Engineering Physics

Quantum Theory and Quantum Mechanics

Study material

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Part-1: Quantum theory

Electromagnetic wave

Electromagnetic waves/radiation are oscillating electric and magnetic fields.

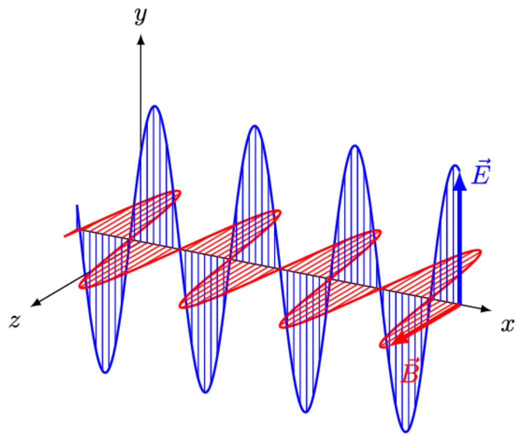
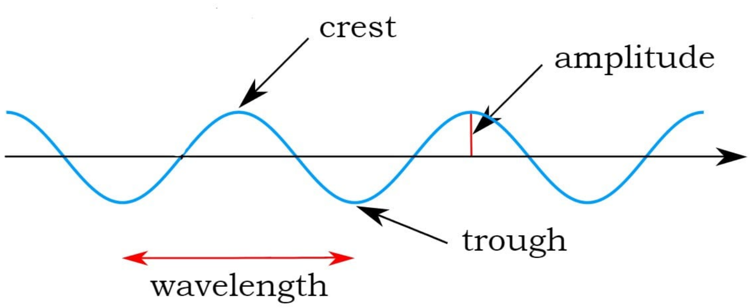
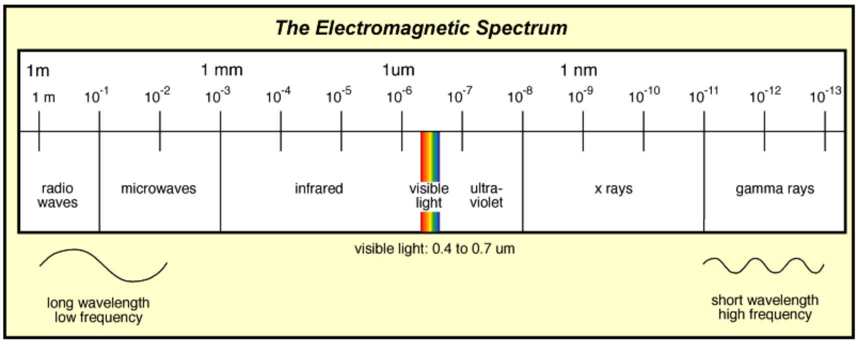


Figure 1: EM wave.



Relation between speed of wave, wavelength and frequency:

$$c = \lambda\nu \implies \lambda = \frac{c}{\nu} \implies \nu = \frac{c}{\lambda}. \tag{1}$$



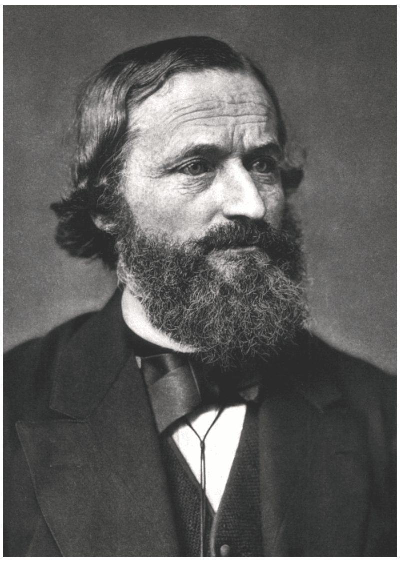
What happens when radiation falls on matter?

Three things can happens:

- Absorption:
  Matter takes up the energy of radiation falling on it.
- Transmission:
  Radiation hits an object and radiation penetrates through the material to travel all the way through.
- Reflection:
  Bouncing back of radiation from the surface of an object.

Any object whose temperature is above zero kelvin (0 K) must emit radiation.

Blackbody



Gustav Kirchhoff (1824 – 1887)

- Kirchhoff in 1860 introduced the theoretical concept of a perfect/ideal blackbody.
- A perfect **blackbody** is a body which absorbs all the incident radiation (of any wavelength) falling on it. It neither reflects nor transmits radiation falling on it.
- For a perfect blackbody, reflectance $(R) = 0$, transmittance $(T) = 0$ & absorptance $(A) = 1$. $(R + T + A = 1)$
- A blackbody absorbs more radiation than any other body at a given temperature. Blackbody is a **perfect absorber**.
- Because blackbody does not reflect any light, it is visually black. All blackbodies are visually black, but all visually black objects are not blackbodies.
- Objects painted with platinum black, gold black, etc absorb radiation like a blackbody.
- Any body with temperature $T > 0\,\mathrm{K}$ must emit radiation. This is also true for a blackbody.

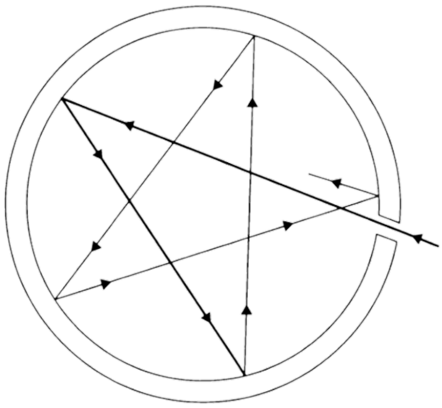


Figure 2: A cavity kept at a constant temperature and having blackened interior walls is connected to the outside by a small hole. To an outside observer, this small hole appears like a blackbody surface.

- At thermal equilibrium, maximum amount of radiation is emitted by a blackbody (otherwise its temperature will change).
- At thermal equilibrium, a blackbody emits more radiation than any other body at a given temperature. Blackbody is a **perfect emitter**. Radiation emitted by blackbody is called **blackbody radiation**.
- Heated tungsten filament, stars, etc emit radiation like a blackbody.

Blackbody radiation

- Kirchhoff proved that the flux of radiation in the cavity is same in all directions. **Blackbody radiation is isotropic**.
- **Blackbody radiation is homogeneous**, namely the same at every point inside the cavity.
- The above two statements are true for any wavelength λ.

Josef Stefan Ludwig Boltzmann

Stefan-Boltzmann law

The energy emitted by a perfect blackbody across all wavelength per unit area per unit time is proportional to fourth power of absolute temperature.

$$R = \sigma T^4. \tag{2}$$

Total emissive power (or total emittance) R has the units of $\mathrm{Wm^{-2}}$.
Stefan's constant $\sigma = 5.67 \times 10^{-8}\,\mathrm{Wm^{-2}K^{-4}}$.

Problem

What is the energy radiated by a blackbody per unit area per unit time which is at a temperature of $T = 1000\,\mathrm{K}$. (Given Stefan's constant $\sigma = 5.67 \times 10^{-8}\,\mathrm{Wm^{-2}K^{-4}}$.)

Solution

Given:
$T = 1000\,\mathrm{K}$.
$\sigma = 5.67 \times 10^{-8}\,\mathrm{Wm^{-2}K^{-4}}$.
Formula:

$$R = \sigma T^4$$
$$R = 5.67 \times 10^{-8} \times (1000)^4$$
$$R = 56\,700\,\mathrm{Wm^{-2}}.$$

Blackbody spectrum

The energy radiated by a blackbody per unit area per unit time for a given temperature and given wavelength, $R(\lambda, T)$ is plotted against wavelength.

- For a given temperature, $R(\lambda, T)$ first increases, reaches a maximum then decreases. We get a bell shaped curve.
- When the curve is drawn for a lesser temperature, height of the curve decreases i.e., $R(\lambda, T)$ corresponding to maximum decreases with decrease in temperature.
- As temperature is lowered, the wavelength corresponding to peak of the curve λ_{max} increases.

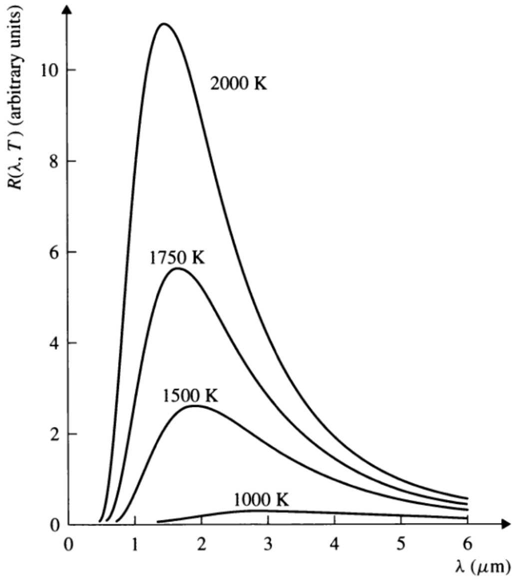


Figure 3: Blackbody spectrum

Wien's displacement law

The wavelength corresponding to where maximum of $R(\lambda, T)$ occurs is inversely proportional to the temperature T of the blackbody.

$$\lambda_{\text{max}} = \frac{b}{T}, \tag{3}$$

Wein's displacement constant $b = 2.898 \times 10^{-3}$ mK.

