures of the two blackbody will be different. If T_1 and T_2 are the temperatures then:

$$\frac{T_1}{T_2} = \frac{[\lambda_{max}]_2}{[\lambda_{max}]_1} = \frac{600}{200} = 3.$$

$$\frac{P_1}{P_2} = \frac{\sigma T_1^4}{\sigma T_2^4} = \left(\frac{T_1}{T_2}\right)^4 = 3^4 = 81.$$

Photoelectric effect:

In 1888 Hertz and afterwards other scientists observed that when the surface of metals like zinc is irradiated with ultraviolet light the metal gets positively charged i.e. the metal loses negative charge. In 1899 P. Lenard (Philipp Lenard, German Physicist, 1862-1947, Supporter of Hitler) showed that the loss of negative charge is due to emission of negatively charged electrons from the metal surface. The following laws were discovered experimentally prior to 1905:

- If the frequency of the incident radiation is smaller than the metal's threshold frequency - a frequency that depends on the properties of the metal—no electron can be emitted regardless of the radiation's intensity (Philipp Lenard, 1902).
- No matter how low the intensity of the incident radiation, electrons will be ejected *instantly* the moment the frequency of the radiation exceeds the threshold frequency ν_0 .

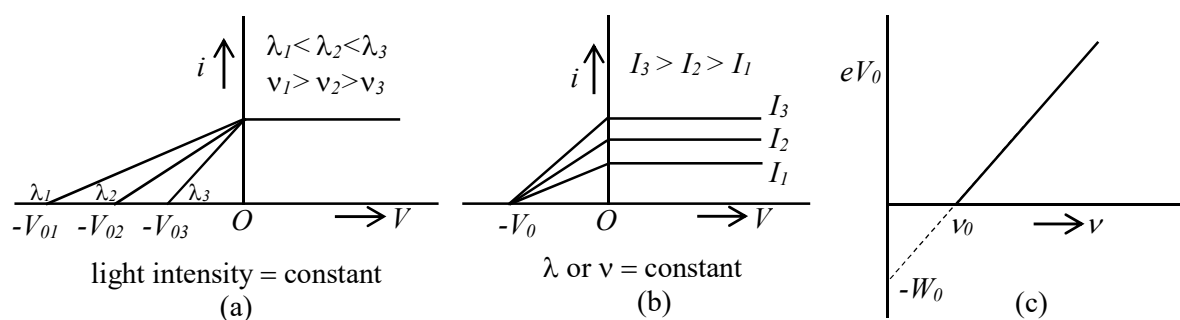


Fig.X

- At any frequency above ν_0 , the photo current and hence the number of electrons ejected per second increases with the intensity of the light but does not depend on the light's frequency.
- The stopping potential (V_0) and so the kinetic energy of the ejected electrons depends on the frequency but not on the intensity of the beam; V_0 and so the maximum kinetic energy of the ejected electrons ($\frac{1}{2}mv_m^2 = eV_0$) increases *linearly* with the incident frequency.

Einstein showed that the plot of maximum kinetic energy of the electrons or of eV_0 with frequency (ν) of the incident light is a straight line (Fig.-X(c)) which can be given by:

$$eV_0 = h\nu - W_0$$

The slope of the straight line graph does not depend on the metal and as determined from experimental results, it is equal to Planck's constant h . If the electron emitting metal surface is clean and oxide free then the intercept W_0 is characteristic of the metal and it is equal to $h\nu_0$.

Einstein, extending Planck's quantum condition to radiation, proposed that light is made up of discrete energy packets or quanta – photons – each of which have energy $h\nu$, where ν is the frequency of light. In photo electric effect a photon, incident on an electron, is completely absorbed by it. At normal temperatures the maximum energy of an electron inside the metal is less than the minimum energy required by an electron to come out of the metal surface by an amount equal to W_0 which is called work function. So if $h\nu < W_0$ the photon absorbing electron cannot come out of the metal surface. But if $h\nu > W_0$ the electron can emit from the metal surface. And the emitted electron possesses a kinetic

energy $h\nu - W_0$ with which it can reach to the anode even if the anode is given no positive potential with respect to the cathode. Moreover to stop such an emitted electron from leaving the metal surface a negative potential (say $-V_0$) should be applied to the anode with respect to the cathode. V_0 is called stopping potential. Clearly $eV_0 = h\nu - W_0$ and it is equal to the maximum kinetic energy of the electrons.

The equation: $eV_0 = h\nu - W_0$ is Einstein's photoelectric equation.

Problems:

JAM 2014

Q.8 In a photoelectric effect experiment, ultraviolet light of wavelength 320 nm falls on the photocathode with work function of 2.1 eV. The stopping potential should be close to

- (A) 1.8 V (B) 1.6 V (C) 2.2 V (D) 2.4 V

Ans. $eV_0 = h\nu - W_0 = \frac{hc}{\lambda} - W_0 = \frac{1240}{320} - 2.1$ electron Volt = 1.775 electron Volt

$\Rightarrow V_0 = \frac{1.775}{e}$ electron Volt = 1.775 Volt \Rightarrow (A).

JAM 2011

Q.6 Light described by the equation $E = (90 \text{ V/m})[\sin(6.28 \times 10^{15} \text{ s}^{-1})t + \sin(12.56 \times 10^{15} \text{ s}^{-1})t]$ is incident on a metal surface. The work function of the metal is 2.0 eV. Maximum kinetic energy of the photoelectrons will be

- (A) 2.14 eV (B) 4.28 eV (C) 6.28 eV (D) 12.56 eV

Ans.: $E = E_0 \sin \omega t$ represents the electric field vector of light having angular frequency ω i.e. frequency $\nu = \omega/2\pi$ where E_0 is the amplitude of the electric field vector.

So $E = (90 \text{ V/m})[\sin(6.28 \times 10^{15} \text{ s}^{-1})t + \sin(12.56 \times 10^{15} \text{ s}^{-1})t]$
 $= (90 \text{ V/m}) \sin(6.28 \times 10^{15} \text{ s}^{-1})t + (90 \text{ V/m}) \sin(12.56 \times 10^{15} \text{ s}^{-1})t$

represents two light waves of frequencies $\nu_1 = \frac{6.28 \times 10^{15}}{2\pi} \text{ s}^{-1} = 10^{15} \text{ s}^{-1} = 10^{15} \text{ Hz}$ and

$\nu_2 = \frac{12.56 \times 10^{15}}{2\pi} \text{ s}^{-1} = 2 \times 10^{15} \text{ s}^{-1} = 2 \times 10^{15} \text{ Hz}$

Clearly the maximum kinetic energy will be determined by the larger frequency. So, in this problem the maximum kinetic energy will be:

$h\nu_2 - W_0 \text{ Joule} = \frac{h\nu_2}{e} - \frac{W_0}{e} \text{ eV}$
 $= \frac{6.626 \times 10^{-34} \times 2 \times 10^{15}}{1.6 \times 10^{-19}} - 2.0 \text{ eV} = 8.28 \text{ eV} - 2.0 \text{ eV} = 6.28 \text{ eV} \Rightarrow$ (C)

JAM 2007:

20. A beam of light of wavelength 400 nm and power 1.55 mW is directed at the cathode of a photoelectric cell. (given: $hc = 1240 \text{ eV nm}$, $e = 1.6 \times 10^{-19} \text{ C}$). If only 10% of the incident photons effectively produce photoelectrons, find the current due to these electrons. If the wavelength of light is now reduced to 200 nm, keeping its power the same, the kinetic energy of the electrons is found to increase by a factor of 5. What are the values of the stopping potentials for the two wavelengths? [21]

Ans. $P_{eff} = 1.55 \times 10^{-3} \times \frac{10}{100} W = 1.55 \times 10^{-4} W$

Number electrons emitted from the cathode per second is equal to the number of photons participating in photoemission per second:

$$\begin{aligned} &= \frac{\text{effective power}}{\text{photon energy}} = \frac{1.55 \times 10^{-4}}{h\nu} = \frac{1.55 \times 10^{-4}}{hc/\lambda} \\ &= \frac{1.55 \times 10^{-4}}{[1240/400] \times 1.6 \times 10^{-19}} = \frac{0.5 \times 10^{-4}}{1.6 \times 10^{-19}} \end{aligned}$$

$$\text{Current} = \frac{0.5 \times 10^{-4}}{1.6 \times 10^{-19}} \times 1.6 \times 10^{-19} = 0.05 \text{ mA.}$$

$$(K.E)_{max} = eV_0 = h\nu - W_0 = \frac{hc}{\lambda} - W_0 \quad \Rightarrow eV_{01} = \frac{hc}{\lambda_1} - W_0; \quad eV_{02} = \frac{hc}{\lambda_2} - W_0$$

$$eV_{02} - eV_{01} = \frac{hc}{\lambda_2} - \frac{hc}{\lambda_1} = \left(\frac{1240}{200} - \frac{1240}{400} \right) \text{ electron Volt} = 3.1 \text{ electron Volt}$$

$$\Rightarrow 5eV_{01} - eV_{01} = 3.1 \text{ electron Volt} \quad \Rightarrow 4eV_{01} = 3.1 \text{ electron Volt} \quad \Rightarrow V_{01} = 3.1/4 \text{ V}$$

$$\Rightarrow V_{01} = 0.7525 \text{ V}; \quad V_{02} = 5 \times 0.775 \text{ eV} = 3.875 \text{ V}$$

Problem of estimation of Plank Constant (Example 1.2, Zettili):

When two ultraviolet beams of wavelengths $\lambda_1 = 80 \text{ nm}$ and $\lambda_2 = 110 \text{ nm}$ fall on a lead surface, they produce photoelectrons with maximum energies 11.390 eV and 7.154 eV, respectively.

(a) Estimate the numerical value of the Planck constant.

(b) Calculate the work function, the cutoff frequency, and the cutoff wavelength of lead.

Solution

(a) From (1.22) we can write the kinetic energies of the emitted electrons as $K_1 = hc/\lambda_1 - W$ and $K_2 = hc/\lambda_2 - W$; the difference between these two expressions is given by $K_1 - K_2 = hc(\lambda_2 - \lambda_1)/(\lambda_1\lambda_2)$ and hence

$$h = \frac{K_1 - K_2}{c} \frac{\lambda_1\lambda_2}{\lambda_2 - \lambda_1}. \quad (1.24)$$

Since $1 \text{ eV} = 1.6 \times 10^{-19} \text{ J}$, the numerical value of h follows at once:

$$h = \frac{(11.390 - 7.154) \times 1.6 \times 10^{-19} \text{ J}}{3 \times 10^8 \text{ m s}^{-1}} \times \frac{(80 \times 10^{-9} \text{ m})(110 \times 10^{-9} \text{ m})}{110 \times 10^{-9} \text{ m} - 80 \times 10^{-9} \text{ m}} \simeq 6.627 \times 10^{-34} \text{ J s.} \quad (1.25)$$

This is a very accurate result indeed.

(b) The work function of the metal can be obtained from either one of the two data

$$\begin{aligned} W = \frac{hc}{\lambda_1} - K_1 &= \frac{6.627 \times 10^{-34} \text{ J s} \times 3 \times 10^8 \text{ m s}^{-1}}{80 \times 10^{-9} \text{ m}} - 11.390 \times 1.6 \times 10^{-19} \text{ J} \\ &= 6.627 \times 10^{-19} \text{ J} = 4.14 \text{ eV.} \end{aligned} \quad (1.26)$$

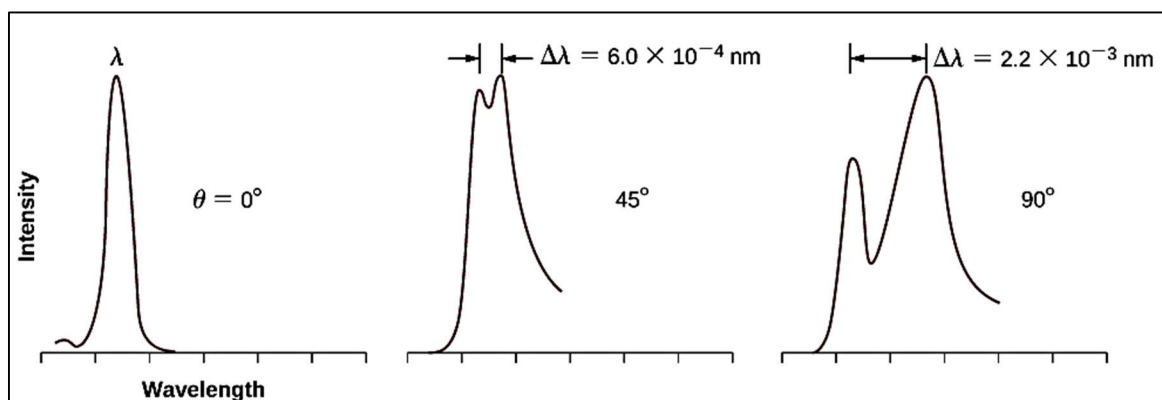
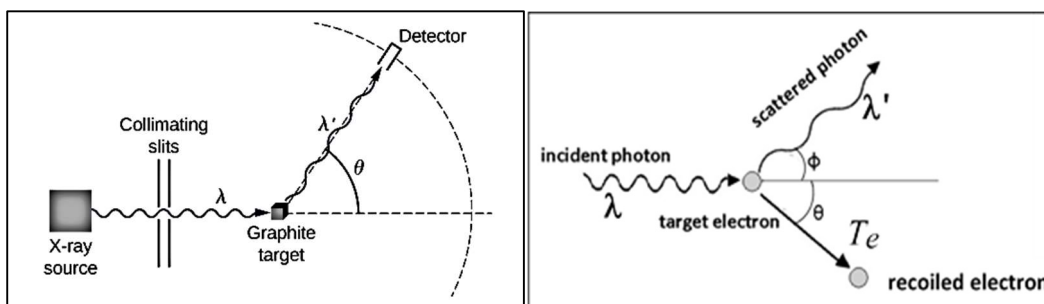
The cutoff frequency and wavelength of lead are

$$\nu_0 = \frac{W}{h} = \frac{6.627 \times 10^{-19} \text{ J}}{6.627 \times 10^{-34} \text{ J s}} = 10^{15} \text{ Hz}, \quad \lambda_0 = \frac{c}{\nu_0} = \frac{3 \times 10^8 \text{ m/s}}{10^{15} \text{ Hz}} = 300 \text{ nm.} \quad (1.27)$$

Compton Effect:

Before starting to study this topic, solve the following problems:

1. An electron has energy E eV. Obtain the expression of de Broglie wavelength ($\lambda = h/p$) of the electron, considering the problem to be (i) relativistic and (ii) non relativistic. Find the value of λ for (a) $E = 10$ eV and (b) $E = 10$ MeV for both relativistic and nonrelativistic treatments.
2. An electron is accelerated through a potential difference V . Obtain the expression of de Broglie wavelength ($\lambda = h/p$) of the electron after acceleration, considering the problem to be (i) relativistic and (ii) non relativistic. Find the value of λ for (a) $V = 10$ V and (b) $E = 100$ kV for both relativistic and nonrelativistic treatments.



*Photons require high energy to produce Compton Effect. Such photons are X-ray and γ -ray photons.

*Electron participating in Compton Effect is assumed to be free.

*Collision is considered to be **elastic**, i.e. both the total kinetic energy and total linear momentum of the colliding particles remain unchanged through the collision.

Conservation of energy:

$$h\nu = h\nu' + T_e = h\nu' + mc^2 - m_0c^2$$

$$\frac{hc}{\lambda} - \frac{hc}{\lambda'} + m_0c^2 = mc^2 \quad \Rightarrow \quad \frac{h}{\lambda} - \frac{h}{\lambda'} + m_0c = mc$$

Squaring

$$\frac{h^2}{\lambda^2} + \frac{h^2}{\lambda'^2} - 2\frac{h^2}{\lambda\lambda'} + 2m_0ch\left(\frac{1}{\lambda} - \frac{1}{\lambda'}\right) + m_0^2c^2 = m^2c^2$$

$$\Rightarrow \frac{h^2}{\lambda^2} + \frac{h^2}{\lambda'^2} - 2\frac{h^2}{\lambda\lambda'} + \frac{2m_0ch}{\lambda\lambda'}(\lambda' - \lambda) = m^2c^2 - m_0^2c^2$$

$$\Rightarrow \frac{h^2}{\lambda^2} + \frac{h^2}{\lambda'^2} - 2 \frac{h^2}{\lambda\lambda'} + \frac{2m_0ch}{\lambda\lambda'} (\lambda' - \lambda) = \frac{m_0^2c^2}{1-\beta^2} - m_0^2c^2 = \frac{m_0^2c^2\beta^2}{1-\beta^2} = \frac{m_0^2v^2}{1-\beta^2}$$

[Where $\beta = v/c$]

$$\Rightarrow \frac{h^2}{\lambda^2} + \frac{h^2}{\lambda'^2} - 2 \frac{h^2}{\lambda\lambda'} + \frac{2m_0ch}{\lambda\lambda'} (\lambda' - \lambda) = m^2v^2 \dots\dots\dots(A)$$

Conservation of momentum:

Relativistic energy relation $\Rightarrow E^2 = p^2c^2 + m_0^2c^4$.