It is more convenient to define monochromatic energy density (energy per unit volume) or **spectral distribution function** $\rho(\lambda, T)$.

$$\rho(\lambda, T) = \frac{4}{c} R(\lambda, T). \tag{4}$$

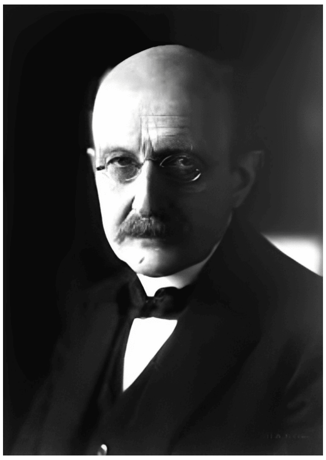
Why we get bell shaped curve for graph of $\rho(\lambda, T)$ versus λ?.
What is the explanation for Wien's displacement law?
How do we account for the blackbody spectrum?
To answer these question we need an expression for $\rho(\lambda, T)$.

$$\rho(\lambda, T) = \lambda^{-5} f(\lambda T) \qquad \text{(Wien's law)}. \tag{5}$$

- Many attempts were made by several physicists to find the form of $\rho(\lambda, T)$.

- Using classical physics; Lord Rayleigh, Sir James Jeans, W. Wien and others give expressions for $\rho(\lambda, T)$ to explain blackbody spectrum. But, they were only partially correct and insufficient.

Planck's radiation law



Max Planck (1858-1947)

In 1900, Max Planck guessed the correct form of $\rho(\lambda, T)$ which correctly fit the experimental data.

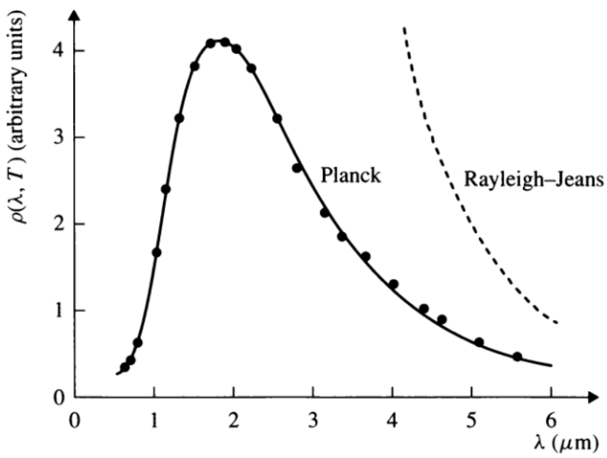


Figure 4: Planck's law fits observed data.

Later, Planck using assumptions outside classical physics, derived the expression for $\rho(\lambda, T)$ (This is the birth of quantum physics).

- The atoms in the walls of the cavity, are treated as harmonic oscillators. Each atom is an electric dipole which vibrates (oscillates) when radiation falls on it.

- Planck postulated that the energy of an oscillator of a given frequency ν cannot take arbitrary values, but can only take on the discrete values nE (where $n = 0, 1, 2, 3, \dots$), E is a fixed amount of energy which must be proportional to frequency ν to satisfy Wien's law.

- The atoms in the walls of the cavity do not absorb radiation continuously. They absorb energy of radiation in discrete units (in the form of packets), i.e., they absorb energy equal to $E, 2E, 3E, \dots$.

$$E = h\nu, \tag{6}$$

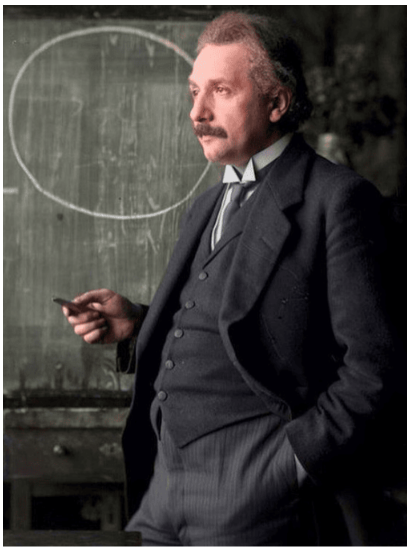
  h is called **Planck's constant**.

- Using the above considerations, Planck derived the expression for $\rho(\lambda, T)$:

$$\rho(\lambda, T) = \frac{8\pi hc}{\lambda^5} \frac{1}{\exp\left(\dfrac{hc}{\lambda kT}\right) - 1}. \tag{7}$$

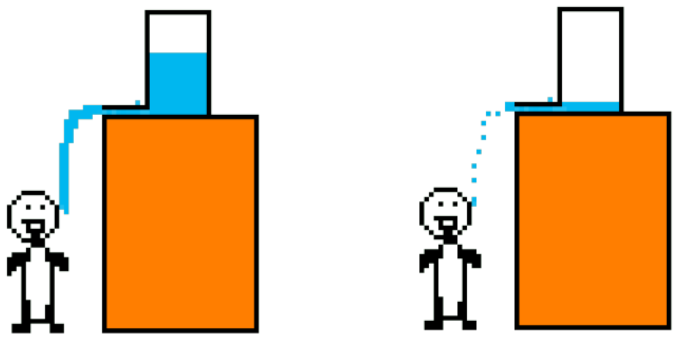
Here $k = 1.38 \times 10^{-23}\,\mathrm{JK}^{-1}$ is Boltzmann constant and $h = 6.626 \times 10^{-34}\,\mathrm{Js}$.

Einstein's extension of Planck's idea



Albert Einstein (1879-1955)

- In Planck's theory, the oscillators representing the EM field could only vibrate with energies given by $nE = nh\nu$.
- Einstein took this idea one step ahead. He said that EM field itself was quantized.
- Planck postulated that, the radiation absorbed by the atoms in walls of the cavity is absorbed (or emitted) not continuously, but is absorbed (or emitted) in the form of packets, hence the oscillators have energy which are quantized.
- But Einstein's argument was that, it is not that radiation is absorbed (or emitted) in the form of packets, radiation itself comes in the form of packets. That is, energy of radiation is quantized.
- This means that radiation has particle nature as well.



(a) Planck's idea (b) Einstein's idea

The photon concept

- Energy of radiation cannot be any arbitrary value. Only certain discrete values are allowed.
- Energy comes in discrete units or packets called **quanta** (*Quantum - singular, Quanta - plural.*) In the case of light they are called **photons** (The quantum of radiation is called photon).
- The energy of each packet (or photon) is $E = h\nu$. Here ν is the frequency of radiation.
- Energy of one photon is $h\nu$, energy of two photons is $2h\nu$, energy of three photons is $3h\nu$. In general if there are n photons, the energy of radiation is $nh\nu$, where $n = 0, 1, 2, 3, \ldots$.

What is quantization?

What is this quantization? Explain again. Quantum scooter (Hypothetical example) Let us say, there is a scooter which can go at only certain allowed speed (multiples of 10). The scooter can go at $0\,\mathrm{km/hr}, 10\,\mathrm{km/hr}, 20\,\mathrm{km/hr}, \ldots,$ but cannot travel at in between speeds like $15\,\mathrm{km/hr}$. The speed of the scooter is $v_n = 10n$, where n is an integer. We say the speed of the scooter is quantized.

Photons have momentum

- Einstein in 1905 also showed that, a particle with mass has energy equivalent to its mass. The energy of a particle equivalent to its mass is called rest mass energy or **rest energy**.
- Rest energy of a particle of mass m is given by

$$\text{Rest energy} = mc^2. \tag{8}$$

- When a particle of mass m, having momentum p is moving with very high speed (close to the speed of light) its total energy E (kinetic energy + rest energy) is given by

$$E^2 = p^2c^2 + m^2c^4 \implies E = \sqrt{p^2c^2 + m^2c^4}. \tag{9}$$

- For a massless particle like photon, rest energy is zero.
- For a photon, $m = 0$. Using this in equation (36), one gets the energy of photon as

$$E^2 = p^2c^2 \tag{10}$$

$$\implies p = \frac{E}{c} = \frac{h\nu}{c} = \frac{h}{\lambda}. \tag{11}$$

- Photons have momentum like particles. While momentum of particles with mass is mv. Photon's momentum depends on wavelength or frequency.

Some properties of photon

1. Quantum of radiation is called photon (particle of light).
2. It has no rest mass.
3. It has no electric charge.

4. In vacuum, they travel at a fixed speed $c = 3 \times 10^8\,\mathrm{ms^{-1}}$.

5. Because it has no electric charge, they do not interact with electric or magnetic field.

6. More the frequency of radiation, more is the photon's energy. Blue photon has more energy than red photon. X-ray photon has more energy than UV photon.

7. They have dual nature i.e., wave-like properties and particle-like properties.

How important is the concept of photon?

- The concept of photon was introduced by Einstein in 1905 and it explained the experimental observations of Photoelectric effect.
- Later, Einstein was awarded the Nobel prize in physics for his work in photoelectric effect.
- The discovery of the concept of photon was central in the development of quantum theory.
- We understood that a **wave like radiation has particle like properties**.
- Later, the photon concept was used to explain Compton effect.

Problem

Calculate the energy of a photon of 5000 Å.
(Given: $h = 6.626 \times 10^{-34}$ Js, $c = 3 \times 10^8\,\mathrm{ms^{-1}}$)
Given:
$\lambda = 5000$ Å
Formula:

$$\begin{aligned}
E &= h\nu \\
E &= \frac{hc}{\lambda} \qquad (\nu = \frac{c}{\lambda}) \\
E &= \frac{6.626 \times 10^{-34} \times 3 \times 10^8}{5000 \times 10^{-10}} \\
E &= 3.97 \times 10^{-19}\,\mathrm{J} \\
E &= 2.48\,\mathrm{eV} \qquad (1\,\mathrm{eV} = 1.6 \times 10^{-19}\,\mathrm{J}).
\end{aligned}$$

Problem

A monochromatic source of light produces radiation of frequency 6.66×10^{14} Hz. If the energy of radiation produced in one second is 1×10^{-3} J. How many photons are produced by the source in one second?(Given: $h = 6.626 \times 10^{-34}$ Js)

Given:

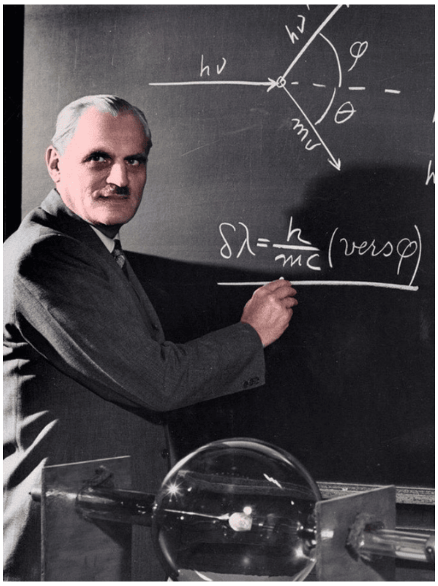
$\nu = 6.66 \times 10^{14}$ Hz

Energy of radiation per second $= \mathcal{E} = 1 \times 10^{-3}$ J

Formula:

$$\begin{aligned} \mathcal{E} &= nh\nu \\ \implies n &= \frac{\mathcal{E}}{h\nu} \\ n &= \frac{1 \times 10^{-3}}{6.626 \times 10^{-34} \times 6.66 \times 10^{14}} \\ n &= 2.26 \times 10^{15} \text{ photons per second.} \end{aligned}$$

Compton Effect



Arthur Compton (1892-1962)

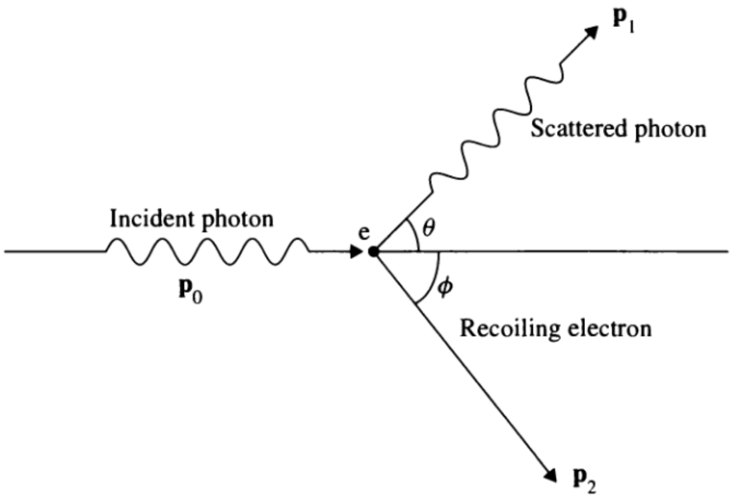


Figure 5: Scattering of X-ray photon with electron.

- Consider an particle like electron with mass m to be at rest.
- Let a photon of momentum $p_0 = h/\lambda_0$ be incident on the electron. The photon is scattered by the electron. The photon scatters at an angle of θ with respect to its initial direction.
- The photon gives a part of its energy to electron. After scattering photon's energy is reduced and hence its wavelength is increased. The photon's momentum has now become $p_1 = h/\lambda_1$.
- Let p_2 be the momentum of electron after scattering.
- Energy of photon before scattering is p_0c.
- Energy of electron before scattering is mc^2.
- Energy of photon after scattering is p_1c.
- Energy of electron after scattering is $\sqrt{p_2^2c^2 + m^2c^4}$.

Conservation of energy:
Energy (photon+e$^-$) before = Energy (photon+e$^-$) after.

$$p_0c + mc^2 = p_1c + \sqrt{p_2^2c^2 + m^2c^4}$$
$$p_0c - p_1c + mc^2 = \sqrt{p_2^2c^2 + m^2c^4}$$

Squaring on both sides

$$(p_0c - p_1c + mc^2)^2 = p_2^2c^2 + m^2c^4. \tag{12}$$

Conservation of momentum:

$$\vec{p}_0 = \vec{p}_1 + \vec{p}_2 \implies \vec{p}_2 = \vec{p}_0 - \vec{p}_1. \tag{13}$$

We know that $\vec{A} \cdot \vec{B} = AB\cos\theta$. From which we have $\vec{A} \cdot \vec{A} = A^2$.

$$p_2^2 = \vec{p}_2 \cdot \vec{p}_2 = (\vec{p}_0 - \vec{p}_1) \cdot (\vec{p}_0 - \vec{p}_1)$$
$$p_2^2 = \vec{p}_0 \cdot \vec{p}_0 - \vec{p}_0 \cdot \vec{p}_1 - \vec{p}_1 \cdot \vec{p}_0 + \vec{p}_1 \cdot \vec{p}_1$$

$$p_2^2 = p_0^2 + p_1^2 - 2p_0p_1\cos\theta. \tag{14}$$

Using equation (14) in equation (12), we get

$$(p_0c - p_1c + mc^2)^2 = (p_0^2 + p_1^2 - 2p_0p_1\cos\theta)c^2 + m^2c^4. \tag{15}$$

$(a+b+c)^2 = a^2 + b^2 + c^2 + 2ab + 2bc + 2ca$. Using this we get

$$\begin{aligned}(p_0c)^2 + (-p_1c)^2 + (mc^2)^2 + 2(p_0c)(-p_1c) + 2(-p_1c)(mc^2)\\ + 2(p_0c)(mc^2) = p_0^2c^2 + p_1^2c^2 - 2p_0p_1\cos\theta c^2 + m^2c^4\end{aligned} \tag{16}$$

Simplifying, we get

$$\begin{aligned}p_0^2c^2 + p_1^2c^2 + m^2c^4 - 2p_0p_1c^2 - 2p_1cmc^2 + 2p_0cmc^2\\ = p_0^2c^2 + p_1^2c^2 - 2p_0p_1\cos\theta c^2 + m^2c^4\end{aligned} \tag{17}$$

$$\begin{aligned}\cancel{p_0^2c^2} + \cancel{p_1^2c^2} + \cancel{m^2c^4} - 2p_0p_1c^2 - 2p_1cmc^2 + 2p_0cmc^2\\ = \cancel{p_0^2c^2} + \cancel{p_1^2c^2} - 2p_0p_1\cos\theta c^2 + \cancel{m^2c^4}\end{aligned} \tag{18}$$

We have

$$-2p_0p_1c^2 - 2p_1cmc^2 + 2p_0cmc^2 = -2p_0p_1\cos\theta c^2. \tag{19}$$

Divide the entire equation by $2c^2$ to get

$$(p_0 - p_1)mc = p_0p_1(1 - \cos\theta). \tag{20}$$

Insert $p_0 = \dfrac{h}{\lambda_0}$ and $p_1 = \dfrac{h}{\lambda_1}$, we have

$$\left(\frac{h}{\lambda_0} - \frac{h}{\lambda_1}\right) mc = \frac{h}{\lambda_0}\frac{h}{\lambda_1}(1-\cos\theta)$$
$$h\left(\frac{\lambda_1 - \lambda_0}{\lambda_0\lambda_1}\right) mc = \frac{h^2}{\lambda_0\lambda_1}(1-\cos\theta)$$
$$\lambda_1 - \lambda_0 = \frac{h}{mc}(1-\cos\theta)$$

$$\boxed{\Delta\lambda = \frac{h}{mc}(1-\cos\theta).} \quad \text{(Compton equation)} \tag{21}$$

Equation (21) is the expression for **Compton shift**. The change in wavelength of the photon after scattering is given by Compton shift. $\frac{h}{mc}$ is called **Compton wavelength**.

Compton's Observation

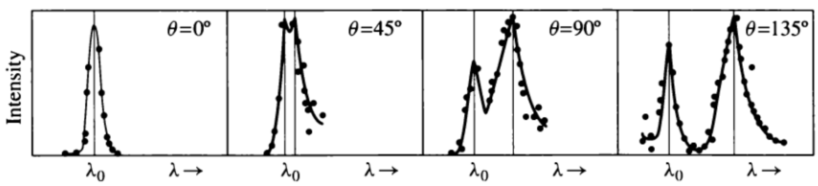


Figure 6: Compton's data of his scattering experiment. Compton carried out the experiment in 1923.

- Compton scattering occurs mostly for X-ray and γ-ray photons.
- When a graph of intensity of scattered light was plotted against wavelength, two peaks are seen (when $\theta \neq 0$).
- The first peak has same wavelength as the incident photon.
- The second peak corresponds to the photon of new wavelength after scattering.
- The distance between the two peaks in the x-axis corresponds to the Compton shift.

Conclusion

- The experimental results is successfully explained by the Compton equation.
- Using different values for θ in Compton equation, the Compton shift observed in experiment can be explained.
- The Compton effect demonstrated that photons have momentum and that energy of radiation is quantized.
- Physicists were more convinced than before that a wave like radiation has particle like properties. That is, light has dual nature.