For photon, $E = h\nu$ and rest mass $m_0 = 0$. Therefore $h\nu = pc$.

$$\Rightarrow \text{photon momentum } p = \frac{h\nu}{c} = \frac{h}{\lambda}.$$

Therefore

$$\frac{h}{\lambda} = \frac{h}{\lambda'} \cos \varphi + mv \cos \theta \quad \Rightarrow \frac{h}{\lambda} - \frac{h}{\lambda'} \cos \varphi = mv \cos \theta \quad \dots\dots\dots(B) \text{ and}$$

$$0 = \frac{h}{\lambda'} \sin \varphi - mv \sin \theta \quad \Rightarrow \frac{h}{\lambda'} \sin \varphi = mv \sin \theta . \quad \dots\dots\dots(C)$$

Squaring and adding (B) and (C):

$$\frac{h^2}{\lambda^2} + \frac{h^2}{\lambda'^2} - 2 \frac{h^2 \cos \varphi}{\lambda\lambda'} = m^2v^2 \dots\dots\dots(D)$$

(A) – (D)

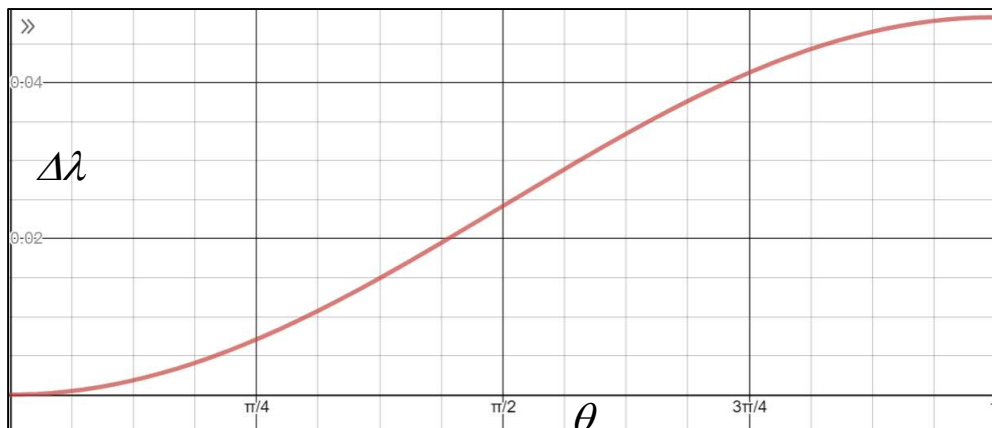
$$-2 \frac{h^2}{\lambda\lambda'} (1 - \cos \varphi) + \frac{2m_0ch}{\lambda\lambda'} (\lambda' - \lambda) = 0$$

Wavelength shift:

$$\Rightarrow \lambda' - \lambda = \frac{h}{m_0c} (1 - \cos \varphi) = \lambda_c (1 - \cos \varphi) \dots\dots\dots (E)$$

$$\Rightarrow \lambda' = \lambda + \lambda_c (1 - \cos \varphi). \dots\dots\dots (F)$$

$$\lambda_c = \frac{h}{m_0c} = \text{Compton wavelength} = \frac{6.626 \times 10^{-34}}{9.11 \times 10^{-31} \times 3 \times 10^8} = 0.02424 \text{ \AA}.$$



Recoil angle of electron:

We have $\frac{h}{\lambda} - \frac{h}{\lambda'} \cos \varphi = mv \cos \theta$ (B)

and $\frac{h}{\lambda'} \sin \varphi = mv \sin \theta$ (C)

$$\tan \theta = \frac{\frac{h}{\lambda'} \sin \varphi}{\frac{h}{\lambda} - \frac{h}{\lambda'} \cos \varphi} = \frac{\sin \varphi}{\frac{\lambda'}{\lambda} - \cos \varphi}$$

From (F), $\frac{\lambda'}{\lambda} = 1 + \frac{\lambda_c}{\lambda} (1 - \cos \varphi) = 1 + \alpha(1 - \cos \varphi)$.

$$\text{Then } \tan \theta = \frac{\sin \varphi}{1 + \alpha(1 - \cos \varphi) - \cos \varphi} = \frac{\sin \varphi}{(1 + \alpha)(1 - \cos \varphi)} = \frac{2 \sin \frac{\varphi}{2} \cos \frac{\varphi}{2}}{2(1 + \alpha) \sin^2 \frac{\varphi}{2}} = \frac{\cos \frac{\varphi}{2}}{(1 + \alpha) \sin \frac{\varphi}{2}}$$

$$\cot \theta = (1 + \alpha) \tan \frac{\varphi}{2} \dots\dots\dots (G)$$

Recoil energy of electron:

$$T_e = hv - hv' = hv \left(1 - \frac{v'}{v}\right) = hv \left(1 - \frac{\lambda}{\lambda'}\right) = hv \left(1 - \frac{1}{1 + \alpha(1 - \cos \varphi)}\right)$$

$$= hv \frac{\alpha(1 - \cos \varphi)}{1 + \alpha(1 - \cos \varphi)}$$

Useful way to calculate T_e if λ (or ν) and φ are given:

First find $\lambda' = \lambda + \lambda_c(1 - \cos \varphi)$

$$\text{Now } T_e = hv - hv' = \frac{hc}{\lambda} - \frac{hc}{\lambda'}$$

Use $hc = 1240 \text{ nm.eV}$

$$\text{Then: } T_e = \frac{hc}{\lambda} - \frac{hc}{\lambda'} = hc \left(\frac{1}{\lambda} - \frac{1}{\lambda'}\right) = 1240 \left(\frac{1}{\lambda \text{ in nm}} - \frac{1}{\lambda' \text{ in nm}}\right) \text{ eV}$$

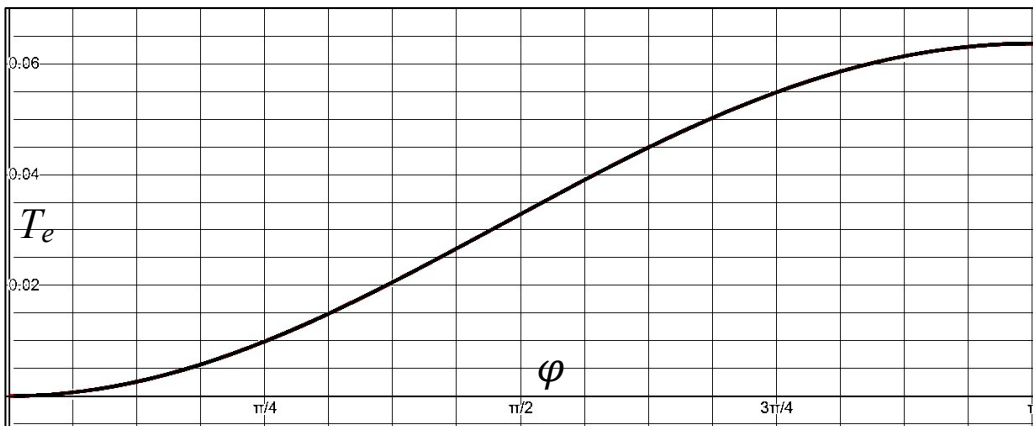
Plot $T_e = \frac{hc}{\lambda} \frac{\alpha(1 - \cos \varphi)}{1 + \alpha(1 - \cos \varphi)}$ vs. φ . Given $\lambda = 0.709 \text{ \AA}$.

$$\text{Ans.: } \alpha = \frac{h}{m_0 c \lambda} = \frac{6.626 \times 10^{-34}}{9.1 \times 10^{-31} \times 3 \times 10^8 \times 0.709 \times 10^{-10}} = 34.2328 \times 10^{-3}$$

$$\frac{hc}{\lambda} = \frac{6.626 \times 10^{-34} \times 3 \times 10^8}{0.709 \times 10^{-10}} = 28.036671 \times 10^{-16} \text{ J}$$

$$T_e = \frac{hc}{\lambda} \frac{\alpha(1 - \cos \varphi)}{1 + \alpha(1 - \cos \varphi)} = \frac{hc}{\lambda} \cdot \frac{34.2328 \times 10^{-3} (1 - \cos \varphi)}{1 + 34.2328 \times 10^{-3} (1 - \cos \varphi)}$$

We plot $\frac{0.034(1 - \cos \varphi)}{1 + 0.034(1 - \cos \varphi)}$ vs. φ



$$(T_e)_\pi = \frac{hc}{\lambda} \frac{\alpha(1-\cos\pi)}{1+\alpha(1-\cos\pi)} = \frac{hc}{\lambda} \cdot \frac{2\alpha}{1+2\alpha}; (T_e)_{\pi/2} = \frac{hc}{\lambda} \cdot \frac{\alpha}{1+\alpha}$$

Comparison between Photoelectric Effect and Compton Effect:

	Photoelectric Effect	Compton Effect
Participating Radiation (photon)	Visible or UV light $\lambda \sim 10^2 \text{ nm}$ $E \sim eV$	X-Rays and γ -Rays $\lambda \sim 10^{-1} - 10^{-3} \text{ nm}$ $E \sim keV - MeV$
What happens to the photon	Completely absorbed by the electron (or other scattering particle) Energy completely transferred to the electron	Energy partly transferred to electron, Direction changes up to 180° , Wavelength increases, For electrons $\Delta\lambda$ may be up to $2\lambda_c = 2 \times 0.002426 \text{ nm}$
Participating electron	Conduction electrons or electrons loosely bound the atoms of a metal	Loosely bound atomic electrons of non-metals e.g. graphite
Electrons free or bound	Electrons have negative energy of several eV In magnitude equal or slightly greater than the work function. Work function of Ag and Na are 4.54 eV & 2.28 eV Magnitude of electron energy is comparable to the energy of photon (eV). So electrons are considered as bound.	Several eV . Magnitude may be greater than that of electrons of Photoelectric effect. Ionisation potential of Carbon is 11.26 eV Magnitude of electron energy is small compared to the photon energy (keV). So electrons are considered as free.
What happens to the electron	Emits from the metal	Recoils. If recoil energy is high then emits from the material.
Energy of emitted / recoiled electron	Several eV . Non-relativistic treatment is allowable	Several eV to keV . Relativistic treatment is required

Problems:

JAM 2017

Q.31 A photon of frequency ν strikes an electron of mass m initially at rest. After scattering at an angle ϕ , the photon loses half of its energy. If the electron recoils at an angle θ , which of the following is (are) true?

(A) $\cos\phi = \left(1 - \frac{mc^2}{h\nu}\right)$

(B) $\sin\theta = \left(1 - \frac{mc^2}{h\nu}\right)$

(C) The ratio of the magnitudes of momenta of the recoiled electron and scattered photon is $\frac{\sin\phi}{\sin\theta}$.

(D) Change in photon wavelength is $\frac{h}{mc}(1 - 2\cos\phi)$.

Ans.: (A) $\lambda' - \lambda = \frac{h}{m_0c}(1 - \cos\phi) \Rightarrow c\left(\frac{1}{\nu'} - \frac{1}{\nu}\right) = \frac{h}{m_0c}(1 - \cos\phi)$

$$\Rightarrow c\left(\frac{2}{\nu} - \frac{1}{\nu}\right) = \frac{h}{m_0c}(1 - \cos\phi)$$

[Since loss of energy = $h\nu - h\nu' = h\nu/2 \Rightarrow \nu' = \nu/2$]

$$\Rightarrow \frac{c}{\nu} = \frac{h}{m_0c}(1 - \cos\phi) \Rightarrow (1 - \cos\phi) = \frac{m_0c}{h} \frac{c}{\nu} = \frac{m_0c^2}{h\nu}$$

$$\Rightarrow \cos\phi = 1 - \frac{m_0c^2}{h\nu} \Rightarrow (A) \text{ is correct.}$$

Loss of energy of Compton scattered photon
 = kinetic energy gained by the recoiled electron

$$= T_e = hv \frac{\alpha(1-\cos\varphi)}{1+\alpha(1-\cos\varphi)}, \text{ where } \alpha = \frac{\lambda_c}{\lambda} = \frac{h/m_0c}{\lambda} = \frac{h/m_0c}{c/v} = \frac{hv}{m_0c^2}.$$

$$\text{Here } T_e = \frac{hv}{2} = hv \frac{\alpha(1-\cos\varphi)}{1+\alpha(1-\cos\varphi)} \Rightarrow 2\alpha(1-\cos\varphi) = 1 + \alpha(1-\cos\varphi);$$

$$\Rightarrow 1 - \cos\varphi = \frac{1}{\alpha} \Rightarrow \cos\varphi = 1 - \frac{1}{\alpha} = 1 - \frac{m_0c^2}{hv} \Rightarrow \Rightarrow \text{(A) is correct.}$$

$$\text{(B) } \tan\theta = \frac{\sin\varphi}{(1+\alpha)(1-\cos\varphi)} = \frac{\sqrt{1-\cos^2\varphi}}{(1+\alpha)/\alpha} = \frac{\sqrt{1-(1-\frac{1}{\alpha})^2}}{(1+\alpha)/\alpha} = \frac{\sqrt{\frac{2}{\alpha} - \frac{1}{\alpha^2}}}{\frac{\alpha+1}{\alpha}} = \frac{\sqrt{\frac{2\alpha-1}{\alpha^2}}}{\frac{\alpha+1}{\alpha}} = \frac{\sqrt{2\alpha-1}}{\alpha+1}$$

$$\sin\theta = \sqrt{\frac{1}{1+\cot^2\theta}} = \sqrt{\frac{1}{1+\frac{(1+\alpha)^2}{2\alpha-1}}} = \sqrt{\frac{1}{\frac{\alpha^2+4\alpha}{2\alpha-1}}} = \sqrt{\frac{2\alpha-1}{\alpha^2+4\alpha}}$$

$$\text{Given relation in (B) : } \sin\theta = 1 - \frac{m_0c^2}{hv} = 1 - \frac{1}{\alpha} \Rightarrow \Rightarrow \text{(B) is wrong.}$$

$$\text{(C) } \text{We have } \frac{h}{\lambda'} \sin\varphi = mv \sin\theta.$$

$$\Rightarrow \frac{mv}{h/\lambda'} = \frac{\sin\varphi}{\sin\theta} \Rightarrow \Rightarrow \text{(C) is correct.}$$

$$\text{(D) } \text{Change in photon wavelength } \lambda' - \lambda = \frac{h}{m_0c} (1 - \cos\varphi) \Rightarrow \Rightarrow \text{(D) is wrong.}$$

JAM 2016

Q.57 X-rays of 20 keV energy is scattered inelastically from a carbon target. The kinetic energy transferred to the recoiling electron by photons scattered at 90° with respect to the incident beam is keV.

(Planck constant = 6.6×10^{-34} Js, Speed of light = 3×10^8 m/s, electron mass = 9.1×10^{-31} kg, Electronic charge = 1.6×10^{-19} C)

$$\text{Ans.: Given: } hv = 20\text{keV}; \text{ Also } \alpha = \frac{hv}{m_0c^2} = \frac{20 \times 1000 \times 1.6 \times 10^{-19}}{9.1 \times 10^{-31} \times (3 \times 10^8)^2} = \frac{2 \times 1.6}{9.1 \times 9} = 0.039072$$

$$T_e = hv \frac{\alpha(1-\cos\varphi)}{1+\alpha(1-\cos\varphi)} \Rightarrow T_e = 20\text{keV} \times \frac{0.039072}{1+0.039072} \approx 0.75\text{keV}$$

$$\text{Alternately: } hv = 20\text{keV} \Rightarrow \lambda = \frac{1240}{20 \times 1000} = 0.062\text{ nm}$$

$$\lambda' = \lambda + \frac{h}{m_0c} (1 - \cos\varphi) = 0.062\text{ nm} + \frac{6.626 \times 10^{-34}}{9.1 \times 10^{-31} \times 3 \times 10^8} = 0.062\text{ nm} + 0.002427\text{ nm}$$

$$= 0.064427\text{ nm}$$

$$hv' = \frac{1240}{0.064427} \text{ eV} = 19.25\text{ keV}$$

$$T_e = hv - hv' = 0.75\text{ keV}$$

JAM 2015: Section C

Q.8 X-rays of wavelength 0.24 nm are Compton scattered and the scattered beam is observed at an angle of 60° relative to the incident beam. The Compton wavelength of the electron is 0.00243 nm. The kinetic energy of scattered electrons in eV is _____.

$$\text{Ans.: } \lambda' - \lambda = \frac{h}{m_0c} (1 - \cos\varphi) = \lambda_c(1 - \cos\varphi) = 0.00243 \times (1 - \cos 60^\circ)$$

$$= 0.00243/2 = 0.001215\text{ nm}$$

$$\lambda' = 0.241215 \text{ nm}$$

Loss of energy of the X-ray is the gain in kinetic energy of the electron. So:

$$T_e = \left(\frac{1240}{0.24} - \frac{1240}{0.241215} \right) eV = (5166.67 - 5140.64) eV = 26.03 eV$$

JAM 2013

- Q.18 A beam of X-rays of wavelength 0.2 nm is incident on a free electron and gets scattered in a direction with respect to the direction of the incident radiation resulting in maximum wavelength shift. The percentage energy loss of the incident radiation is

$$\text{Ans.: } \lambda' - \lambda = \frac{h}{m_0 c} (1 - \cos \varphi) = \lambda_c (1 - \cos \varphi) = 0.002426 \times (1 - \cos 180^\circ)$$

$$= 0.004856 \text{ nm}$$

$$\lambda' = 0.204856 \text{ nm}$$

% loss of energy of the X-rays:

$$\left(\frac{1240}{0.2} - \frac{1240}{0.204856} \right) / \frac{1240}{0.2} \% = (6200 - 6053.03) / 6200 \% = 2.37 \%$$

JAM 2010

- Q.19 (a) A photon of initial momentum p_0 collides with an electron of rest mass m_0 moving with relativistic momentum P and energy E . The change in wavelength of the photon after scattering by an angle θ is given by, $\Delta\lambda = 2c\lambda_0 \frac{p_0 + P}{E - cP} \sin^2 \frac{\theta}{2}$, where c is the speed of light and λ_0 is the wavelength of the incident photon before scattering. What will be the value of $\Delta\lambda$ when the electron is moving in a direction opposite to that of the incident photon with momentum P and energy E ? Show that the value of $\Delta\lambda$ becomes independent of the wavelength of the incident photon when the electron is at rest before collision. (12)
- (b) In a Compton experiment, the ultraviolet light of wavelength 2000 Å is scattered from an electron at rest. What should be the minimum resolving power of an optical instrument to measure the Compton shift, if the observation is made at 90° with respect to the direction of the incident light? (9)

Ans.: (a) In case of head on collision the photon will bounce back by 180° .

$$\text{Then } \Delta\lambda = 2c\lambda_c \frac{p_0 + P}{E - cP} \sin^2 \frac{\theta}{2} = 2c\lambda_c \frac{p_0 + P}{E - cP} \sin^2 \frac{\pi}{2} = 2c\lambda_c \frac{p_0 + P}{E - cP}$$

If the electron is initially at rest then: $P = 0$.

$$\text{Then } \Delta\lambda = 2c\lambda_c \frac{p_0 + P}{E - cP} \sin^2 \frac{\theta}{2} = 2c\lambda_c \frac{p_0}{E} \sin^2 \frac{\theta}{2} = 2c\lambda_c \frac{h/\lambda}{E} \sin^2 \frac{\theta}{2}$$

$$(b) \text{ Resolving power} = \frac{\lambda}{\Delta\lambda} = \frac{\lambda}{\lambda_c (1 - \cos \theta)} = \frac{2000}{0.02426 \times (1 - \cos 90^\circ)} = \frac{2000}{0.02426} = 82440.23$$

JAM 2008

- Q.11 A photon of wavelength λ is incident on a free electron at rest and is scattered in the backward direction. The fractional shift in its wavelength in terms of the Compton wavelength λ_c of the electron is

$$(A) \frac{\lambda_c}{2\lambda}$$

$$(B) \frac{2\lambda_c}{3\lambda}$$

$$(C) \frac{3\lambda_c}{2\lambda}$$

$$(D) \frac{2\lambda_c}{\lambda}$$

Ans.: $\frac{\lambda' - \lambda}{\lambda} = \frac{\lambda_c}{\lambda} (1 - \cos \varphi) = \frac{\lambda_c}{\lambda} (1 - \cos \pi) = \frac{2\lambda_c}{\lambda}$.

JAM 2006:

23. A photon of energy E_{ph} collides with an electron at rest and gets scattered at an angle 60° with respect to the direction of the incident photon. The ratio of the relativistic kinetic energy T of the recoiled electron and the incident photon energy E_{ph} is 0.05.

(a) Determine the wavelength of the incident photon in terms of the Compton wavelength $\lambda_c \left(= \frac{h}{m_e c} \right)$, where h , m_e , c are Planck's constant, electron rest mass and velocity of light respectively. [12]

(b) What is the total energy E_e of the recoiled electron in units of its rest mass? [9]

Ans.: (a) $0.05 = \frac{T_e}{h\nu} = \frac{h\nu - h\nu'}{h\nu} = 1 - \frac{\nu'}{\nu} = 1 - \frac{\lambda}{\lambda'}$

$$\lambda = 0.95\lambda' = 0.95\Delta\lambda + 0.95\lambda \Rightarrow 0.05\lambda = 0.95\Delta\lambda \Rightarrow \lambda = 19\Delta\lambda$$

$$\lambda = 19\Delta\lambda = 19\lambda_c(1 - \cos \varphi) = 19\lambda_c(1 - \cos 60^\circ) = \frac{19}{2}\lambda_c = 9.5\lambda_c.$$

(b) $E_e = T_e + m_0c^2 = 0.05h\nu + m_0c^2 = \frac{0.05hc}{\lambda} + m_0c^2 = \frac{0.05hc}{9.5\lambda_c} + m_0c^2$

$$= \frac{0.05hcm_0c}{9.5h} + m_0c^2 = \frac{0.05}{9.5} m_0c^2 + m_0c^2 = \frac{m_0c^2}{190} + m_0c^2.$$

$$= \frac{191m_0c^2}{190} J = \frac{191c^2}{190} \text{ in the units of rest mass}$$

Zettili: Page-21

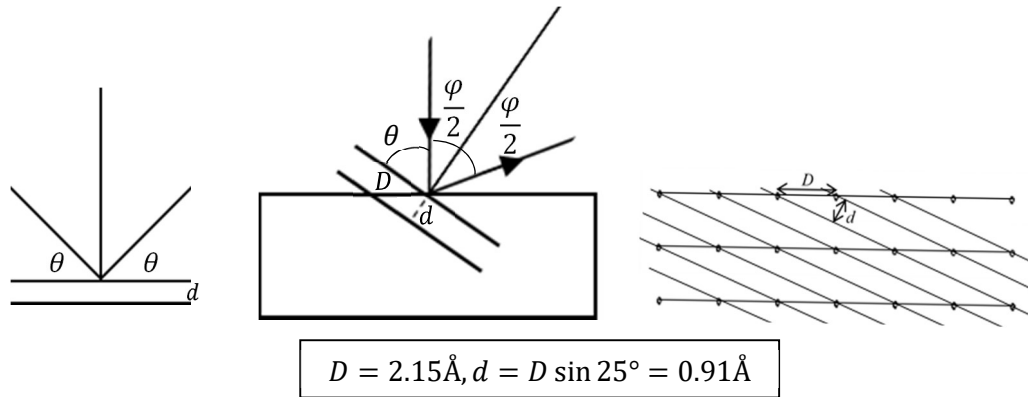
Calculate the de Broglie wavelength for

- (a) a proton of kinetic energy 70 MeV kinetic energy and
 (b) a 100 g bullet moving at 900 m s^{-1} .
-

Wave nature of particle

Davisson-Germer Experiment (1923-27):

Bombarding the surface of nickel single crystal normally with collimated beam of electrons and detecting the number of electrons scattered in different angles with the incident beam. It was observed that scattering was maximum for an angle $\varphi = 50^\circ$ when the electron energy was 54 eV .



To explain their result Davisson and Germer used the concept of wave nature of particle, here electrons, postulated by de Broglie. So the de Broglie wavelength of the electrons:

$$\frac{h}{p} = \frac{h}{\sqrt{2mE_k}} = \frac{6.626 \times 10^{-34}}{\sqrt{2 \times 9 \times 10^{-31} \times 54 \times 1.6 \times 10^{-19}}} \quad m = 1.67 \text{ \AA}$$

Verify for relativistic relations

Again when waves, like X-rays, are incident on the atomic planes of a crystal at different angles they suffers intense reflection like scattering for some particular angles given by Bragg's equation:

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

where θ is the angle of the incident beam with the set of parallel atomic planes (glancing angle) responsible for scattering, d is the inter-planar spacing between these planes and n is a positive integer, called order number. It is to be noted that intensity of scattered beam is small for large n .

In the Davisson-Germer experiment angle of incident $\varphi/2 = 50^\circ/2 = 25^\circ$ and so $\theta = 90^\circ - \varphi/2 = 65^\circ$. Thus the atomic planes responsible for the Bragg like scattering are oriented at an angle 25° with the surface of the crystal. Inter planer spacing of these planes was $d = 0.91 \text{ \AA}$.

Thus taking $n = 1$, since a single scattering maximum was observed,

$$\lambda = 2d \sin \theta = 2 \times 0.91 \times \sin 65^\circ \text{ \AA} = 1.65 \text{ \AA}$$

which matches quite well with the de Broglie wavelength of the electrons (1.67 \AA) within experimental errors. Thus the results of Davisson-Germer experiment confirms de Broglie relation $\lambda = h/p$.

*****Story (Wikipedia):** Davisson began work in 1921 to study electron bombardment and secondary electron emissions. A series of experiments continued through 1925.

Davisson and Germer's actual objective was to study the surface of a piece of nickel by directing a beam of electrons at the surface and observing how many electrons bounced off at various angles. They expected that because of the small size of electrons, even the smoothest crystal surface would be too rough and thus the electron beam would experience diffused reflection.

The experiment consisted of firing an electron beam at a nickel crystal, perpendicular to the surface of the crystal, and measuring how the number of reflected electrons varied as the angle between the detector and the nickel surface varied. To measure the number of electrons that were scattered at different angles, an electron detector that could be moved on an arc path about the crystal was used. The detector was designed to accept only elastically scattered electrons.

During the experiment, air accidentally entered the chamber, producing an oxide film on the nickel surface. To remove the oxide, Davisson and Germer heated the specimen in a high temperature oven, not knowing that this caused the formerly polycrystalline structure of the nickel to form large single crystal areas with crystal planes continuous over the width of the electron beam.

When they started the experiment again and the electrons hit the surface, they were scattered by nickel atoms in crystal planes (so the atoms were regularly spaced) of the crystal. This, in 1925, generated a diffraction pattern with unexpected peaks.

On a break, Davisson attended the Oxford meeting of the British Association for the Advancement of Science in summer 1926. At this meeting, he learned of the recent advances in quantum mechanics. To Davisson's surprise, Max Born gave a lecture that used diffraction curves from Davisson's 1923 research which he had published in Science that year, using the data as confirmation of the de Broglie hypothesis.

He learned that in prior years, other scientists – Walter Elsasser, E. G. Dymond, and Blackett, James Chadwick, and Charles Ellis – had attempted similar diffraction experiments, but were unable to generate low enough vacuums or detect the low-intensity beams needed.

Returning to the United States, Davisson made modifications to the tube design and detector mounting, adding azimuth in addition to colatitude. Following experiments generated a strong signal peak at 65 V and an angle $\theta = 45^\circ$. He published a note to Nature titled, "The Scattering of Electrons by a Single Crystal of Nickel".

Questions still needed to be answered and experimentation continued through 1927.

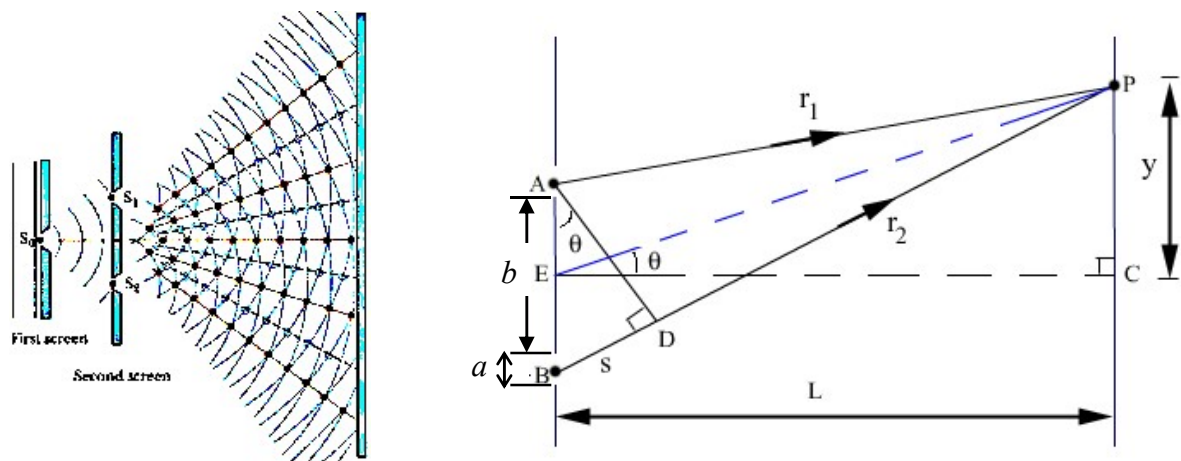
By varying the applied voltage to the electron gun, the maximum intensity of electrons diffracted by the atomic surface was found at different angles. The highest intensity was observed at an angle $\theta = 50^\circ$ with a voltage of 54 V, giving the electrons a kinetic energy of 54 eV.

According to the de Broglie relation, electrons with kinetic energy of 54 eV have a wavelength of 0.167 nm. The experimental outcome was 0.165 nm via Bragg's law, which closely matched the predictions.

Davisson and Germer's accidental discovery of the diffraction of electrons was the first direct evidence confirming de Broglie's hypothesis that particles can have wave properties as well.***

Double slit experiment with light (photons) and with electrons:

Double slit experiment with parallel monochromatic beam of light:



Path difference: $\delta = (a + b) \sin \theta$, where a & b are respectively the widths of the slits and the separation between the slits. θ is the angular position of a point on the screen with respect to the central line between the slits.

Condition of maximum intensity:

$$(a + b) \sin \theta_n = n\lambda \Rightarrow \sin \theta_n = \frac{n\lambda}{a+b}; \text{ Now for small } \theta_n, \sin \theta_n \approx \tan \theta_n = \frac{y_n}{D}$$

$$\text{So } \frac{y_n}{D} = \frac{n\lambda}{a+b}; \quad y_n = \frac{D}{a+b} n\lambda$$

$$\text{Fringe width} = \beta = y_n - y_{n-1} = \frac{D}{a+b} \lambda = \frac{D}{d} \lambda = \text{constant.}$$

where $d = a + b$ is the distance between the centres of the slits.

Resultant intensity on the screen (**considering the slits to be extremely narrow**):

$$\psi_1 = Ae^{i(kx-\omega t)}; \quad \psi_2 = Ae^{i(k(x+\delta)-\omega t)}$$

$$\psi = \psi_1 + \psi_2 ;$$

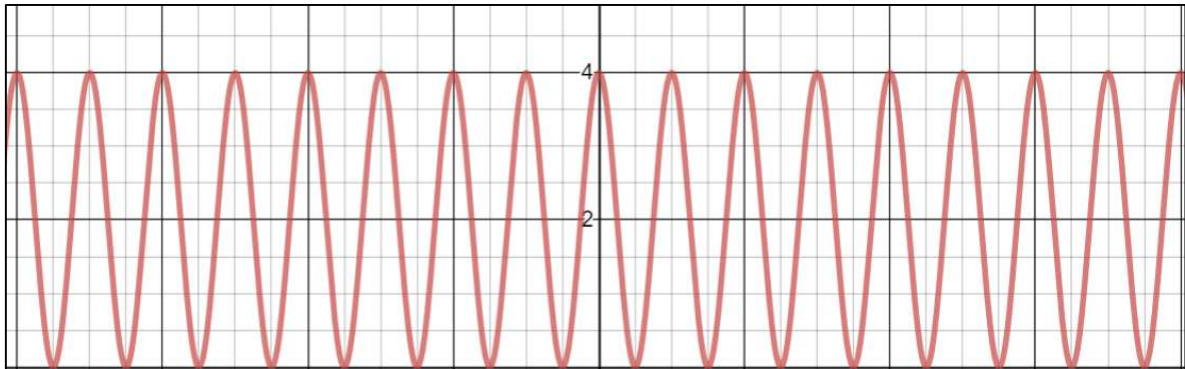
$$I = |\psi|^2 = (\psi_1 + \psi_2)(\psi_1^* + \psi_2^*) = |\psi_1|^2 + |\psi_2|^2 + |\psi_1||\psi_2|(e^{-ik\delta} + e^{ik\delta})$$

$$= |\psi_1|^2 + |\psi_2|^2 + 2|\psi_1||\psi_2| \cos(k\delta)$$

$$I = I_1 + I_2 + 2\sqrt{I_1 I_2} \cos[k(a + b) \sin \theta]$$

For $I_1 = I_2 = I_0$, we have:

$$I = 2I_0 + 2I_0 \cos[k(a + b) \sin \theta] = 4I_0 \cos^2 \beta, \text{ where } \beta = \frac{k(a+b)}{2} \sin \theta.$$