Problem

Calculate the Compton wavelength of electron. Given $h = 6.626 \times 10^{-34}$ Js, $c = 3 \times 10^8\,\mathrm{ms^{-1}}$ and $m_e = 9.1 \times 10^{-31}$ kg.
Formula:
Compton wavelength $\lambda_C = \dfrac{h}{m_e c}$.

$$\begin{aligned}\lambda_C =& \frac{6.626 \times 10^{-34}}{9.1 \times 10^{-31} \times 3 \times 10^8}\\ =& 2.426 \times 10^{-12}\,\mathrm{m}.\end{aligned}$$

Problem

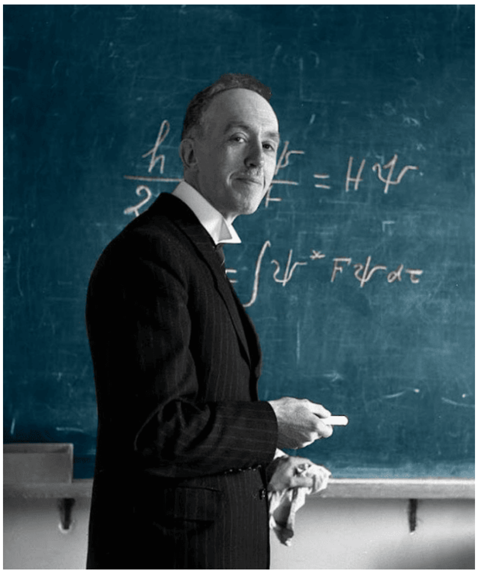
X-rays of wavelength 22 pm are scattered from a carbon target, and the scattered rays are detected at 85^o to the incident beam. What is the Compton shift of the scattered rays? What is the wavelength of photon after scattering (Given: $h = 6.626 \times 10^{-34}$ Js, $c = 3 \times 10^8\,\mathrm{ms^{-1}}$ and $m_e = 9.1 \times 10^{-31}$ kg.)
Given:
$\lambda = 22\,\mathrm{pm}$
$\theta = 85^o$
Formula:

$$\begin{aligned}\Delta\lambda =& \frac{h}{m_e c}(1 - \cos\theta)\\ =& \frac{6.626 \times 10^{-34} \times (1 - \cos 85^o)}{9.1 \times 10^{-31} \times 3 \times 10^8}\\ =& 2.2 \times 10^{-12}\,\mathrm{m}.\end{aligned}$$

The wavelength of photon after scattering will be
$\lambda_1 = \lambda + \Delta\lambda$

$\lambda_1 = 22\,\text{pm} + 2.2\,\text{pm}$
$\lambda_1 = 24.2\,\text{pm}.$

Wave-particle dualism



Louis de Broglie (1892-1987)

- A young Louis de Broglie, asked an important question. There are two things in our known universe - matter and radiation.
- If radiation has dual nature i.e., has wave-like and particle-like properties, why should matter have only particle like properties?
- If nature is symmetric in this aspect, then matter must also have dual nature.
- De Broglie asked, if a wave like radiation has particle like properties then, does matter have wave like properties?
- In 1924, de Broglie proposed an idea which unified the concepts of radiation and matter.

De Broglie hypothesis

- De Broglie hypothesized that, matter (material particles) have wave-like properties in addition to its particle nature.

- Waves associated with matter are called **matter waves** or **de Broglie waves**. The wavelength associated with a matter wave is called **de Broglie wavelength**.
- De Broglie postulated that the de Broglie wavelength is given by
$$\lambda = \frac{h}{p}, \tag{22}$$
which is same as that used for a photon. But, for a material particle $p = mv$ (when $v << c$). Therefore, the de Broglie wavelength of a particle of mass m moving with speed v is
$$\lambda = \frac{h}{mv}. \tag{23}$$

The frequency associated with matter wave (material particle) of energy E is
$$\nu = \frac{E}{h}. \tag{24}$$

- For a photon, we know about its wave properties like frequency and wavelength, hence we express its particle properties in terms of its wave properties. $E = h\nu$ and $p = h/\lambda$.
- For a material particle, we know its particle properties like momentum and energy of a particle, hence we express its wave properties in terms of its particle properties. $\nu = E/h$ and $\lambda = h/p$.
- Even though the form of the equation appears same for both photons and matter waves, their meanings are different.

De Broglie waves

What will be the de Broglie wavelength associated with an object of mass m at rest?
$$\lambda = \frac{h}{mv} = \frac{6.626 \times 10^{-34}\ \text{Js}}{m \times 0} = \infty.$$
What will be the de Broglie wavelength associated with an object of zero mass moving at speed v?
$$\lambda = \frac{h}{mv} = \frac{6.626 \times 10^{-34}\ \text{Js}}{0 \times v} = \infty.$$

We understand that, de Broglie wavelength of an object at rest or of a massless object has no meaning and cannot be practically measured. **de Broglie wavelength is finite only when the particle is moving and has mass.**

Suppose there is golf ball of 50 g moving with a speed of 36 $\mathrm{ms^{-1}}$. Let us see what will be the de Broglie wavelength of this golf ball.

$$\begin{aligned}\lambda =& \frac{h}{mv} \\ \lambda =& \frac{6.626 \times 10^{-34}\,\mathrm{Js}}{50 \times 10^{-3}\,\mathrm{kg} \times 36\,\mathrm{ms^{-1}}} \\ \lambda =& 3.68 \times 10^{-34}\,\mathrm{m}.\end{aligned}$$

The de Broglie wavelength associated with a moving golf ball is very very very small. It is so small that it cannot be practically measured. This number is so small that it is smaller than any objects in the physical world. Therefore, wave nature of a golf ball has no significance.

Now, suppose that an electron is moving with a speed of $7 \times 10^6\,\mathrm{ms^{-1}}$. What will be the de Broglie wavelength of this electron?

$$\begin{aligned}\lambda =& \frac{h}{mv} \\ \lambda =& \frac{6.626 \times 10^{-34}\,\mathrm{Js}}{9.1 \times 10^{-31}\,\mathrm{kg} \times 7 \times 10^{6}\,\mathrm{ms^{-1}}} \\ \lambda =& 1.04 \times 10^{-10}\,\mathrm{m} \approx 10^{-10}\,\mathrm{m}.\end{aligned}$$

The de Broglie wavelength associated with a moving electron is about the size of an atom. Because the de Broglie wavelength of a moving electron is comparable to the size of an atom, the wave nature of electrons become significant.

What do we understand from this?

- We understand that, the wave nature of large objects (classical object) like golf balls, cars, humans, planets, stars, etc are of no significance.
- The wave nature of very small objects (quantum objects) like atoms, electrons, neutrons, etc have very much significance.
- Matter has both wave and particle nature. But in the classical world particle nature dominates, in the quantum world wave nature dominates.
- Because of this classical physics (Newton's laws) is sufficient to describe the dynamics of the macroscopic world. But classical physics cannot be applied to quantum particles. We need a new mechanics to describe the quantum world. This mechanics is called **quantum mechanics**.

Alternate forms of de Broglie wavelength:

$\lambda = \dfrac{h}{p}$. For a particle of mass m moving with speed v, its kinetic energy $E_K = \dfrac{1}{2}mv^2 = \dfrac{1}{2m}m^2v^2 = \dfrac{p^2}{2m}$. From which one gets, $p = \sqrt{2mE_K}$. Using this in de Broglie wavelength, we have

$$\lambda = \frac{h}{\sqrt{2mE_K}}. \tag{25}$$

If a charged particle of charge q is kept at a potential difference of V, its kinetic energy is $E_K = qV$.

$$\lambda = \frac{h}{\sqrt{2mqV}}. \tag{26}$$

Problem

Calculate the de Broglie wavelength of a proton moving with a speed of $4 \times 10^7\,\mathrm{ms^{-1}}$. Given $m_p = 1.67 \times 10^{-27}\,\mathrm{kg}$.
Given:
$v = 4 \times 10^7\,\mathrm{ms^{-1}}$
$m_p = 1.67 \times 10^{-27}\,\mathrm{kg}$
Formula:

$$\begin{aligned}\lambda =& \frac{h}{mv}\\ =& \frac{6.626 \times 10^{-34}}{1.67 \times 10^{-27} \times 4 \times 10^7}\\ =& 9.91 \times 10^{-15}\,\mathrm{m}\end{aligned}$$

Problem

Calculate the de Broglie wavelength of an electron accelerated through a potential difference of $1\,\mathrm{V}$.
Given:
$V = 1\,\mathrm{V}$.
Formula:

$$\lambda = \frac{h}{\sqrt{2mqV}}.$$

$$\lambda = \frac{6.626 \times 10^{-34}}{\sqrt{2 \times 9.1 \times 10^{-31} \times 1.6 \times 10^{-19} \times 1}}$$
$$= 1.22\,\mathrm{nm}.$$

Problem

A proton has a de Broglie wavelength of 0.5 Å. Calculate its kinetic energy.
Given:
$\lambda = 0.5\,\text{Å}$
Formula:

$$\lambda = \frac{h}{\sqrt{2mE_K}}.$$

$$\implies E_K = \frac{h^2}{2m\lambda^2}$$

$$E_K = \frac{(6.626 \times 10^{-34})^2}{2 \times 1.67 \times 10^{-27} \times (0.5 \times 10^{-10})^2}$$

$$= 0.328\,\text{eV}.$$

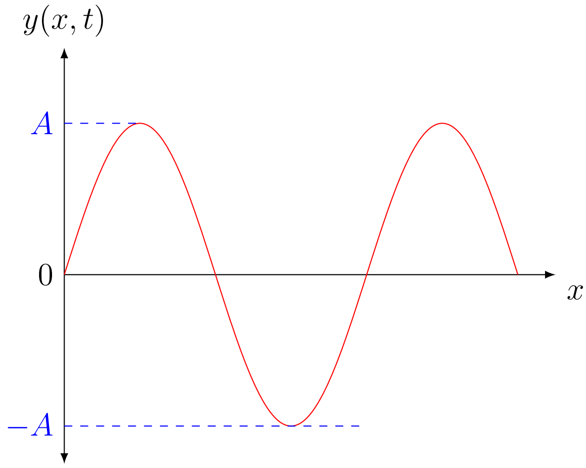
Experimental confirmation of matter waves

- In 1927, C. J. Davisson and L. H. Germer and independently by G. P. Thomson experimentally confirmed that matter has wave properties.
- Instead of using X-rays, they used electrons to determine lattice constant of crystals.
- The experiment showed that electrons undergo diffraction, which is a wave phenomena, confirming the wave nature of matter.
- J. J. Thomson discovered the electron and showed it has particle properties. His son G. P. Thomson showed electron has wave properties (There is wave-particle duality between father and son!).