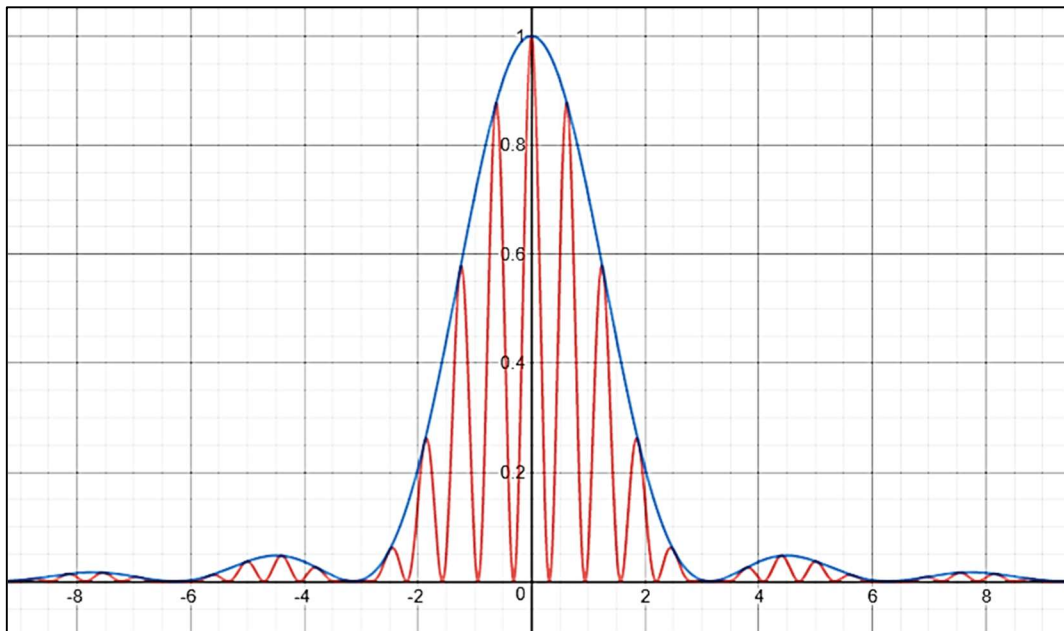


Again the intensity distribution on the screen, for a single slit of finite width a , is given by:

$$I = I_0 \frac{\sin^2 \alpha}{\alpha^2}, \text{ where } \alpha = \frac{ka}{2} \sin \theta = \frac{\pi a}{\lambda} \sin \theta .$$

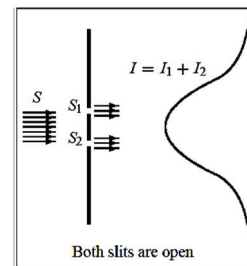
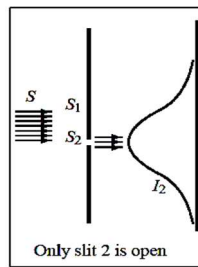
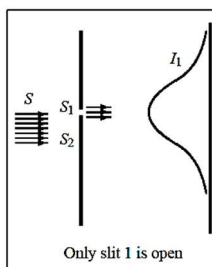
It can be shown that in case of the double slit experiment if the finite width of the slits is considered, then intensity distribution will be given by:

$$I = 4I_0 \frac{\sin^2 \alpha}{\alpha^2} \cos^2 \beta.$$



Double slit experiment with macroscopic particles:

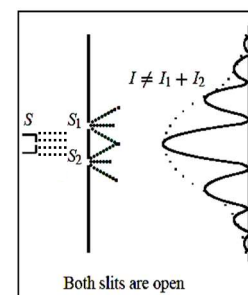
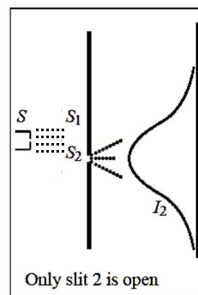
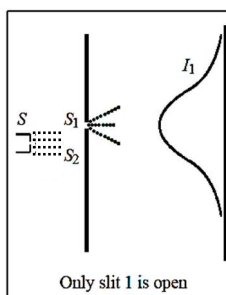
$$I = I_1 + I_2$$



Quantum Mechanics Concepts and Applications - Nouredine Zettili

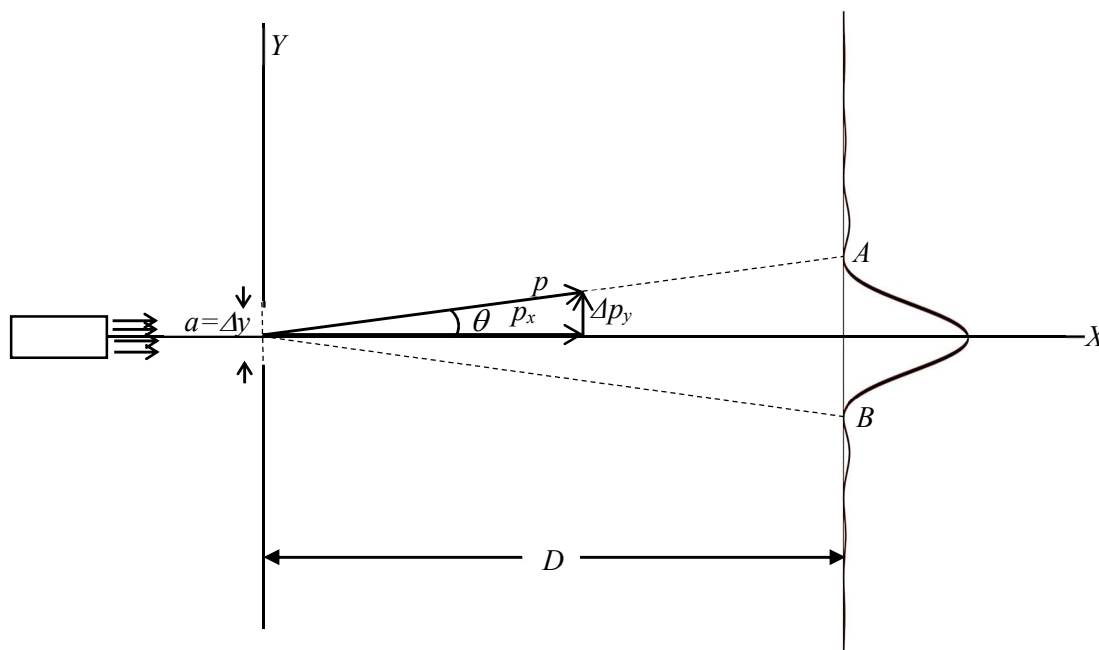
Double slit experiment with parallel mono-energetic beam of electrons:

1. $I \neq I_1 + I_2$
2. Count distribution pattern on the screen is similar to the double slit diffraction pattern of light of wavelength $\lambda = h/p$, where p is the linear momentum of the electrons and h is Planck constant.
3. The count distribution pattern remains same if even one electron at a time is fired from the electron gun.



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Single slit diffraction of light:



The intensity of light on the screen is given by:

$I = I_0 \frac{\sin^2 \alpha}{\alpha^2}$, where $\alpha = \frac{ka}{2} \sin \theta = \frac{\pi a}{\lambda} \sin \theta$, θ being the angular position on the slit with respect to the centre of the slit.

Condition of minima is $\frac{dI}{d\alpha} = 0, \frac{d^2I}{d\alpha^2} = +ve \Rightarrow \sin \alpha = 0 \Rightarrow \alpha = \frac{\pi a}{\lambda} \sin \theta = n\pi$.

$\Rightarrow a \sin \theta = n\lambda; n = \pm 1, \pm 2, \pm 3 \dots; n \neq 0$, as $n = 0$ corresponds to the central maximum.

For the first minimum on the both sides of the central maximum $|\sin \theta| = \frac{\lambda}{a}$.

Before passing through the slit, the beam of light is parallel and so have no angular spread. But after passing through the narrow slit, the beam of light gets some angular spread. In the figure the angular spread of the central maximum is $2\theta \approx 2 \sin \theta$ (since θ is small) $= \frac{2\lambda}{a}$. Thus the angular spread of the central maximum increases if the width of the slit (a) decreases.

Single slit diffraction of electrons and Heisenberg uncertainty principle:

Now let in the place of light/photons electrons are used for the diffraction experiment. Let detectors are placed at every point on the screen which can count the number of electrons hitting that point. The distribution pattern of electron counts on the screen will be similar to that for light of wavelength $\lambda = h/p$, where p is the momentum of the mono-energetic electrons incident on the slits.

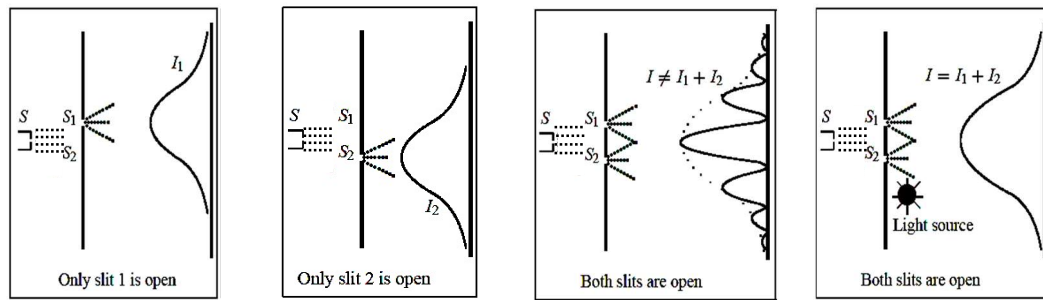
The electrons, emitting from the source, move in positive X direction. So we can write $p = p_x$. But after passing through the slit the electrons gain a little momentum in Y direction, which causes angular spread of the diffracted electron beam. Let $\pm \Delta p_y$ are the y-components of momentum gained by the electrons reaching to the first minima on the both sides of the central maximum. Then we can say that, the electrons reaching the screen within the central peak AB have gained at the slit an uncertainty Δp_y in y-component of momentum in either positive or negative y-direction. These electrons have passed through any point in the slit of width a . So, at the slit, the uncertainty in their y-coordinate is $\Delta y = a$.

Now: $\frac{\Delta p_y}{p_x} = \tan \theta \approx \theta \approx \sin \theta$ (since θ is small) $= \frac{\lambda}{a} = \frac{\lambda}{\Delta y}$

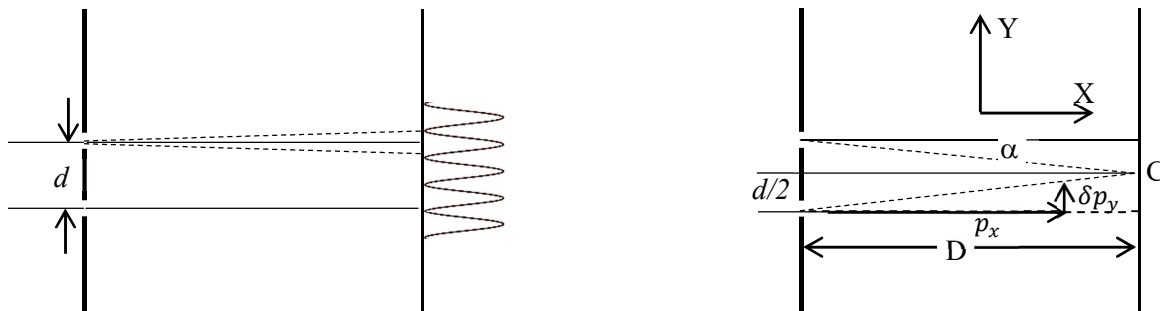
So, at the slit, $\Delta y \Delta p_y \approx \lambda p_x \Rightarrow \Delta y \Delta p_y \approx \lambda \frac{h}{\lambda} \Rightarrow \Delta y \Delta p_y \approx h$.

i.e. the product of the uncertainties in y-component of momentum and position is $h > \frac{\hbar}{2}$. Thus Heisenberg uncertainty principle is obeyed.

From uncertainty principle show that, in the double slit diffraction of electrons, it is not possible to determine the slit, through which the electron passes and to produce the diffraction pattern in a single experiment.



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Ans.: Fringe width of the interference fringes in the double slit diffraction experiment is given by:

$$\beta = y_n - y_{n-1} = \frac{D}{d} \lambda.$$

For the fringe system to be stationary the uncertainty in measurement of the position (y -coordinate) of the slit plate must be small compared to the fringe width β .

$$\text{i.e. } \Delta y \ll \beta \quad \Rightarrow \Delta y \ll \frac{D}{d} \lambda. \quad \dots \dots \dots (A)$$

Now let we want to determine through which the electron passes to reach a point C on the screen. If the electron passes through the lower slit, it would have to gain a momentum, say δp_y , in $+ve Y$ direction and if it passes through the upper slit, it would have to gain a momentum, say δp_y , in $-ve Y$ direction. In the two cases the slit plate will recoil in opposite directions and measuring the recoil momentum of the slit plate it will be possible to determine through which slit the electron passes. But to measure the recoil momenta of the slit plate in these two cases distinctly the uncertainty in measurement of the momentum of the slit plate must be much small compared to the difference of these two recoil momenta.

$$\text{i.e. } \Delta p_y \ll \delta p_y - (-\delta p_y), \quad \text{or, } \Delta p_y \ll 2\delta p_y.$$

Now from figure:

$$\frac{\delta p_y}{p_x} = \tan \alpha = \frac{d/2}{D} = \frac{d}{2D}. \quad \text{Therefore } \delta p_y = p_x \frac{d}{2D} = \frac{h}{\lambda} \frac{d}{2D}.$$

$$\text{So, } \Delta p_y \ll 2 \frac{h}{\lambda} \frac{d}{2D},$$

$$\text{or, } \Delta p_y \ll \frac{h}{\lambda} \frac{d}{D} \quad \dots \dots \dots (B)$$

Thus to measure through which slit the electron passes and also to have a diffraction pattern at the same time, we must have both the conditions (A) and (B) satisfied at the same time. Or in other words: $\Delta p_y \Delta y \ll \frac{h}{\lambda} \frac{D}{d} \lambda;$

$$\text{Or, } \Delta p_y \Delta y \ll h \dots \dots (C).$$

Equation (C) is clear violation of uncertainty principle and so impossible. Therefore measuring through which the electron passes and having a diffraction pattern at the same time is impossible. Or in other words, any successful trial of 'seeing' through which slit the electrons pass will destroy the diffraction pattern.

Problems of Waveparticle Duality, Uncertainty Principle, Two Slit Experiment:

JAM 2017

- Q.57 In an electron microscope, electrons are accelerated through a potential difference of 200 kV. What is the best possible resolution of the microscope?
(Specify your answer in picometers to two digits after the decimal point.)

Ans.: Rest mass energy of the electron is 0.511 MeV Kinetic energy gained by the electron is 200 keV = 0.2 MeV, which is of the order of the rest mass energy. Therefore relativistic treatment is required.

Kinetic energy gained by the electron is 200 keV = 3.2×10^{-14} J

$$K.E = E - m_0c^2 = \sqrt{p^2c^2 + m_0^2c^4} - m_0c^2$$

$$\sqrt{p^2c^2 + m_0^2c^4} = K.E + m_0c^2$$

$$p^2 = \frac{(K.E + m_0c^2)^2 - m_0^2c^4}{c^2}$$

$$p = \frac{\sqrt{(K.E + m_0c^2)^2 - m_0^2c^4}}{c} = \frac{\sqrt{K.E(K.E + 2m_0c^2)}}{c}$$

$$p = \frac{\sqrt{3.2 \times 10^{-14}(3.2 \times 10^{-14} + 2 \times 8.187 \times 10^{-14})}}{2.9979 \times 10^8}$$

$$= \frac{7.91}{2.9979 \times 10^8} \times 10^{-14}$$

$$= \frac{7.91}{2.9979 \times 10^8} \times 10^{-14} = 2.64 \times 10^{-22} \text{ kg.m/s}$$

$$\lambda = \frac{h}{p} = \frac{6.626 \times 10^{-34}}{2.64 \times 10^{-22}} = 2.5 \times 10^{-12} \text{ m}$$

Best possible resolution = $\lambda = 2.5 \times 10^{-1} \text{ m}$

JAM 2016

- Q.17 Consider a free electron (e) and a photon (ph) both having 10 eV of energy. If λ and P represent wavelength and momentum respectively, then
(mass of electron = 9.1×10^{-31} kg; speed of light = 3×10^8 m/s)
- (A) $\lambda_e = \lambda_{ph}$ and $P_e = P_{ph}$. (B) $\lambda_e < \lambda_{ph}$ and $P_e > P_{ph}$.
(C) $\lambda_e > \lambda_{ph}$ and $P_e < P_{ph}$. (D) $\lambda_e < \lambda_{ph}$ and $P_e < P_{ph}$.