Wave concepts

Consider a travelling in the positive x-direction of angular frequency $\omega = 2\pi\nu$ and angular wave number $k = 2\pi/\lambda$.

$$y(x,t) = A\cos(\omega t - kx)$$



- $y(x,t)$ is the displacement of the wave at a position x in space at an instant of time t.
- Speed with which the wave travels is known as **phase velocity** v_p.
- $\omega t - kx = \phi =$ constant is called the **phase** of the wave at a particular position x at an instant t.

Proof that phase is constant

$$\begin{aligned}
\phi =& \omega t - kx \implies \frac{\mathrm{d}\phi}{\mathrm{d}t} = \omega - k\frac{\mathrm{d}x}{\mathrm{d}t} \\
\frac{\mathrm{d}\phi}{\mathrm{d}t} =& \omega - kv_p = 2\pi\nu - \frac{2\pi}{\lambda}v_p \\
=& 2\pi\nu - 2\pi\nu = 0 \\
\implies& \phi \text{ is a constant with time.}
\end{aligned}$$

Phase velocity

The phase velocity can be written in terms of ω and k.

Formula for phase velocity v_p

$$\begin{aligned}\frac{\mathrm{d}\phi}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t}\left(\omega t - kx\right) &= 0\\ \omega - k\frac{\mathrm{d}x}{\mathrm{d}t} &= 0\\ \frac{\mathrm{d}x}{\mathrm{d}t} = v_p &= \frac{\omega}{k}.\end{aligned}$$

$$v_p = \frac{\omega}{k} = \nu\lambda. \tag{27}$$

Problem

A sinusoidal wave whose displacement is given by $y = 0.5\cos(24t - 4x)$, where the displacement is in SI units. Find the amplitude of this wave, and with what speed is the wave travelling?
Comparing the given equation with the standard sinusoidal wave equation $y = A\cos(\omega t - kx)$, we get
$A = 0.5\,\mathrm{m}$.
$\omega = 24\,\mathrm{rads}^{-1}$.
$k = 4\,\mathrm{radm}^{-1}$.
Phase velocity $v_p = \dfrac{\omega}{k} = \dfrac{24}{4} = 6\,\mathrm{ms}^{-1}$.
Therefore, amplitude of the wave is $0.5\,\mathrm{m}$ and its speed is $6\,\mathrm{ms}^{-1}$.

Phase velocity

- $E = \dfrac{mc^2}{\sqrt{1-\frac{v^2}{c^2}}}$ and $p = \dfrac{mv}{\sqrt{1-\frac{v^2}{c^2}}}$ are expressions for total energy and momentum of particle whose speed v is close to the speed of light c.
  What will be the speed of matter waves?
- Naturally, one might think the speed of matter wave is the phase velocity $v_p = \nu\lambda$.
  Let us verify!
  $v_p = \nu\lambda = \dfrac{E}{h} \times \dfrac{h}{p} = \dfrac{mc^2/\sqrt{1-v^2/c^2}}{mv/\sqrt{1-v^2/c^2}} = c^2/v.$
- Therefore, $v_p \neq v$.
- **The velocity of the particle is not the phase velocity of the wave.**

Wave packet

- Intuitively, the wave associated with a particle cannot be a sinusoidal wave. Rather, it must be a wave packet because a particle is localized in space.

Figure 7: Wave packet.

- A wave packet has an appreciable amplitude only in a small region and is zero or nearly zero everywhere else.
- A wave packet is obtained by superposition of waves of different wavelength.
- The amplitude within the packet gives the likelihood of locating the particle's position at an instant.
- The entire wave packet moves at a speed called the **group velocity** v_g. The waves within the wave packet have speed equal to the phase velocity v_p.
- The particle's speed v is equal to the group velocity v_g.
- **Group of waves shows particle behavior**.

Expression for group velocity v_g

Consider superposition of two waves,

$$y_1 = A\cos(\omega t - kx),$$
$$y_2 = A\cos[(\omega + \Delta\omega)t - (k + \Delta k)x].$$

The resultant wave is $y = y_1 + y_2$. We use the formulae

$$\cos\alpha + \cos\beta = 2\cos\left(\frac{\alpha+\beta}{2}\right)\cos\left(\frac{\alpha-\beta}{2}\right),$$

and $\cos(\theta) = \cos(-\theta)$ to obtain

$$y = 2A\cos\frac{1}{2}\left[(2\omega + \Delta\omega)t - (2k + \Delta k)x\right]\cos\frac{1}{2}(\Delta\omega t - \Delta kx).$$

When $\Delta\omega$ and Δk are very small, we can write

$$2\omega + \Delta\omega \approx 2\omega,$$
$$2k + \Delta k \approx 2k.$$

The expression for y get simplified to

$$y = 2A\cos(\omega t - kx)\cos\frac{1}{2}(\Delta\omega t - \Delta kx).$$

Writing the above equation in the form $y = A_R\cos(\omega t - kx)$, we have

$$y = 2A\cos\frac{1}{2}(\Delta\omega t - \Delta kx)\cos(\omega t - kx),$$

where $A_R = 2A\cos\frac{1}{2}(\Delta\omega t - \Delta kx)$ is the modulated amplitude.

From the expression phase velocity $v_p = \omega/k$ and group velocity v_g is

$$v_g = \frac{\Delta\omega}{\Delta k}.$$

In the limit $\Delta k \to 0$, we have

$$v_g = \lim_{\Delta k\to 0}\frac{\Delta\omega}{\Delta k} = \frac{\mathrm{d}\omega}{\mathrm{d}k}.$$

Homework

Derive the relation between group velocity and phase velocity for a wave packet.

$$v_g = v_p - \lambda\frac{\mathrm{d}v_p}{\mathrm{d}\lambda}.$$

To show that $v_g = v$.

Angular frequency

$$\omega = 2\pi\nu = \frac{2\pi E}{h}.$$

Differentiating, we get

$$\mathrm{d}\omega = \frac{2\pi}{h}\mathrm{d}E.$$

Next, angular wave number

$$k = \frac{2\pi}{\lambda} = \frac{2\pi p}{h}.$$

Differentiating, we get

$$\mathrm{d}k = \frac{2\pi}{h}\mathrm{d}p.$$

We know that

$$v_g = \frac{\mathrm{d}\omega}{\mathrm{d}k} = \frac{2\pi \mathrm{d}E/h}{2\pi \mathrm{d}p/h} = \frac{\mathrm{d}E}{\mathrm{d}p}.$$

Kinetic energy

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

Differentiating, we get

$$\mathrm{d}E = \frac{2p\ \mathrm{d}p}{2m} \implies \frac{\mathrm{d}E}{\mathrm{d}p} = \frac{p}{m}$$

$$v_g = \frac{p}{m} = \frac{mv}{m} = v.$$

Therefore, $\boxed{v_g = v}$.
The velocity of the particle is the group velocity of the wave packet.

Summary

Concepts learnt

- Blackbody and blackbody spectrum.
- Planck's radiation law.
- Einstein's concept of photon.
- Compton effect.
- Wave-particle duality.
- De Broglie hypothesis of matter waves.
- Wave packet and other aspects.

Formulae for problems

- $R = \sigma T^4$.
- $E = h\nu$ and $p = h/\lambda$ for photons.
- $\Delta\lambda = \dfrac{h}{mc}(1 - \cos\theta)$.

- $\nu = E/h$ and $\lambda = h/p$ for matter waves.
- $\lambda = \dfrac{h}{\sqrt{2mE_K}}$.
- $\lambda = \dfrac{h}{\sqrt{2mqV}}$.
- $v_p = \dfrac{\omega}{k}$.
- $v_g = \dfrac{\mathrm{d}\omega}{\mathrm{d}k}$.
- $v_g v_p = c^2$.

Practice questions

1. Derive the expression for Compton shift.
2. Obtain the formula for group velocity of a wave packet.
3. Show that the group velocity of a wave packet is equal to particle's velocity.
4. Describe the photon concept. Mention the properties of photon.
5. What is blackbody? Explain the features of blackbody spectrum.
6. What is de Broglie hypothesis? Is the wave nature of macroscopic objects significant? Explain.
7. Problems.

Suggested reading and references

[1] M. R. Srinivasan. *Physics For Engineers.*

[2] R. K. Gaur and S. L. Gupta. *Engineering Physics.*

[3] B. H. Bransden and C. J. Joachain. *Quantum mechanics.*

[4] R. Resnik, J. Walker and D. Halliday. *Fundamentals of Physics.*

[5] H. Young and R. Freedman. *University Physics.*

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Part-2: Quantum mechanics

- We have understood that matter has waves properties in addition to its particle properties.
- The wave nature of macroscopic objects is not signifiacant. Hence, Newton's laws are sufficient to describe them.
- We also understood that the wave nature of matter is significant for particles like electrons, atoms, etc. Hence, classical mechanics cannot be applied.
- We need a new mechanics to describe quantum systems. This is called **Quantum Mechanics**.