Ans.: Rest mass energy of electron is 0.511 MeV. Given kinetic energy of the electron is 10 eV is much less than the rest mass energy of the electron. Therefore nonrelativistic treatment can be done.

$$P_e = \sqrt{2mE} = \sqrt{2 \times 9.1 \times 10^{-31} \times 1.6 \times 10^{-19} \times 10} = 1.7065 \times 10^{-24} \text{ kg.ms}^{-1}.$$

$$\lambda_e = \frac{h}{P_e} = \frac{6.626 \times 10^{-34}}{1.7065 \times 10^{-24}} = 3.88 \times 10^{-10} \text{ m} = 0.388 \text{ nm}$$

$$\lambda_{ph} = \frac{1240}{10} = 124 \text{ nm}$$

$$P_{ph} = \frac{h}{\lambda_{ph}} = \frac{6.626 \times 10^{-34}}{124 \times 10^{-9}} = 5.34 \times 10^{-27} \text{ kg.ms}^{-1}$$

$$P_{ph} = \frac{E}{c} = \frac{10 \times 1.6 \times 10^{-19}}{3 \times 10^8} = 5.33 \times 10^{-27} \text{ kg.ms}^{-1}$$

Thus $\lambda_e < \lambda_{ph}$ & $P_e > P_{ph}$

JAM 2016

Q.39 A slit has width 'd' along the x-direction. If a beam of electrons, accelerated in y-direction to a particular velocity by applying a potential difference of 100 ± 0.1 kV passes through the slit, then, which of the following statement(s) is(are) correct?

(A) The uncertainty in the position of electrons in x-direction before passing the slit is zero.

(B) The momentum of electrons in x-direction is $\sim \hbar/d$ immediately after passing the slit.

(C) The uncertainty in the position of electrons in y-direction before passing the slit is zero.

(D) The presence of the slit does not affect the uncertainty in momentum of electrons in y-direction.

Ans.: (A) If (A) would be true then the momentum of the electrons in x-direction would be completely indeterminable. Then one could not say that they are accelerated in y-direction.

(B) From Heisenberg uncertainty relation, if the position in x-direction has an uncertainty d, then uncertainty in momentum in x-direction will be $\Delta p_x \approx \frac{\hbar}{2d} \approx \frac{\hbar}{d}$. So (B) is correct.

(C) Uncertainty in momentum along y-direction:

Energy of the electron is $E = 100 \pm 0.1 \text{ eV} = (100 \pm 0.1) \times 1.6 \times 10^{-19} \text{ eV}$

Nonrelativistic treatment:

$$\begin{aligned} \Delta p_y &= \sqrt{2me(V + \Delta V)} - \sqrt{2me(V - \Delta V)} \\ &= \sqrt{2 \times 9.1 \times 10^{-31} \times 1.6 \times 10^{-19}} \left[\sqrt{(V + \Delta V)} - \sqrt{(V - \Delta V)} \right] \\ &= 5.3963 \times 10^{-25} \left[\sqrt{V} \left(1 + \frac{1}{2} \frac{\Delta V}{V} \right) - \sqrt{V} \left(1 - \frac{1}{2} \frac{\Delta V}{V} \right) \right] \\ &= 5.3963 \times 10^{-25} \times \sqrt{V} \times \frac{\Delta V}{V} = 5.3963 \times 10^{-25} \times 10 \times \frac{0.1}{100} \text{ kg.ms}^{-1} \\ &= 5.3963 \times 10^{-27} \text{ kg.ms}^{-1}. \end{aligned}$$

Relativistic treatment:

$$\begin{aligned} \Delta p_y &= \frac{\sqrt{e(V+\Delta V)(e(V+\Delta V)+2m_0c^2)}}{c} - \frac{\sqrt{e(V-\Delta V)(e(V-\Delta V)+2m_0c^2)}}{c} \\ &= \frac{\sqrt{e(V+\Delta V)(eV+2m_0c^2+e\Delta V)}}{c} - \frac{\sqrt{e(V-\Delta V)(eV+2m_0c^2-e\Delta V)}}{c} \\ &= \frac{\sqrt{eV(eV+2m_0c^2)} \left(1 + \frac{\Delta V}{V} \right) \left(1 + \frac{e\Delta V}{eV+2m_0c^2} \right)}{c} - \frac{\sqrt{eV(eV+2m_0c^2)} \left(1 - \frac{\Delta V}{V} \right) \left(1 - \frac{e\Delta V}{eV+2m_0c^2} \right)}{c} \\ &= \frac{\sqrt{eV(eV+2m_0c^2)}}{c} \left[\left(1 + \frac{\Delta V}{V} \right) \left(1 + \frac{e\Delta V}{2(eV+2m_0c^2)} \right) - \left(1 - \frac{\Delta V}{V} \right) \left(1 - \frac{e\Delta V}{2(eV+2m_0c^2)} \right) \right] \\ &= \frac{\sqrt{eV(eV+2m_0c^2)}}{c} \left[\left(1 + \frac{\Delta V}{2V} + \frac{e\Delta V}{2(eV+2m_0c^2)} \right) - \left(1 - \frac{\Delta V}{2V} - \frac{e\Delta V}{2(eV+2m_0c^2)} \right) \right] \end{aligned}$$

$$= \frac{\sqrt{eV(eV+2m_0c^2)}}{c} \left[\frac{\Delta V}{V} + \frac{e\Delta V}{(eV+2m_0c^2)} \right]$$

$$= \frac{\sqrt{100(100e+2 \times 51100)}}{c} \left[\frac{0.1}{100} + \frac{0.1e}{(100e+2 \times 51100e)} \right],$$

(since $m_0c^2 = 0.511 \text{ MeV} = 511000 \times e \text{ Joule}$)

$$= \frac{e\sqrt{100 \times 1022100}}{c} \times \frac{1022200}{100 \times 1022100} \times 0.1 = 5.39247 \times 10^{-27} \text{ kg.m/s}$$

$$\Delta y \approx \frac{\hbar}{2\Delta p_y} = \frac{6.626 \times 10^{-34}}{2\pi \times 2 \times 5.3963 \times 10^{-27}} = 9.776 \text{ nm} \neq 0$$

(D) The presence of the slit has no influence on the y-direction motion of the electrons. So it does not effect the momentum of the electrons in y-direction.

JAM 2016

Q.55 The de Broglie wavelength of a relativistic electron having 1 MeV of energy is $\frac{\quad}{\quad} \times 10^{-12} \text{ m}$. (Take the rest mass energy of the electron to be 0.5 MeV. Planck constant = $6.63 \times 10^{-34} \text{ Js}$, Speed of light = $3 \times 10^8 \text{ m/s}$, Electronic charge = $1.6 \times 10^{-19} \text{ C}$)

Ans.: $E^2 = p^2c^2 + m_0^2c^4 \Rightarrow p^2 = \frac{E^2}{c^2} + m_0^2c^2$

$$\Rightarrow p = \sqrt{\frac{E^2}{c^2} + m_0^2c^2} = \sqrt{\frac{(10^6 \times 1.6 \times 10^{-19})^2}{(3 \times 10^8)^2} + (9.1 \times 10^{-31} \times 3 \times 10^8)^2}$$

$$= \sqrt{(0.53 \times 10^{-21})^2 + (27.3 \times 10^{-2})^2}$$

$$= 10^{-21} \times \sqrt{(0.53)^2 + (0.273)^2} = 0.59 \times 10^{-21} \text{ kg m s}^{-1}$$

$$\lambda = \frac{h}{p} = \frac{6.63 \times 10^{-34}}{0.59 \times 10^{-21}} = 11.23 \times 10^{-13} \text{ m} = 1.123 \times 10^{-12} \text{ m}.$$

JAM 2015: Section A

Q.26 A nucleus has a size of 10^{-15} m . Consider an electron bound within a nucleus. The estimated energy of this electron is of the order of

- (A) 1 MeV (B) 10^2 MeV
 (C) 10^4 MeV (D) 10^6 MeV

Ans.: Minimum uncertainty in momentum $\approx (\hbar/2)/\text{Maximum uncertainty in position}$

$$\Delta p \approx \frac{\hbar}{2\Delta x} = \frac{h}{2\pi \times 2\Delta x} = \frac{6.63 \times 10^{-34}}{2\pi \times 2\Delta x} \approx \frac{10^{-3}}{2 \times 10^{-15}} \approx \frac{10^{-1}}{2} \text{ kg.ms}^{-1}.$$

Minimum momentum of the electron is:

$$p_{min} = \Delta p \approx \frac{10^{-19}}{2} \text{ kg.ms}^{-1}.$$

If non relativistic treatment is done then the velocity of the electron comes to be:

$$v = p_{min}/m_0 \approx \frac{10^{-1}}{2 \times 9.1 \times 10^{-31}} \approx 10^{11} \text{ m/s} \gg c \text{ and is impossible.}$$

Therefore relativistic treatment is to be done.

$$E_{min} = \sqrt{p_{min}^2c^2 + m_0^2c^4}$$

$$E_{min} = c\sqrt{p_{min}^2 + m_0^2c^2} = 3 \times 10^8 \times \sqrt{\left(\frac{10^{-19}}{2}\right)^2 + (9.1 \times 10^{-31})^2 (3 \times 10^8)^2}$$

$$= 3 \times 10^8 \times 10^{-1} \sqrt{0.25 + 27.3 \times 10^{-8}} \approx 3 \times 10^8 \times 10^{-19} \times 0.5 = 1.5 \times 10^{-11} \text{ J}$$

$$= \frac{1.5 \times 10^{-11}}{1.6 \times 10^{-19}} \text{ eV} = 10^8 \text{ eV} = 10^2 \text{ MeV}$$

JAM 2007:

12. The speed of an electron, whose de Broglie wavelength is equal to its Compton wavelength, is (c is the speed of light)

(A) c

(B) $c/\sqrt{2}$

(C) $c/2$

(D) $c/3$

Ans.: $\lambda = \text{Compton wavelength} = \lambda_c = \frac{h}{m_0 c}$

$$p = \frac{h}{\lambda} = m_0 c$$

$$p = mv = \frac{m_0 v}{\sqrt{1-v^2/c^2}} = \frac{m_0 v}{\sqrt{1-v^2/c^2}}$$

$$\frac{m_0 v}{\sqrt{1-v^2/c^2}} = m_0 c \Rightarrow v^2/c^2 = 1 - v^2/c^2 \Rightarrow 2v^2/c^2 = 1 \Rightarrow v = \frac{c}{\sqrt{2}}$$

QX. Zero point energy of harmonic oscillator from uncertainty principle:

If Δp_x is the standard deviation of measurement of p_x then: $(\Delta p_x)^2 = \langle p_x^2 \rangle - \langle p_x \rangle^2 = \langle p_x^2 \rangle$

Similarly if Δx is the standard deviation of measurement of x then: $(\Delta x)^2 = \langle x^2 \rangle - \langle x \rangle^2 = \langle x^2 \rangle$

Now $E = \frac{p_x^2}{2m} + \frac{1}{2}kx^2$

So $\langle E \rangle = \frac{\langle p_x^2 \rangle}{2m} + \frac{1}{2}k\langle x^2 \rangle = \frac{(\Delta p_x)^2}{2m} + \frac{1}{2}k(\Delta x)^2 = \frac{(\Delta p_x)^2}{2m} + \frac{m\omega^2}{2}(\Delta x)^2$

Uncertainty Principle: $(\Delta x)(\Delta p_x) \geq \frac{\hbar}{2}$

$$\Rightarrow (\Delta x)^2(\Delta p_x)^2 \geq \frac{\hbar^2}{4}$$

$$\Rightarrow (\Delta p_x)^2 \geq \frac{\hbar^2}{4(\Delta x)^2}$$

Thus $\langle E \rangle \geq \frac{\hbar^2}{8m(\Delta x)^2} + \frac{m\omega^2}{2}(\Delta x)^2$

The r.h.s will be minimum if $\frac{\partial(\text{r.h.s})}{\partial[(\Delta x)^2]} = 0$; i.e. if $-\frac{\hbar^2}{8m(\Delta x)^4} + \frac{m\omega^2}{2} = 0$; i.e. if $(\Delta x)^2 = \frac{\hbar}{2m\omega}$

So $\langle E \rangle_{\min} = \frac{\hbar^2}{8m} \frac{2m}{\hbar} + \frac{m\omega^2}{2} \frac{\hbar}{2m}$

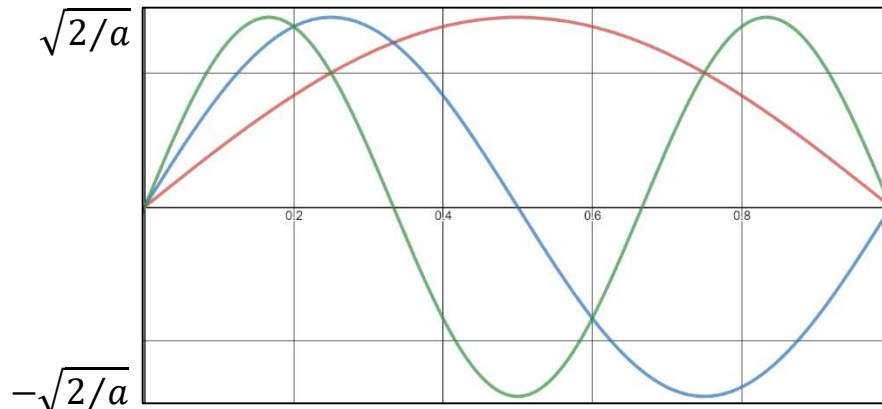
$$= \frac{1}{2} \hbar \omega = \text{zero point energy of quantum harmonic oscillator.}$$

SOME PROBLEMS ON WAVE PACKET

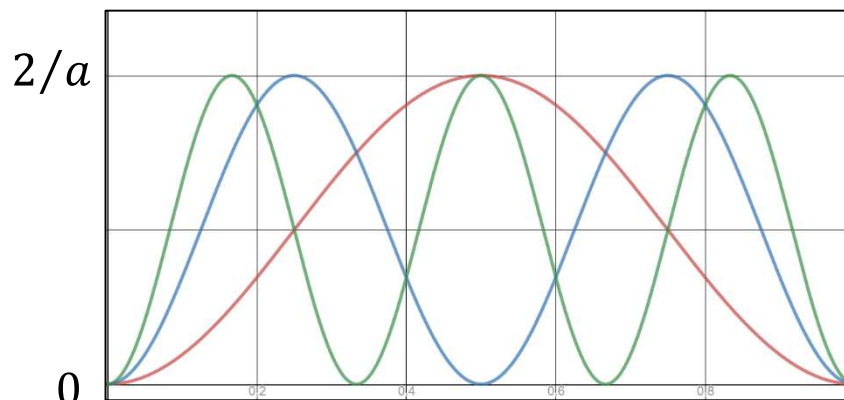
Eigen functions of particle in a one dimensional infinite potential well:

$$\Psi(x, t) = \sum_{n=0}^{\infty} c_n \psi_n(x, t) = \sum_{n=0}^{\infty} c_n \psi_n(x) e^{-iE_n t/\hbar} = \sqrt{\frac{2}{a}} \sum_{n=0}^{\infty} c_n \sin\left(\frac{n\pi x}{a}\right) e^{-i\left(\frac{n^2 \pi^2 \hbar^2}{2ma^2}\right)t/\hbar}$$

Where $\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$ are the eigen functions or stationary states.



Plot of $\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$ for $a = 1$, $n = 1, 2, 3$



Plot of $P_n(x) = \frac{2}{a} \sin^2\left(\frac{n\pi x}{a}\right)$ for $a = 1$, $n = 1, 2, 3$

The functions $\psi_n(x, t) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) e^{-i\left(\frac{n^2 \pi^2 \hbar^2}{2ma^2}\right)t/\hbar}$, are not of the form $f(x \pm vt)$ or $f(kx \pm \omega t)$. So they do not represent propagating waves. They actually represent standing waves with amplitude $\sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$ and wavelength $\frac{2a}{n}$. The probability density is $P_n(x) = \frac{2}{a} \sin^2\left(\frac{n\pi x}{a}\right)$ for $n = 1, 2, 3, \dots$

Free particle:

$$\frac{-\hbar^2}{2m} \frac{\partial^2 \Psi(x, t)}{\partial x^2} = i\hbar \frac{\partial \Psi(x, t)}{\partial t}$$

Using separation of variables: $\Psi(x, t) = \psi(x)\eta(t)$

$$\frac{i\hbar}{\eta(t)} \frac{d\eta(t)}{dt} = E \quad \Rightarrow \quad \frac{d\eta}{\eta} = -\frac{iE}{\hbar} dt \quad \Rightarrow \quad \eta(t) = e^{-\frac{iE}{\hbar}t}$$

Since $\eta(t)$ must not blow up at $t = \infty$, so E must have to be real.

$$\frac{-\hbar^2}{2m\psi(x)} \frac{d^2\psi(x)}{dx^2} = E \quad \Rightarrow \quad \frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}\psi = 0 \quad \Rightarrow \quad \frac{d^2\psi}{dx^2} + k^2\psi = 0; \quad \left[k = \sqrt{\frac{2mE}{\hbar^2}} \right] \quad \Rightarrow \quad \psi(x) = Ae^{-ikx} + Be^{+ikx}$$

$\Rightarrow \psi_k(x) = A_k e^{ikx}$ with $k = \pm \sqrt{\frac{2mE}{\hbar^2}}$ for waves travelling to right and to left respectively... (A)

Since $\psi_k(x)$ must not blow up at $x = \pm\infty$, so k must have to be real.

$$\psi_k(x, t) = A_k e^{i(kx - \frac{E}{\hbar}t)} = A_k e^{i\left(\pm\sqrt{\frac{2mE}{\hbar^2}}x - \frac{E}{\hbar}t\right)} \dots\dots (B)$$

For free particle there are no boundary conditions. Therefore values of k or $E = \frac{\hbar^2 k^2}{2m}$ are not discrete. Rather they have continuous values.