Werner Heisenberg (1901-1976)

Heisenberg's Uncertainty principle

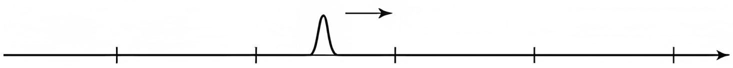


Figure 8: A wave with a (fairly) well-defined position, but an ill-defined wavelength.

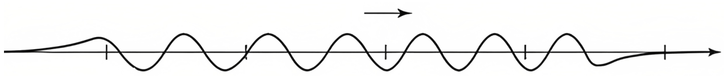


Figure 9: A wave with a (fairly) well-defined wavelength, but an ill-defined position.

- The more knowledge we have about particle's position, the less knowledge we have about its wavelength and vice-versa.
- De Broglie has shown that the wavelength of matter wave is related to the momentum of the particle, $\lambda = \dfrac{h}{p}$.
- Therefore, when wavelength is ill-defined, momentum is also ill-defined. When wavelength is well-defined, momentum is also well-defined.
- When the position of a particle is well-defined, its momentum is ill-defined. When momentum of a particle is well-defined, its position is ill-defined.
- In other words, **simultaneous knowledge of position and momentum of a particle is forbidden** in quantum mechanics.
- Is it because that, we humans do not have sophisticated instruments to simultaneously measure position and momentum of a particle?
- NO! Nature itself forbids us from measuring position and momentum together. It has nothing to do with instruments.
- How do we express this in a mathematical statement?

Understanding with an example

Let us consider measuring position of an electron. Say there are five electrons in the same state, subject to identical conditions. The positions of the electrons may be like

Trial	Position, x	$x - \langle x \rangle$
1	2	-1
2	6	3
3	1	-2
4	4	1
5	2	-1

The average position of the electron is

$$\langle x \rangle = \frac{2+6+1+4+2}{5} = 3\,\text{units}.$$

Mean of $x - \langle x \rangle$ is zero. (This is true for any data) Because the mean of $x - \langle x \rangle$ is zero. We define a quantity called **standard deviation**.

Standard deviation

Standard deviation is defined the the square root of the mean of the square of the deviation from average. Standard deviation of X is $\Delta X = \sqrt{\langle (X - \langle X \rangle)^2 \rangle}$

Standard deviation measures the deviation from the average value of a quantity. More the standard deviation of quantity, we have less information about that quantity, and vice-versa.
When $\Delta X = 0 \implies X = \langle X \rangle$, we have full knowledge about X.

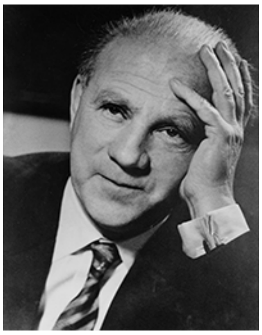
- Let us do a thought experiment. Consider a large collections of electrons, which are all in the same state subjected to identical conditions. Say there are 20,000 electrons in the same state.
- On the first 10,000 electrons measure position and from that calculate standard deviation of position.
- On the next 10,000 electrons measure momentum and from that calculate standard deviation of momentum.
- Uncertainty principle states that the product of standard deviation of position and standard deviation of momentum is greater than or equal to $h/4\pi$.
- Standard deviation is often referred as uncertainty.
- This principle applies not only for electrons but applies for any material particle whose wave nature is significant.

Statement of Uncertainty principle

The product of standard deviation of position and standard deviation of momentum of a quantum particle is never less than $\hbar/2$.

$$\Delta x \Delta p \geq \frac{\hbar}{2}. \tag{28}$$

Here $\hbar$ is reduced Planck's constant $\hbar = \dfrac{h}{2\pi}$.
It is clear that, when $\Delta x = 0 \implies \Delta p \sim \infty$.
When $\Delta p = 0 \implies \Delta x \sim \infty$. That is, when the position of the particle is known with full knowledge, momentum is ill-defined and vice-versa.



"It was about three o' clock at night when the final result of the calculation [which gave birth to quantum mechanics] lay before me. At first I was deeply shaken... I was soo excited that I could not think of sleep. So I left the house and awaited the sunrise on top of a rock".
–Werner Heisenberg, Physics and Beyond.

If we consider a particle like electron in 3D space, then the Uncertainty principle holds for each coordinate

$$\Delta x \Delta p_x \geq \frac{\hbar}{2},$$
$$\Delta y \Delta p_y \geq \frac{\hbar}{2},$$
$$\Delta z \Delta p_z \geq \frac{\hbar}{2}.$$

Application of Uncertainty principle

Why electron does not exist inside the nucleus of an atom?

- The typical size of nucleus is of the order of 5×10^{-15} m. We will prove by method of contradiction that electron does exist inside the nucleus of an atom.
- Suppose if the electron exists inside a nucleus, the uncertainty in its position Δx should not exceed 5×10^{-15} m.

- Using Heisenberg's Uncertainty principle, uncertainty in electron's momentum is:
$\Delta p \geq \hbar/2\Delta x \geq 1.055 \times 10^{-20}\,\text{kgms}^{-1}$.

- Using Δp, one can calculate kinetic energy of electron to be KE $\geq 20\,\text{MeV}$.

- But, no experiments have shown that electrons are emitted with energies $\geq 20\,\text{MeV}$. Therefore, our assumption that electron exist inside the nucleus is wrong.

Does the Uncertainty principle hold only for position and momentum?

Energy-time uncertainty principle

Suppose there is large collection of identical systems whose standard deviation of its lifetime is Δt, and the standard deviation of its energy is ΔE, then

$$\Delta E \Delta t \geq \frac{\hbar}{2}. \tag{29}$$

What is the meaning of this? Say there is a large collection of atoms in identical states. Measure the lifetime t of an atomic state for first 50% of the collection. and calculate Δt. Measure the energy E of an atom for rest 50% and calculate ΔE. The product of ΔE and Δt is never less than $\hbar/2$.
This implies that, **more accurately we know about lifetime of an atomic state, less accurately we know about its energy and vice-versa.**

More about uncertainty principle

- In general the Uncertainty principle holds for any two physical observables which do not commute.

- In quantum mechanics, physical observables are operators.

- What do we mean by observables which do not commute?
Any two operators $\hat{A}$ and $\hat{B}$ are said to be non-commutative (do not commute) when $\hat{A}\hat{B} \neq \hat{B}\hat{A}$. Then for such operators $\hat{A}$ and $\hat{B}$, uncertainty principle holds.

- What do we mean by operators?

Operators

- Heisenberg realized that, if position and momentum are satisfying uncertainty principle then they are non-commutative. If so, then they cannot be mere numbers. They must be operators.

- An operator is an instruction to do something.
  Examples: $\frac{\mathrm{d}}{\mathrm{d}x}$, $\frac{\mathrm{d}}{\mathrm{d}t}$, $\frac{\mathrm{d}^2}{\mathrm{d}x^2}$, x, k, etc.

- An operator, operates on a function to give another function.
  Examples:

$$\frac{\mathrm{d}}{\mathrm{d}x}(\sin x) = \cos x,$$
$$\int e^x \mathrm{d}x = e^x,$$
$$2.(x^2) = 2x^2, \text{ etc.}$$

Operators in quantum mechanics

What are the operators in quantum mechanics?

- Position operator $\hat{x} = x$.

- Momentum operator $\hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x}$.

- Kinetic energy operator will be

$$\frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}.$$

- Potential energy operator $\hat{V} = V(x)$.

- Operator for total energy (the **Hamiltonian operator**), will be KE + PE

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x).$$

Eigenvalue equation

Consider an operator $\hat{A}$ acting on a function $f(x)$. The function $f(x)$ is called **eigenfunction** if it satisfies

$$\hat{A}f(x) = \lambda f(x). \tag{30}$$

Equation (30) is called the **eigenvalue equation**. Here λ is a constant called the **eigenvalue**.

Examples:

- $\dfrac{\mathrm{d}}{\mathrm{d}x}(e^{2x}) = 2e^{2x}$.
- $\dfrac{\mathrm{d}^2}{\mathrm{d}x^2}(\sin x) = -\sin x$.
- $x.(x+1) = x^2 + x$. NOT an eigenvalue equation.
- $\int e^{2x}\mathrm{d}x = \dfrac{e^{2x}}{2}$.

Story so far

- Because of wave nature of matter, we understand that position and momentum do not have simulataneous reality.
- Further, for position and momentum to satisfy the uncertainty principle they must be non-commutative operators.
- We learnt about operators in quantum mechanics.
- A wave is defined as the propagation of a disturbance. Such disturbances carry energy from point to another.
- In water waves, the disturbance is oscillation of water molecules. In sound waves, the disturbance is change in air pressure. In EM waves, the disturbance is oscillating electric and magnetic field.
- What is the disturbance in matter wave ? Oscillations of what constitutes a matter wave ?

Max Born (1882-1970)

Wave function Ψ

- The physical interpretation of matter wave was given by Max Born.
- The quantity whose variations make up the matter wave is called **wave function** Ψ.
- Wave function Ψ is a complex valued function. $\Psi \in \mathbb{C}$.
- Wave function is not a physical quantity, hence cannot be measured in experiment.
- Wave function represents the state of a quantum system. It contains all the information of a quantum system.
- Wave function depends on position of the particle (x, y, z) at a given instant of time t. We denote wave function at (x, y, z, t) as $\Psi(x, y, z, t)$.

Born interpretation of Ψ

We shall consider one dimensional case for Ψ for the remainder of this chapter.

- $\Psi(x, t)$ alone has no physical meaning.
- According to Born, the absolute squared of Ψ at position x at an instant of time t gives the probability of experimentally finding the particle at x at an instant of time t.