Comparing the equation $\psi_k(x, t) = A_k e^{i(kx - \frac{E}{\hbar}t)} = A_k e^{ik(x - \frac{E}{\hbar k}t)}$ with the standard wave equation $f = f(x - vt)$ we see that the velocity of the wave is:

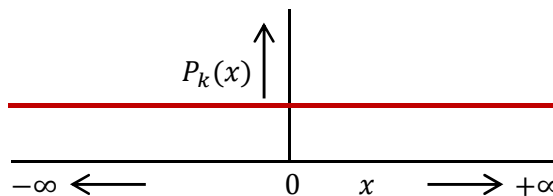
$$v_{wave} = \frac{E}{\hbar k} = \frac{E}{\hbar} \sqrt{\frac{\hbar^2}{2mE}} = \sqrt{\frac{E}{2m}} \dots\dots\dots (C).$$

But the particle velocity $v_{particle} = \sqrt{\frac{2E}{m}} \dots\dots (D) \quad \left[\text{From } E = \frac{1}{2}mv^2 \right].$

Therefore, $\frac{v_{wave}}{v_{particle}} = \sqrt{\frac{E}{2m}} \times \sqrt{\frac{m}{2E}} = \frac{1}{2}.$

The ‘eigen function’ (A) [or (B)] do not represent the stationary states of a free particle since:

(i) $P_k = |\psi_k(x, t)|^2 = |A_k|^2$ is independent of x and the probability of finding the particle at anywhere between $x = -\infty$ to $+\infty$ is the same (see Fig.). Therefore the eigen function does not represent a localised particle.



(ii) $\int_{-\infty}^{\infty} P_k(x) dx = |A_k|^2 \int_{-\infty}^{\infty} dx = \infty.$ i.e the ‘eigen functions’ ψ_k are not square integrable and total probability becomes infinite which is impossible.

(iii) The wave, representing the particle, moves with a velocity which is half of the velocity of the particle.

Thus these ‘eigen functions’ [eqn. (A) or (B)] “do not represent the physically realisable states”[Griffiths]. In other words “a free particle cannot exist in a stationary state” or “there is no such thing as a free particle with a definite energy”[Griffiths].

Now the general solution will be the linear combination of all the eigen functions or of all the solutions $\exp\left(i\left(kx - \frac{\hbar k^2}{2m}t\right)\right).$ Since k or E are continuous so the summation in the linear combination will be replaced by integration:

$$\Psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \varphi(k) e^{i\left(kx - \frac{\hbar k^2}{2m}t\right)} dk,$$

where $\frac{1}{\sqrt{2\pi}} \varphi(k)$ play the role of the coefficients of the linear combination.

$\varphi(k)$ can be determined from the initial wave function $\Psi(x, 0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \varphi(k) e^{ikx} dk$ with the help of Fourier Transform:

$$\varphi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \Psi(x, 0) e^{-ikx} dx$$

Fourier Transform:

If $f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} F(k) e^{ikx} dk \dots \dots (i)$ then $F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} f(x) e^{-ikx} dx \dots \dots (ii)$ and vice versa. (ii) is called the Fourier Transform of (i) and (i) is called inverse Fourier transform of (ii).

Thus the free particle wave function at $t = 0$ and at $t = t$ are:

$$\Psi(x, 0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \varphi(k) e^{ikx} dk$$

$$\text{and } \Psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \varphi(k) e^{i\left(kx - \frac{\hbar k^2}{2m}t\right)} dk = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \varphi(k) e^{i\left(kx - \frac{\hbar k^2}{2m}t\right)} dk$$

$$\text{with } \varphi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \Psi(x, 0) e^{-ikx} dx.$$

Now we see that $|\Psi(x, 0)|^2 = P(x, 0) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} |\varphi(k)|^2 dk$ and

$$\frac{1}{2\pi} \int_{-\infty}^{+\infty} P(x, 0) dx = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} |\varphi(k)|^2 dk dx \text{ is not infinite essentially.}$$

What does $\Psi(x, 0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \varphi(k) e^{ikx} dk$ represent?

The type or shape of the wave represented by $\Psi(x, 0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \varphi(k) e^{ikx} dk$ depends on $\varphi(k)$. To have an idea about what is represented by $\Psi(x, 0)$, let us first solve the following problems (A) to (D).

Problem A. (From: Int. to Q. M. 2nd edn. D. J. Griffiths Problem 2.20 (a)):

Dirichlet's theorem says that 'any' function $f(x)$ on the interval $[-a, a]$ can be expanded as a Fourier series:

$$f(x) = \sum_{n=0}^{\infty} \left[a_n \sin\left(\frac{n\pi x}{a}\right) + b_n \cos\left(\frac{n\pi x}{a}\right) \right]$$

Show that this can be written equivalently as: $f(x) = \sum_{n=-\infty}^{\infty} c_n e^{\frac{i n \pi x}{a}} \dots \dots (A)$

where $c_n = b_n$ for $n = 0$; $c_n = \frac{1}{2}(-ia_n + b_n)$ for $n = 1, 2, \dots \infty$

and $c_n = \frac{1}{2}(ia_{-n} + b_{-n})$ for $n = -1, -2, \dots -\infty$.

$$\begin{aligned} \text{Ans.: } f(x) &= \sum_{n=0}^{\infty} \left[a_n \sin\left(\frac{n\pi x}{a}\right) + b_n \cos\left(\frac{n\pi x}{a}\right) \right] = \sum_{n=0}^{\infty} \left[a_n \frac{e^{\frac{i n \pi x}{a}} - e^{-\frac{i n \pi x}{a}}}{2i} + b_n \frac{e^{\frac{i n \pi x}{a}} + e^{-\frac{i n \pi x}{a}}}{2} \right] \\ &= \sum_{n=0}^{\infty} \left[\left(\frac{a_n}{2i} + \frac{b_n}{2} \right) e^{\frac{i n \pi x}{a}} + \left(-\frac{a_n}{2i} + \frac{b_n}{2} \right) e^{-\frac{i n \pi x}{a}} \right] \end{aligned}$$

$$\begin{aligned}
&= \sum_{n=0}^{\infty} \frac{1}{2} (-ia_n + b_n) e^{\frac{i n \pi x}{a}} + \sum_{n=0}^{\infty} \frac{1}{2} (ia_n + b_n) e^{-\frac{i n \pi x}{a}} \\
&= \frac{1}{2} (-ia_0 + b_0) + \frac{1}{2} (ia_0 + b_0) + \sum_{n=1}^{\infty} \frac{1}{2} (-ia_n + b_n) e^{\frac{i n \pi x}{a}} + \sum_{n=1}^{\infty} \frac{1}{2} (ia_n + b_n) e^{-\frac{i n \pi x}{a}} \\
&= \sum_{n=1}^{\infty} \frac{1}{2} (-ia_n + b_n) e^{\frac{i n \pi x}{a}} + b_0 e^{\frac{i \cdot 0 \cdot \pi x}{a}} + \sum_{n=-1}^{-\infty} \frac{1}{2} (ia_{-n} + b_{-n}) e^{+\frac{i n \pi x}{a}} \\
&= \sum_{n=-\infty}^{-1} \frac{1}{2} (ia_{-n} + b_{-n}) e^{+\frac{i n \pi x}{a}} + b_0 e^{\frac{i \cdot 0 \cdot \pi x}{a}} + \sum_{n=1}^{\infty} \frac{1}{2} (-ia_n + b_n) e^{\frac{i n \pi x}{a}} \\
&= \sum_{n=-\infty}^{\infty} c_n e^{\frac{i n \pi x}{a}}
\end{aligned}$$

Problem B. (From: Int. to Q. M. 2nd edn. D. J. Griffiths Problem 2.20 (b)):

Show that: $c_n = \frac{1}{2a} \int_{-a}^{+a} f(x) e^{-\frac{i n \pi x}{a}} dx \dots\dots\dots$ (B)

Ans.: $f(x) = \sum_{n=-\infty}^{\infty} c_n e^{\frac{i n \pi x}{a}}$

$$\int_{-a}^a f(x) e^{-\frac{i m \pi x}{a}} dx = \sum_{n=-\infty}^{\infty} \int_{-a}^a c_n e^{\frac{i n \pi x}{a}} e^{-\frac{i m \pi x}{a}} dx = \sum_{n=-\infty}^{\infty} \int_{-a}^a c_n e^{\frac{i(n-m)\pi x}{a}} dx \dots\dots\dots (X)$$

For $n = m$,

$$\int_{-a}^a c_n e^{\frac{i(n-m)\pi x}{a}} dx = \int_{-a}^a c_m e^0 dx = 2ac_m$$

For $n \neq m$,

$$\begin{aligned}
\int_{-a}^a c_n e^{\frac{i(n-m)\pi x}{a}} dx &= \frac{a}{i(n-m)\pi} c_n \left[e^{\frac{i(n-m)\pi a}{a}} - e^{-\frac{i(n-m)\pi a}{a}} \right] = \frac{a}{i(n-m)\pi} c_n [e^{i(n-m)\pi} - e^{-i(n-m)\pi}] \\
&= \frac{a}{i(n-m)\pi} c_n [(-1)^{(n-m)} - (-1)^{-(n-m)}] \quad (\text{Since } e^{i\pi} = -1) \\
&= 0
\end{aligned}$$

Therefore all the terms of the summation of the r.h.s of (X) vanish except for $n = m$ and:

$$\int_{-a}^a f(x) e^{-\frac{i m \pi x}{a}} dx = \sum_{n=-\infty}^{\infty} \int_{-a}^a c_n e^{\frac{i(n-m)\pi x}{a}} dx = 2ac_m.$$

$$\text{Hence } c_n = \frac{1}{2a} \int_{-a}^a f(x) e^{-\frac{i n \pi x}{a}} dx.$$

Problem C. (From: Int. to Q. M. 2nd edn. D. J. Griffiths Problem 2.20 (c)):

Let $k = \frac{n\pi}{a}$, Δk is the increment in k for increment in n by 1 and $c_n = \frac{1}{a} \sqrt{\frac{\pi}{2}} F(k)$. Show that (A) and (B) reduce to:

$$f(x) = \frac{1}{\sqrt{2\pi}} \sum_{n=-\infty}^{\infty} F(k) e^{ikx} \Delta k \dots\dots\dots (C) \quad \text{and} \quad F(k) = \frac{1}{\sqrt{2\pi}} \int_{-a}^{+a} f(x) e^{-ikx} dx. \dots\dots\dots (D)$$

Ans.: We have $f(x) = \sum_{n=-\infty}^{\infty} c_n e^{\frac{i n \pi x}{a}}$

With the substitutions $k = \frac{n\pi}{a}$, and $c_n = \frac{1}{a} \sqrt{\frac{\pi}{2}} F(k)$ we have:

$$f(x) = \sum_{n=-\infty}^{\infty} \frac{1}{a} \sqrt{\frac{\pi}{2}} F(k) e^{ikx} = \frac{1}{\sqrt{2\pi}} \sum_{n=-\infty}^{\infty} \frac{1}{a} \sqrt{2\pi} \sqrt{\frac{\pi}{2}} F(k) e^{ikx} = \frac{1}{\sqrt{2\pi}} \sum_{n=-\infty}^{\infty} \frac{\pi}{a} F(k) e^{ikx}$$

Now Δk is the increment in k for increment in n by 1. i.e. $\Delta k = \frac{\pi}{a}$. Then:

$$f(x) = \frac{1}{\sqrt{2\pi}} \sum_{n=-\infty}^{\infty} \frac{\pi}{a} F(k) e^{ikx} = \frac{1}{\sqrt{2\pi}} \sum_{n=-\infty}^{\infty} F(k) e^{ikx} \Delta k. \dots\dots (C)$$

$$\text{Also we have: } c_n = \frac{1}{2a} \int_{-a}^a f(x) e^{-\frac{in\pi x}{a}} dx \Rightarrow \frac{1}{a} \sqrt{\frac{\pi}{2}} F(k) = \frac{1}{2a} \int_{-a}^a f(x) e^{-ikx} dx$$

$$\Rightarrow F(k) = \frac{1}{2a} a \sqrt{\frac{2}{\pi}} \int_{-a}^a f(x) e^{-ikx} dx = \frac{1}{\sqrt{2\pi}} \int_{-a}^a f(x) e^{-ikx} dx \dots\dots (D)$$

Problem D. (From: Int. to Q. M. 2nd edn. D. J. Griffiths Problem 2.20 (d)):

Show that for $a \rightarrow \infty$ (C) and (D) reduce to:

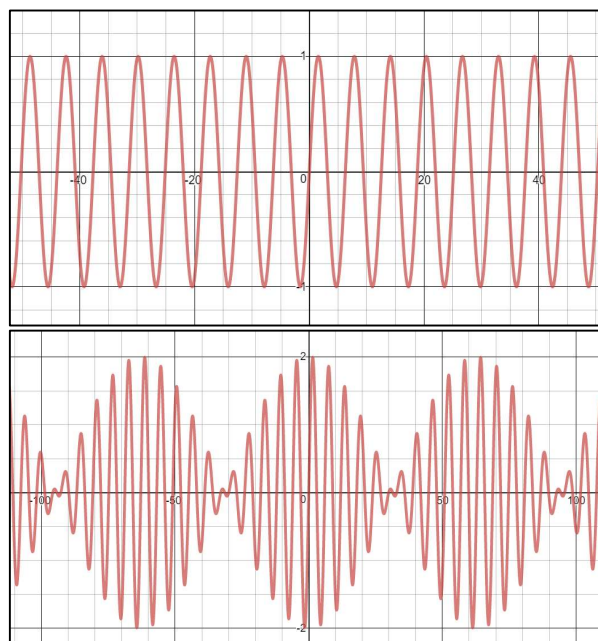
$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} F(k) e^{ikx} dk \dots\dots (E) \text{ and } F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} f(x) e^{-ikx} dx. \dots\dots (F)$$

Ans.: For $a \rightarrow \infty$, from (D) we have: $F(k) = \frac{1}{\sqrt{2\pi}} \int_{-a}^a f(x) e^{-ikx} dx = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} f(x) e^{-ikx} dx$

From (C) $f(x) = \frac{1}{\sqrt{2\pi}} \sum_{n=-\infty}^{\infty} F(k) e^{ikx} \Delta k$. Now for $a \rightarrow \infty$, $\Delta k = \frac{\pi}{a} \rightarrow 0$. Therefore the summation is to be replaced by integration: $f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} F(k) e^{ikx} dk$.

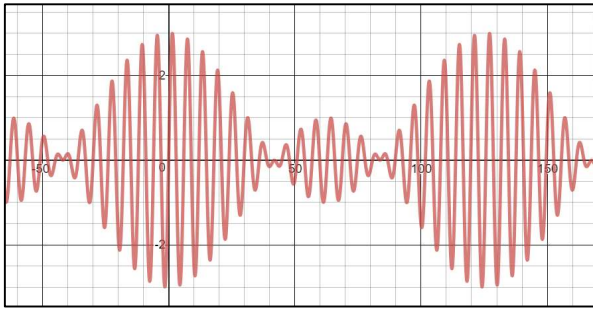
Wave Packet:

Now let us plot the wave obtained by adding sine waves having uniformly varying propagation constants within a finite range [for example, we may take $1 \leq k \leq 1.1$] i.e. $\sum \sin kx$, where $1 \leq k \leq 1.1$. We see that [Fig.1-7] the resultant wave is a series of wave groups. As the number of component waves within the finite range of propagation constants increases, the resultant wave groups increase in height, decrease in width and the separation between the groups increases. The small wave groups in between can be neglected in the present discussion since they decrease in height and thus become insignificant with increase in the number of component waves. If the number of component waves tends to infinity then the separation between the groups will increase to infinity and we will get a single wave group or wave packet. The height of the group or packet will be very large and width will be very small. If the resultant wave represents the wave function of a particle, then the probability density of the particle, i.e. the square of the resultant wave function will be very high at a very narrow region i.e. within the width of the wave group and the particle will be well localised.

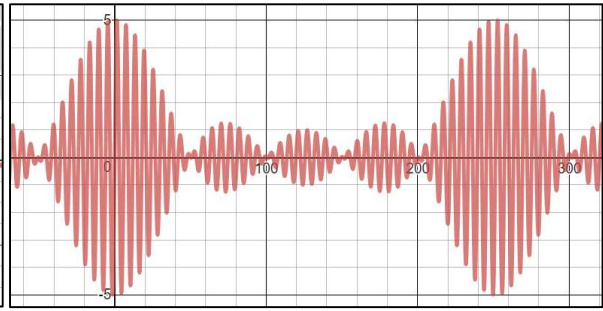


$y = \sin(x)$

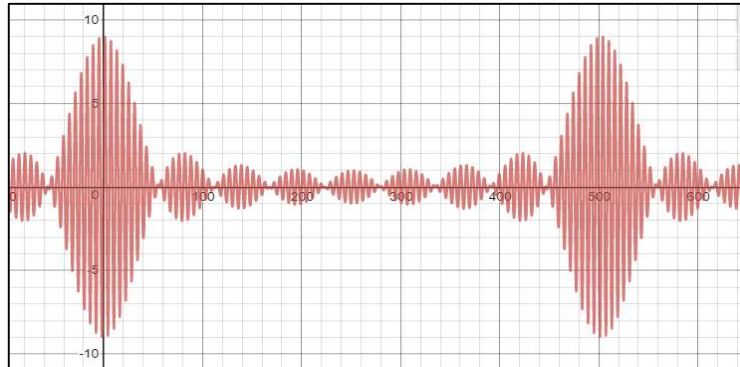
$y = \sin(x) + \sin(1.1x)$



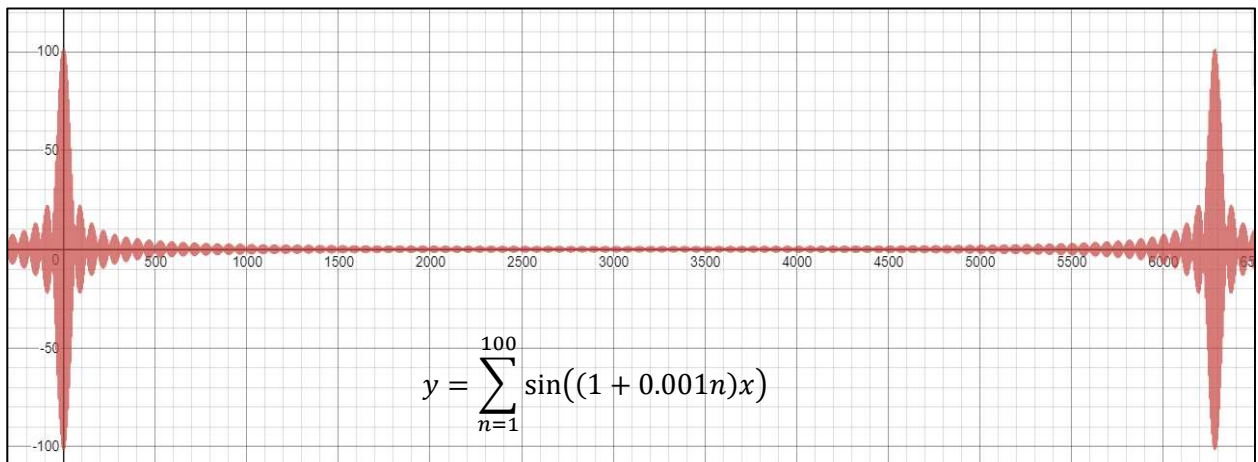
$$y = \sin(x) + \sin(1.05x) + \sin(1.1x) + \sin(1.1x)$$



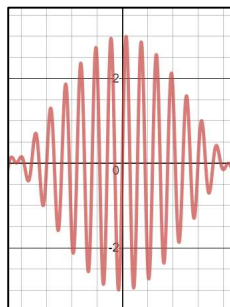
$$y = \sin(x) + \sin(1.025x) + \sin(1.05x) + \sin(1.075x) + \sin(1.1x)$$



$$y = \sin(x) + \sin(1.0125x) + \sin(1.025x) + \sin(1.0375x) + \sin(1.05x) + \sin(1.0625x) + \sin(1.075x) + \sin(1.0875x) + \sin(1.1x)$$



We see that the wave packet is composed of waves of smaller wavelength modulated by a profile or envelope which gives the shape of the group (Fig.-8).



QQ: Let two superposing sine waves have wave lengths λ_1 and λ_2 . Let at any particular instant of time their peaks coincide at $x = 0$. Show that at the same instant their peaks will also coincide at:

$$x = n \times \text{LCM}(\lambda_1, \lambda_2), \text{ where } n \text{ is an integer.}$$

From the problems (A) to (D) it is clear that the set of sine waves forming the above wave groups can be obtained as special case from $f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} F(k)e^{ikx} dk$ in proceeding back from problem (D) to (A) i.e. from $f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} F(k)e^{ikx} dk$ to $f(x) = \sum_{n=0}^{\infty} \left[a_n \sin\left(\frac{n\pi x}{a}\right) + b_n \cos\left(\frac{n\pi x}{a}\right) \right]$ and by suitably choosing n and the coefficients a_n and b_n . Therefore $\Psi(x, 0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \varphi(k)e^{ikx} dk$ represents a localised wave packet or group, whose shape depends on $\varphi(k)$ and may be different from those given in the above figures. This will be clear from the following problems (E) & (F). However since the wave packet

Problem E. (From: Int. to Q. M. 2nd edn. D. J. Griffiths Problem 2.21):

A free particle has initial wave function $\Psi(x, 0) = Ae^{-a|x|}$, where A and a are constants with a a real and positive.

- (i) Normalise $\Psi(x, 0)$.
- (ii) Find $\Psi(x, t)$ in integral form.
- (iii) Discuss the cases for a very large and a very small.

Ans.: (i) Normalise $\Psi(x, 0)$:

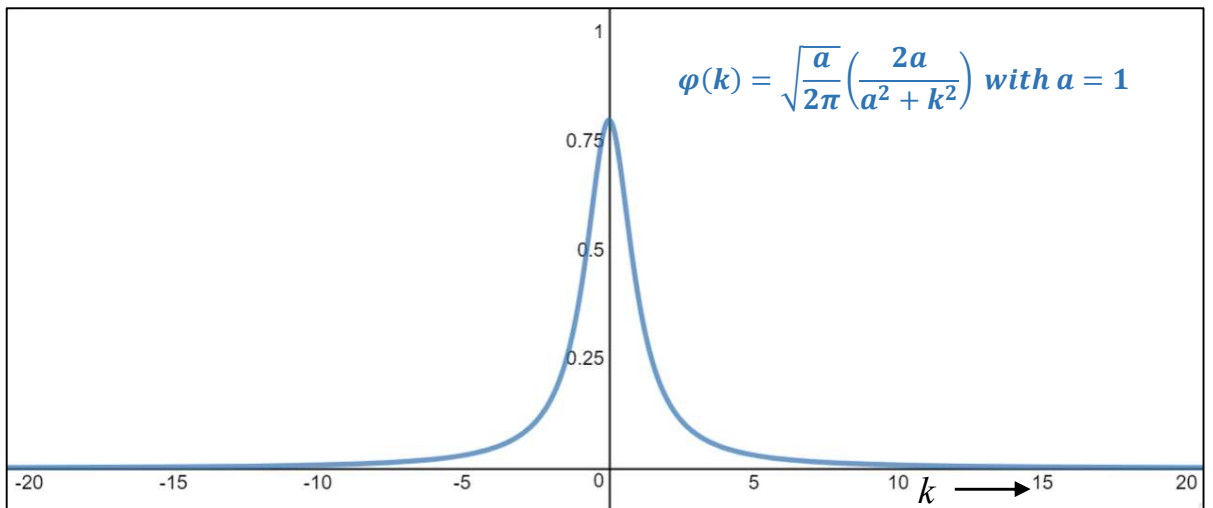
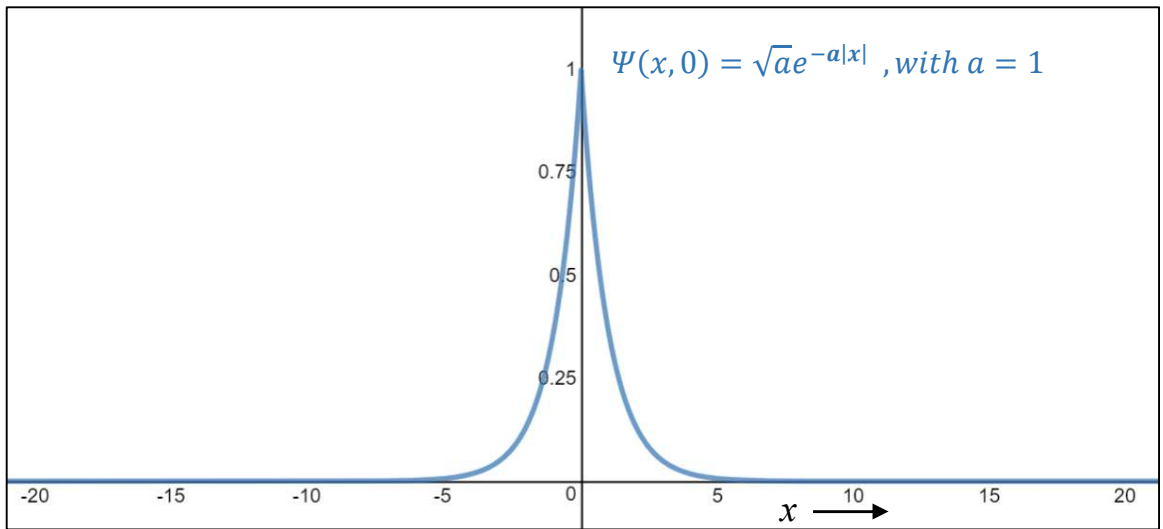
$$\begin{aligned} \int_{-\infty}^{+\infty} |\Psi(x, 0)|^2 dx &= 1 \Rightarrow A^2 \int_{-\infty}^{+\infty} e^{-2a|x|} dx = 1 \\ \Rightarrow A^2 \left(\int_{-\infty}^0 e^{2ax} dx + \int_0^{+\infty} e^{-2ax} dx \right) &= 1 \Rightarrow A^2 \frac{1}{2a} \left(\int_{-\infty}^0 e^y dy + \int_0^{+\infty} e^{-y} dy \right) = 1 \\ \Rightarrow A^2 \frac{1}{2a} \left([e^y]_{-\infty}^0 - [e^{-y}]_0^{+\infty} \right) &= 1 \\ \Rightarrow A^2 \frac{1}{2a} (e^0 - e^{-\infty} - e^{-\infty} + e^0) &= 1 \\ \Rightarrow \frac{2A^2}{2a} = 1 \Rightarrow A &= \sqrt{a}. \end{aligned}$$

$$\text{So } \Psi(x, 0) = \sqrt{a}e^{-a|x|}.$$

$$\begin{aligned} \text{(ii) } \Psi(x, 0) &= \sqrt{a}e^{-a|x|} \\ \varphi(k) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \Psi(x, 0)e^{-ikx} dx = \frac{1}{\sqrt{2\pi}} \sqrt{a} \int_{-\infty}^{+\infty} e^{-a|x|} e^{-ikx} dx \\ &= \sqrt{\frac{a}{2\pi}} \left[\int_{-\infty}^0 e^{-(-ax+ikx)} dx + \int_0^{+\infty} e^{-(ax+ikx)} dx \right] \\ &= \sqrt{\frac{a}{2\pi}} \left(\frac{1}{a-ik} [e^{ax-ikx}]_{-\infty}^0 + \frac{1}{-(a+ik)} [e^{-(ax+ikx)}]_0^{+\infty} \right) \\ &= \sqrt{\frac{a}{2\pi}} \left(\frac{1}{a-ik} - \frac{1}{-(a+ik)} \right) \\ &= \sqrt{\frac{a}{2\pi}} \left(\frac{1}{a-ik} + \frac{1}{a+ik} \right) = \sqrt{\frac{a}{2\pi}} \left(\frac{2a}{a^2+k^2} \right) \\ \varphi(k) &= \sqrt{\frac{a}{2\pi}} \left(\frac{2a}{a^2+k^2} \right) \end{aligned}$$

$$\Psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \varphi(k)e^{i\left(kx - \frac{\hbar k^2}{2m}t\right)} dk = \frac{a^{3/2}}{\pi} \int_{-\infty}^{+\infty} \frac{1}{a^2+k^2} e^{i\left(kx - \frac{\hbar k^2}{2m}t\right)} dk$$

- (iii) For very large a , $\Psi(x, 0) = Ae^{-a|x|}$ is a very narrow spike at $x = 0$. But for small a , $\Psi(x, 0) = Ae^{-a|x|}$ is flat.



Problem F. (From: Int. to Q. M. 2nd edn. D. J. Griffiths Problem 2.22, with modification):

A free particle has initial wave function $\Psi(x, 0) = \frac{1}{(\pi\sigma_0^2)^{1/4}} e^{-\frac{1}{2\sigma_0^2}x^2} e^{ik_0x} = Ae^{-ax^2} e^{ik_0x}$, where A and a are constants with a real and positive.

- (i) Show that $\Psi(x, 0) = \frac{1}{(\pi\sigma_0^2)^{1/4}} e^{-\frac{1}{2\sigma_0^2}x^2} e^{ik_0x}$ is normalised.
- (ii) Normalise $\Psi(x, 0) = Ae^{-ax^2} e^{ik_0x}$ to show that $A = \left(\frac{2a}{\pi}\right)^{\frac{1}{4}}$.
- (iii) Plot $\text{Im}(\Psi(x, 0))$ and $|\Psi(x, 0)|$ for $a = 1, k_0 = 100$.
- (iv) Show that the expression of $\varphi(k)$ in the Fourier expansion of $\Psi(x, 0)$ is:

$$\varphi(k) = \frac{1}{\sqrt{2a}} \left(\frac{2a}{\pi}\right)^{\frac{1}{4}} e^{-\frac{(k-k_0)^2}{4a}}.$$
- (v) Plot $\varphi(k)$ vs. k for $a = 1$.
- (vi) Find the expression of $\Psi(x, t)$.
- (vii) Find the expression of $|\Psi(x, t)|^2$. Comment on it. Plot $|\Psi(x, t)|^2$ vs. t . What happens to $|\Psi(x, t)|^2$ as time goes on.

(viii) *At what time does the system come closest to uncertainty limit?*

Ans.: (i)

(ii) Normalise $\Psi(x, 0) = Ae^{-ax^2} e^{ik_0x}$:

$$\int_{-\infty}^{+\infty} |\Psi(x, 0)|^2 dx = 1 \Rightarrow A^2 \int_{-\infty}^{+\infty} e^{-2ax^2} dx = 1$$

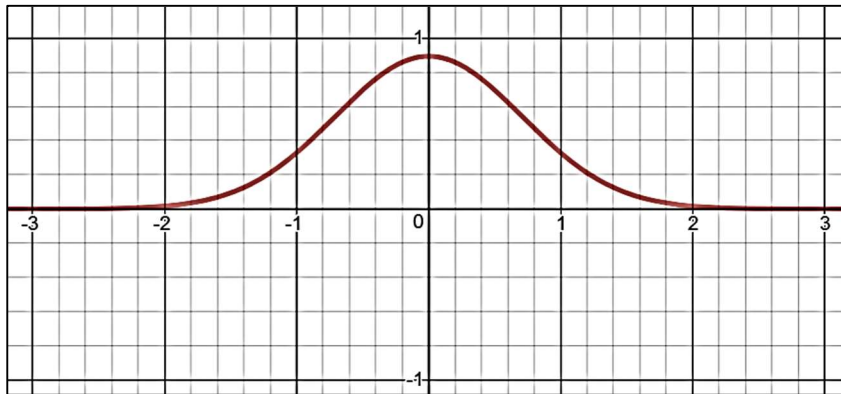
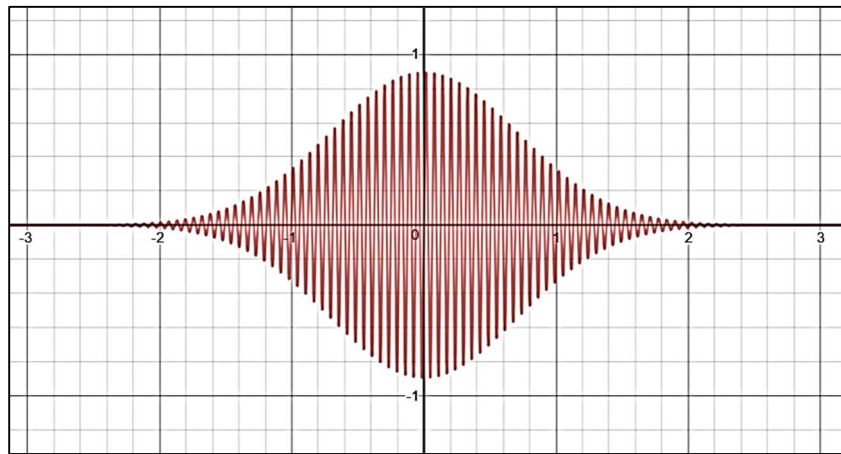
$$\text{Let } 2ax^2 = y \Rightarrow 4ax dx = dy \Rightarrow dx = \frac{dy}{4ax} = \frac{\sqrt{2a} dy}{4a\sqrt{y}} = \frac{y^{-1/2} dy}{2\sqrt{2a}}$$

$$\Rightarrow \frac{2A^2}{2\sqrt{2a}} \int_0^{+\infty} y^{1/2-1} e^{-y} dy = 1 \Rightarrow \frac{2A^2}{2\sqrt{2a}} \Gamma\left(\frac{1}{2}\right) = 1 \Rightarrow \frac{2A^2}{2\sqrt{2a}} \Gamma\left(\frac{1}{2}\right) \Rightarrow A = \left(\frac{2a}{\pi}\right)^{\frac{1}{4}}$$