- The absolute squared of Ψ is written as $|\Psi|^2 = \Psi^*\Psi$. Here Ψ^* denotes complex conjuagate of Ψ.
- $|\Psi|^2$ is called **probability density**.
- If $|\Psi|^2$ represents probability then we must have

$$\int_{-\infty}^{\infty} |\Psi(x,t)|^2 \mathrm{d}x = 1. \quad \text{(Normalization)} \tag{31}$$

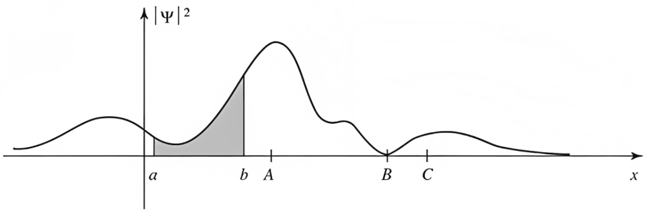


Figure 10: The shaded area represents the probability of finding the particle between a and b. The particle would be relatively likely to be found near A, and unlikely to be found near B.

$$\boxed{\int_a^b |\Psi(x,t)|^2 \mathrm{d}x = \begin{cases} \text{Probability of finding the particle} \\ \text{between } a \text{ and } b \text{ at time } t. \end{cases}}$$

- It is clear from Born's interpretation that, even when the wave function of a quantum system is known, we cannot predict the position of the particle with 100% precision. We can only calculate the probability of finding a particle in a given region.
- But when we do an experiment the particle is found at a point (say C). Where was the particle before the measurement ?
- The particle wasn't really anywhere. Measurement forced the particle to the position C. This is referred to as the **collapse of the wave function**.

Expectation values

- We have seen that in quantum mechanics, it is not possible to specify the position of a particle with 100% precision (in classical mechanics we can).

- In quantum mechanics one can calculate the average of the physical observables like position, momentum, angular momentum, etc.
- In general, to calculate average of a quantity one needs probability density function.

Average of a quantity

If $\rho(x)$ is probability density then average of a quantity A is

$$\langle A \rangle = \int A\,\rho(x)\mathrm{d}x. \tag{32}$$

Expectation value of position

In quantum mechanics the probability density is $\Psi^*\Psi = |\Psi|^2$. The expectation value (average) of position of a particle is

$$\langle x \rangle = \int_{-\infty}^{\infty} \Psi^*(x,t)\, x\, \Psi(x,t)\, \mathrm{d}x \tag{33}$$

What is the meaning of this ?
Consider a large collection of particles, all in the state $\Psi(x,t)$. Measure the position of each particle of the collection and take the average. This average value is the expectation value $\langle x \rangle$.

Expectation value of momentum

The expectation value (average) of momentum of a particle is

$$\langle p \rangle = \int_{-\infty}^{\infty} \Psi^*(x,t)\, \frac{\hbar}{i}\frac{\partial}{\partial x}\left(\Psi(x,t)\right) \mathrm{d}x \tag{34}$$

What is the meaning of this ?
Consider a large collection of particles, all in the state $\Psi(x,t)$. Measure the momentum of each particle of the collection and take the average. This average value is the expectation value $\langle p \rangle$.

Expectation value of physical observable

The expectation value (average) of any physical observable Q of a particle is

$$\langle Q \rangle = \int_{-\infty}^{\infty} \Psi^*(x,t)\, \hat{Q}\left(\Psi(x,t)\right) \mathrm{d}x \tag{35}$$

To calculate the expectation value of a physical observable we sandwich the appropriate operator between Ψ^* and Ψ, and integrate.

Story so far

- The disturbance in matter wave is called wave function.
- Wave function contains full information about the quantum system considered.
- We can only calculate probability of finding the particle in a region.
- Using $|\Psi|^2$ one can calculate the expectation values of a physical observable.
- If matter is a wave, then there must be a wave equation for matter wave.

What is the wave equation for matter wave ?
How do find the wave function for a particle ?
Like how Newton's second law describes dynamics of particle in classical mechanics, what is the equation that describes dynamics of particle in quantum mechanics ?

Erwin Schrödinger (1887-1961)

Schrödinger equation

In 1926, Erwin Schrödinger formulated quantum mechanics known as wave mechanics.

The wave equation for matter wave is given by the Schrödinger equation:

$$i\hbar\frac{\partial\Psi}{\partial t} = \hat{H}\Psi. \tag{36}$$

Here $\hat{H}$ is the Hamiltonian operator. The above equation is often referred as **time dependent Schrödinger equation**. What is the use of this equation?

The Schrödinger equation describes the time evolution of a particle in quantum mechanics. By solving the Schrödinger equation we get the wave function, from which expectation values of physical observables can be calculated.

If the particle has only kinetic and potential energies then we may write equation (36) in one dimension as

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\Psi(x,t) \tag{37}$$

Here m is the mass of the particle having potential energy $V(x)$, and kinetic energy $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$.

Using equation (37), let us derive time independent Schrödinger equation for one dimension.

Time independent Schrödinger equation

Consider the wave function of a particle in one dimension

$$\Psi(x,t) = A\exp[-i(\omega t - kx)]. \tag{38}$$

$$\Psi(x,t) = A\exp\left[-\frac{i}{\hbar}(Et - px)\right]. \tag{39}$$

Since $\omega = E/\hbar$ and $k = p/\hbar$. $\Psi(x,t)$ is a separable function i.e., it can be written in the form

$$\Psi(x,t) = \psi(x)\,\phi(t). \tag{40}$$

$\psi(x)$ is the spatial part of the wave function and $\phi(t)$ is the temporal part of the wave function.

In many textbooks $\psi(x)$ itself is called the wave function. Specifically we must call it space part of wave function.

$$\Psi(x,t) = Ae^{-iEt/\hbar}e^{ipx/\hbar}. \tag{41}$$

$$\Psi(x,t) = \psi(x)e^{-iEt/\hbar}. \tag{42}$$

Differentiate equation (42) partially wrt x twice, we get

$$\frac{\partial^2}{\partial x^2}\left(\Psi(x,t)\right) = \frac{\partial^2 \psi(x)}{\partial x^2}\, e^{-iEt/\hbar}. \tag{43}$$

Differentiate equation (42) partially wrt t, we get

$$\frac{\partial}{\partial t}\left(\Psi(x,t)\right) = \psi(x)\left(-\frac{iE}{\hbar}\right) e^{-iEt/\hbar}. \tag{44}$$

Substitute equations (43) and (44) in

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t) + V(x)\Psi(x,t). \tag{45}$$

We get

$$i\hbar\psi(x)\left(-\frac{iE}{\hbar}\right) e^{-iEt/\hbar} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2}e^{-iEt/\hbar} + V(x)\psi(x)e^{-iEt/\hbar}. \tag{46}$$

$$i\cancel{\hbar}\psi(x)\left(-\frac{iE}{\cancel{\hbar}}\right) \cancel{e^{-iEt/\hbar}} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2}\cancel{e^{-iEt/\hbar}} + V(x)\psi(x)\cancel{e^{-iEt/\hbar}}. \tag{47}$$

Simplifying equation (47), we get

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) + V(x)\psi(x) = E\psi(x). \tag{48}$$

Because there is only one variable x, partial derivative becomes total derivative. Equation (48) can be written as

$$\left[-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)\right]\psi(x) = E\psi(x). \tag{49}$$

This equation becomes

$$\hat{H}\psi(x) = E\psi(x). \tag{50}$$

This is an eigenvalue equation. $\hat{H}$ is the operator, $\psi(x)$ is the eigenfunction and E is eigenvalue. Here the eigenvalue is the energy of the particle. Equation (48) can be rearranged and written in the form:

$$\boxed{\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2} + \frac{2m}{\hbar^2}\left[E - V(x)\right]\psi(x) = 0}. \tag{51}$$

This equations (48), (49), (50) and (51) are all the same equation with different arrangements. This equation is called **time independent Schrödinger equation**.

- The function $\psi(x)$ are also called **stationary states**, as they do not evolve with time.
- The properties mentioned for wave function $\Psi(x, t)$ in Born interpretation also apply for $\psi(x)$. Except for the fact that $\psi(x)$ is time independent.
- $|\psi(x)|^2$ represents the probability of finding the particle at position x.
- We must also have the condition that

$$\int_{-\infty}^{\infty} |\psi(x)|^2 \mathrm{d}x = 1 \tag{52}$$

  because the probabilities sum up to one.

It is easy to show that $|\psi(x)|^2 = |\Psi(x, t)|^2$.

Conditions that $\psi(x)$ must satisfy

There are conditions that the space part of wave function and its derivative must satisfy to be physically realizable.

1. $\psi(x)$ and $\mathrm{d}\psi(x)/\mathrm{d}x$ must be finite.
2. $\psi(x)$ and $\mathrm{d}\psi(x)/\mathrm{d}x$ must be single valued.
3. $\psi(x)$ and $\mathrm{d}\psi(x)/\mathrm{d}x$ must be continuous in all regions where the potential of the particle is finite.
4. $\psi(x)$ must be normalized:

$$\int_{-\infty}^{\infty} |\psi(x)|^2 \mathrm{d}x = 1. \tag{53}$$

Particle in a 1D box

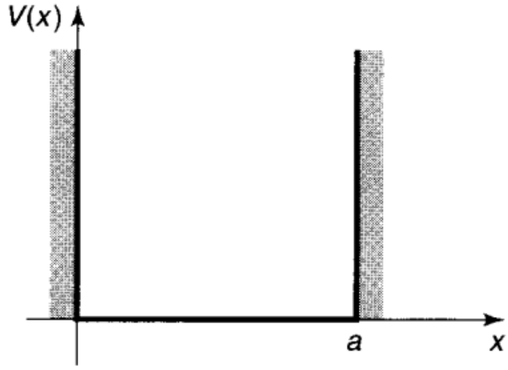


Figure 11: The figure depicts potential $V(x)$ vs position x for particle in a box. This problem is also called infinite square well potential.