(iii) $\Psi(x, 0) = \left(\frac{2a}{\pi}\right)^{\frac{1}{4}} e^{-ax^2} e^{ik_0x}$

$$\text{Im}(\Psi(x, 0)) = \left(\frac{2a}{\pi}\right)^{\frac{1}{4}} e^{-ax^2} \sin(k_0x) = \left(\frac{2}{\pi}\right)^{\frac{1}{4}} e^{-x^2} \sin(100x).$$

$$|\Psi(x, 0)| = \left(\frac{2a}{\pi}\right)^{\frac{1}{4}} e^{-ax^2} = \left(\frac{2}{\pi}\right)^{\frac{1}{4}} e^{-x^2}.$$



(iv) $\Psi(x, 0) = \left(\frac{2a}{\pi}\right)^{\frac{1}{4}} e^{-ax^2} e^{ik_0x}$

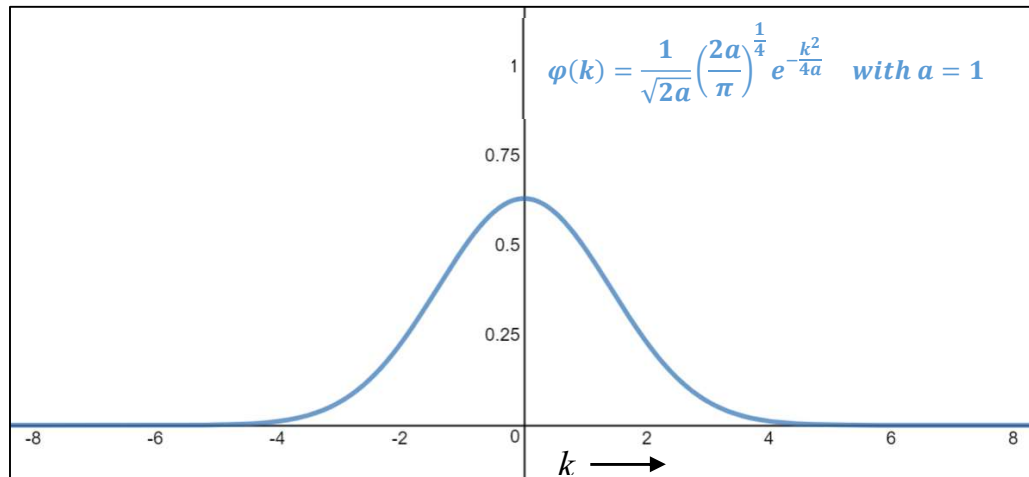
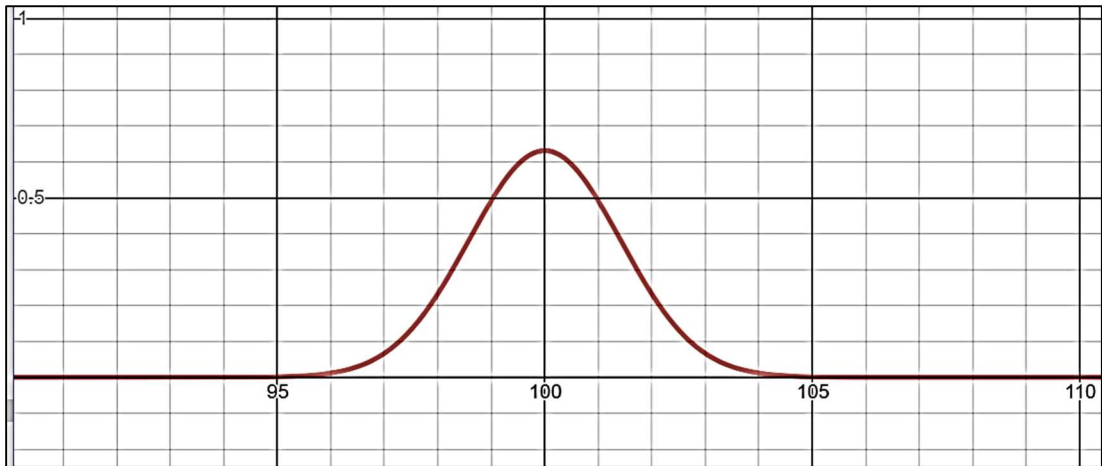
$$\varphi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \Psi(x, 0) e^{-ikx} dx = \frac{1}{\sqrt{2\pi}} \left(\frac{2a}{\pi}\right)^{\frac{1}{4}} \int_{-\infty}^{+\infty} e^{-ax^2} e^{-i(k-k_0)x} dx$$

$$= \frac{1}{\sqrt{2\pi}} \left(\frac{2a}{\pi}\right)^{\frac{1}{4}} \int_{-\infty}^{+\infty} e^{-[ax^2 + i(k-k_0)x]} dx$$

$$\int_{-\infty}^{+\infty} e^{-(ax^2+bx)} dx = \int_{-\infty}^{+\infty} e^{-a\left(x^2+\frac{b}{a}x\right)} dx = \int_{-\infty}^{+\infty} e^{-a\left(x^2+2x\frac{b}{2a}+\frac{b^2}{4a^2}\right)+\frac{b^2}{4a}} dx$$

$$= e^{\frac{b^2}{4a}} \int_{-\infty}^{+\infty} e^{-a\left(x+\frac{b}{2a}\right)^2} dx = \frac{2}{\sqrt{a}} e^{\frac{b^2}{4a}} \int_0^{\infty} e^{-y^2} dy = \frac{2}{\sqrt{a}} e^{\frac{b^2}{4a}} \frac{\sqrt{\pi}}{2} = \sqrt{\frac{\pi}{a}} e^{\frac{b^2}{4a}}$$

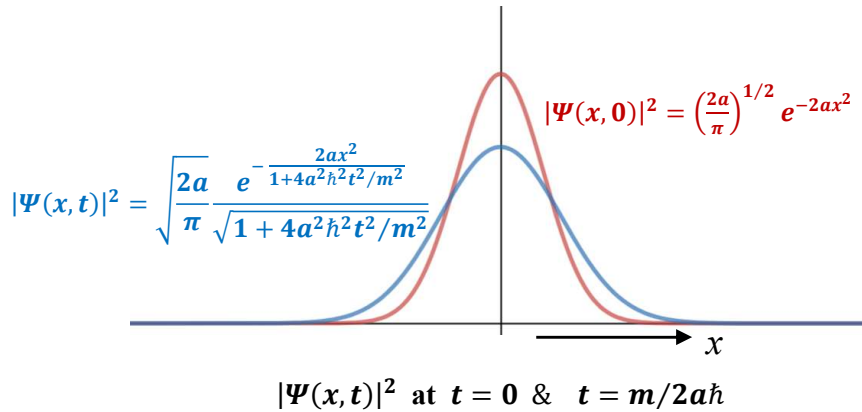
$$\varphi(k) = \frac{1}{\sqrt{2\pi}} \left(\frac{2a}{\pi}\right)^{\frac{1}{4}} \sqrt{\frac{\pi}{a}} e^{-\frac{(k-k_0)^2}{4a}} = \frac{1}{\sqrt{2a}} \left(\frac{2a}{\pi}\right)^{\frac{1}{4}} e^{-\frac{(k-k_0)^2}{4a}}.$$



$$\begin{aligned} \Psi(x, t) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \varphi(k) e^{i\left(kx - \frac{\hbar k^2}{2m}t\right)} dk = \frac{1}{\sqrt{2\pi}} \frac{1}{\sqrt{2a}} \left(\frac{2a}{\pi}\right)^{\frac{1}{4}} \int_{-\infty}^{+\infty} e^{-\frac{(k-k_0)^2}{4a}} e^{i\left(kx - \frac{\hbar k^2}{2m}t\right)} dk \\ &= \frac{1}{\sqrt{2\pi}} \frac{1}{\sqrt{2a}} \left(\frac{2a}{\pi}\right)^{\frac{1}{4}} \int_{-\infty}^{+\infty} e^{-\left(\frac{i\hbar t}{2m} + \frac{1}{4a}\right)k^2 - \left(ix + \frac{k_0}{2a}\right)k + \frac{k_0^2}{4a}} dk \\ &= \frac{1}{\sqrt{2\pi}} \frac{1}{\sqrt{2a}} \left(\frac{2a}{\pi}\right)^{\frac{1}{4}} e^{-\frac{k_0^2}{4a}} \int_{-\infty}^{+\infty} e^{-\left(\frac{i\hbar t}{2m} + \frac{1}{4a}\right)k^2 - \left(ix + \frac{k_0}{2a}\right)k} dk \\ &= \frac{1}{\sqrt{2\pi}} \frac{1}{\sqrt{2a}} \left(\frac{2a}{\pi}\right)^{\frac{1}{4}} e^{-\frac{k_0^2}{4a}} \sqrt{\frac{\pi}{\left(\frac{i\hbar t}{2m} + \frac{1}{4a}\right)}} e^{\left(ix + \frac{k_0}{2a}\right)^2 / 4\left(\frac{i\hbar t}{2m} + \frac{1}{4a}\right)} \\ &= \left(\frac{2a}{\pi}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2\pi}} \frac{1}{\sqrt{2a}} e^{-\frac{k_0^2}{4a}} \sqrt{\frac{4a\pi}{1 + 2ai\hbar t/m}} e^{a\left(ix + \frac{k_0}{2a}\right)^2 / (1 + 2ai\hbar t/m)} \\ &= \left(\frac{2a}{\pi}\right)^{\frac{1}{4}} e^{-\frac{k_0^2}{4a}} \frac{1}{\sqrt{1 + 2ai\hbar t/m}} e^{a\left(-x^2 + \frac{ix}{a} + \frac{k_0^2}{4a^2}\right) / (1 + 2ai\hbar t/m)} \end{aligned}$$

$$\begin{aligned}
&= \left(\frac{2a}{\pi}\right)^{\frac{1}{4}} \frac{1}{\sqrt{1+2ai\hbar t/m}} e^{\frac{a\left(-x^2+\frac{ix_0}{a}+\frac{k_0^2}{4a^2}\right)-(1+2ai\hbar t/m)\frac{k_0^2}{4a}}{(1+2ai\hbar t/m)}} \\
&= \left(\frac{2a}{\pi}\right)^{\frac{1}{4}} \frac{1}{\sqrt{1+2ai\hbar t/m}} e^{\frac{a\left(-x^2+\frac{ixk_0}{a}\right)-\frac{i\hbar k_0^2 t}{2m}}{(1+2ai\hbar t/m)}} \\
&= \frac{1}{\sqrt{2\pi}} \frac{1}{\sqrt{2a}} \left(\frac{2a}{\pi}\right)^{\frac{1}{4}} \sqrt{\frac{\pi}{\left(\frac{i\hbar t}{2m}+\frac{1}{4a}\right)}} e^{-\frac{x^2}{4\left(\frac{i\hbar t}{2m}+\frac{1}{4a}\right)}} = \left(\frac{2a}{\pi}\right)^{1/4} \frac{e^{-ax^2/(1+2ai\hbar t/m)}}{\sqrt{1+2ai\hbar t/m}}.
\end{aligned}$$

(iii) $|\Psi(x, t)|^2 = \left(\frac{2a}{\pi}\right)^{1/2} \frac{e^{-[ax^2/(1+2ai\hbar t/m)+ax^2/(1-2ai\hbar t/m)]}}{\sqrt{(1+2ai\hbar t/m)(1-2ai\hbar t/m)}} = \left(\frac{2a}{\pi}\right)^{1/2} \frac{e^{-2ax^2/(1+4a^2\hbar^2 t^2/m^2)}}{\sqrt{1+4a^2\hbar^2 t^2/m^2}}.$



Phase velocity, group velocity and particle velocity:

Phase velocity:

Eigen functions of free particle: $\psi_k(x, t) = A_k e^{i(kx - \omega t)}$; where $k = \frac{p}{\hbar}$, $\omega = \frac{E}{\hbar}$, $E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$.
Let the wave form, which was at position x at time t , appears at position $x + dx$ at time $t + dt$.
In other words:

$$\psi_k(x, t) = \psi_k(x + dx, t + dt),$$

$$\text{Or, } A_k e^{i\left(kx - \frac{E}{\hbar}t\right)} = A_k e^{i\left(k(x+dx) - \frac{E}{\hbar}(t+dt)\right)}$$

$$\text{Or, } k(x + dx) - \frac{E}{\hbar}(t + dt) = kx - \frac{E}{\hbar}t;$$

$$\text{Or, } v_p = \frac{dx}{dt} = \frac{E}{\hbar k} = \frac{\hbar^2 k^2 / 2m}{\hbar k} = \frac{\hbar k}{2m} = \frac{p}{2m} = \frac{v}{2}.$$

Thus the velocity of the wave form, or phase velocity, is equal to half of the particle velocity.

We see that the phase velocity of the monochromatic (particular k) eigen functions of the free particle is half of the particle velocity. Now let us calculate the group velocity i.e. the velocity of the envelope of the wave group or packet in the following cases:

Group velocity:

1. Wave packet composed of two plane waves: Consider two sine waves of equal amplitudes but slightly different propagation constants and frequencies –

$$\psi_1(x, t) = A \sin(kx + \omega t) \text{ and}$$

$$\psi_2(x, t) = A \sin((k + dk)x + (\omega + d\omega)t)$$

The wave group formed by these waves will be: $\psi_1(x, t) = \sin(kx + \omega t)$ and

$$\psi = \psi_1(x, t) + \psi_2(x, t) = A \sin(kx + \omega t) + A \sin((k + dk)x + (\omega + d\omega)t)$$

$$= 2A \sin\left[\left(k + \frac{dk}{2}\right)x + \left(\omega + \frac{d\omega}{2}\right)t\right] \cos\left(\frac{dk}{2}x + \frac{d\omega}{2}t\right)$$

$$\approx 2A \sin(kx + \omega t) \cos\left(\frac{dk}{2}x + \frac{d\omega}{2}t\right)$$

$$= 2A \cos\left(\frac{dk}{2}x + \frac{d\omega}{2}t\right) \sin(kx + \omega t)$$

This is not a plane wave, but a sine wave $[\sin(kx + \omega t)]$ of propagation constant k and frequency ω whose amplitude is modulated or enveloped by the function $2A \cos\left(\frac{dk}{2}x + \frac{d\omega}{2}t\right)$.

The $\sin(kx + \omega t) = \sin k\left(x + \frac{\omega}{k}t\right)$ part oscillates with frequency ω and moves with velocity ω/k as the component waves but its amplitude or envelope $2A \cos\left(\frac{dk}{2}x + \frac{d\omega}{2}t\right) =$

$2A \cos\frac{dk}{2}\left(x + \frac{d\omega}{dk}t\right)$ is slowly varying with small frequency $d\omega/2$ moves with velocity $\frac{d\omega}{dk}$.

$v_{ph} = \omega/k$ represents the velocity of the phase of the part $\sin k\left(x + \frac{\omega}{k}t\right)$ and is called the

phase velocity and $v_g = \frac{d\omega}{dk}$ represents the velocity of the envelope of the wave and is called the group velocity of the wave.

2. Fourier Packet:

$$\Psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \varphi(k) e^{i(kx - \omega t)} dk, \text{ where propagation vector } \mathbf{k} = \frac{\mathbf{p}}{\hbar}$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \varphi(k) e^{i\left(\frac{p}{\hbar}x - \frac{E}{\hbar}t\right)} dk$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \varphi(k) e^{i\left(kx - \frac{\hbar k^2}{2m}t\right)} dk$$

Given:

The Gaussian wave packet $\Psi(x, 0) = Ae^{-ax^2}$ can be written in terms of Fourier transform as:

$$\Psi(x, 0) = Ae^{-ax^2} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \varphi(k) e^{ikx} dk, \text{ with } \varphi(k) = \frac{1}{\sqrt{2a}} \left(\frac{2a}{\pi}\right)^{\frac{1}{4}} e^{-\frac{k^2}{4a}}.$$

Where $\psi_k(x) = e^{ikx}$ are plane wave solutions of the Schrodinger eqn. for a free particle.

Question:

Let: $J_k = \frac{i\hbar}{2m} \left(\psi_k \frac{d\psi_k^*}{dx} - \psi_k^* \frac{d\psi_k}{dx} \right)$ and $J = \frac{i\hbar}{2m} \left(\Psi \frac{d\Psi^*}{dx} - \Psi^* \frac{d\Psi}{dx} \right)$ and in a problem of step potential $R_k = \frac{|J_{rk}|}{|J_{ik}|}$, $T_k = \frac{|J_{tk}|}{|J_{ik}|}$ and $R = \frac{|J_r|}{|J_i|}$, $T = \frac{|J_t|}{|J_i|}$.

Verify whether: $R_k = R$, $T_k = T$.