Consider a particle trapped inside a 1D box of length a. Let the potential inside the box be zero. Outside the box the potential be infinite. That is, the particle cannot come out of the box.

$$V(x) = \begin{cases} 0 & 0 \leq x \leq a \\ \infty & \text{otherwise.} \end{cases} \tag{54}$$

Since the particle cannot be outside the box, $\psi(x) = 0$. Probability of finding the particle outside the box is zero.
Inside the box, $V(x) = 0$ and the time independent Schrödinger equation becomes

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + \frac{2mE}{\hbar^2}\psi = 0. \tag{55}$$

This can be written in the form

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + \kappa^2\psi = 0. \quad (\kappa^2 = \frac{2mE}{\hbar^2}) \tag{56}$$

The general solution of $\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + \kappa^2\psi = 0$ is

$$\psi(x) = A\sin(\kappa x) + B\cos(\kappa x), \tag{57}$$

where A and B are arbitrary constants, which we have to determine.
Because $\psi(x)$ is zero outside, in order to satisfy the continuity condition, $\psi(x)$

must also to zero at $x = 0$ and $x = a$.
From continuity of $\psi(x)$:

$$\psi(0) = \psi(a) = 0. \tag{58}$$

Using $\psi(0) = 0$ in (57), we get $B = 0$. Therefore,

$$\psi(x) = A\sin(\kappa x). \tag{59}$$

Using $\psi(a) = 0$ in equation (59), we get

$$\begin{aligned} \psi(a) &= 0 = A\sin\kappa a \\ \sin\kappa a &= 0 \\ \implies \kappa a &= 0, \pi, 2\pi, 3\pi, \dots \\ \kappa &= \frac{n\pi}{a} \quad n = 1, 2, 3, \dots \end{aligned}$$

We neglect the solution $\kappa a = 0$ because this implies $\psi(x) = 0$.
Therefore,

$$\psi_n(x) = A\sin\left(\frac{n\pi x}{a}\right), \quad (n \in \mathbb{N}). \tag{60}$$

Using normalization condition:

$$\int_0^a |\psi(x)|^2 \mathrm{d}x = 1, \tag{61}$$

we have

$$\begin{aligned} A^2\int_0^a \sin^2\left(\frac{n\pi x}{a}\right)\mathrm{d}x = 1 \\ \frac{A^2}{2}\int_0^a \left[1 - \cos\left(\frac{2n\pi x}{a}\right)\right]\mathrm{d}x = 1 \\ \frac{A^2}{2}\int_0^a \mathrm{d}x - \frac{A^2}{2}\int_0^a \cos\left(\frac{2n\pi x}{a}\right)\mathrm{d}x = 1 \\ \frac{A^2}{2}\,x\bigg|_0^a - \frac{A^2}{2}\,\frac{\sin(2n\pi x/a)}{2n\pi/a}\bigg|_0^a = 1. \end{aligned}$$

Simplifying, we get

$$\begin{aligned} \frac{A^2 a}{2} &= 1 \\ A &= \sqrt{\frac{2}{a}}. \end{aligned}$$

Finally, we have

$$\boxed{\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)}, \qquad \text{with } n = 1, 2, 3, \ldots. \tag{62}$$

What are the energy eigenvalues of $\psi_n(x)$?

$$\kappa = \frac{n\pi}{a} \implies \kappa^2 = \frac{n^2\pi^2}{a^2}$$

$$\kappa^2 = \frac{2mE}{\hbar^2}$$

$$\frac{n^2\pi^2}{a^2} = \frac{2mE}{\hbar^2}.$$

$$\boxed{E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}}. \tag{63}$$

E_1 is the energy of the particle in state $\psi_1(x)$
E_2 is the energy of the particle in state $\psi_2(x)$
E_3 is the energy of the particle in state $\psi_3(x)$ and so on.

The energy eigenvalues are

$$E_1 = \frac{\pi^2\hbar^2}{2ma^2}, \qquad E_2 = \frac{4\pi^2\hbar^2}{2ma^2},$$

$$E_3 = \frac{9\pi^2\hbar^2}{2ma^2}, \qquad E_4 = \frac{16\pi^2\hbar^2}{2ma^2}$$

corresponding to the states

$$\psi_1(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right), \qquad \psi_2(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{2\pi x}{a}\right),$$

$$\psi_3(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{3\pi x}{a}\right), \qquad \psi_4(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{4\pi x}{a}\right)$$

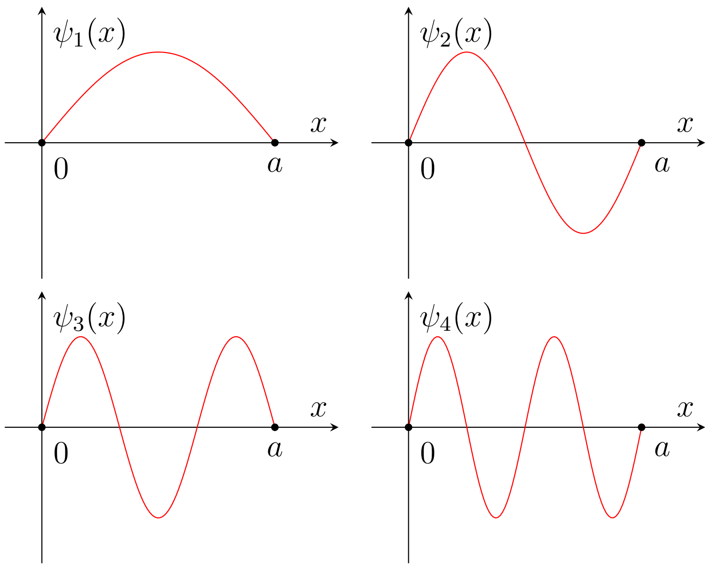
respectively.

- The wave function of the particle when it is in $\psi_1(x)$ is $\Psi_1(x,t) = \psi_1(x)e^{-iE_1t/\hbar}$.
- The wave function of the particle when it is in $\psi_2(x)$ is $\Psi_2(x,t) = \psi_2(x)e^{-iE_2t/\hbar}$.
- The wave function of the particle when it is in $\psi_3(x)$ is $\Psi_3(x,t) = \psi_3(x)e^{-iE_3t/\hbar}$ and so on.

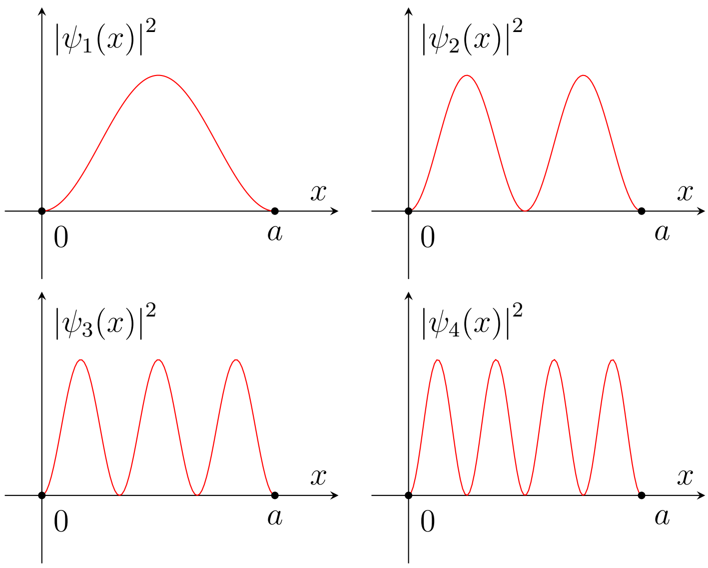
The general solution is a linear combination of all the possible wave functions.

$$\Psi(x,t) = c_1\Psi_1(x,t) + c_2\Psi_2(x,t) + \ldots \tag{64}$$

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n\Psi_n(x,t). \tag{65}$$



$\psi_n(x)$ plotted for $n = 1, 2, 3, 4$ for particle in a box.



$|\psi_n(x)|^2$ plotted for $n = 1, 2, 3, 4$ for particle in a box.

Concepts learnt

- Uncertainty Principle.
- Operators in quantum mechanics.
- Eigenvalue equation.
- Wave function.
- Born interpretation.
- Expectation value.
- Schrödinger equation for one dimension.
- Particle in a 1D box.

Practice questions

1. Write a note on Heisenberg uncertainty principle and its significance.
2. Write a note on probability density and normalization of wave function.
3. Prove that a free electron cannot exist inside a nucleus using the Heisenberg uncertainty principle.
4. Derive Schrödinger wave equation.
5. What is eigenvalue and eigenfunction? Derive the expression for eigenfunction and eigenvalue energies for a particle in a infinite potential well of finite width (Particle in a box problem).
6. What are eigenvalues and eigenfunctions?
7. Discuss the wave functions and probability density for particle in an infinite potential well, for first two states.
8. What are the properties of wave functions?
9. Find the eigenfunctions and eigenvalues for a particle in one dimensional potential well of infinite height discuss the solutions (Particle in a box problem).
10. Set-up time independent Schrodinger wave equation.

11. Write the physical significance of wave function (Born interpretation).

12. Problems.

Suggested reading and references

[1] M. R. Srinivasan. *Physics For Engineers.*

[2] R. K. Gaur and S. L. Gupta. *Engineering Physics.*

[3] P. S. Aithal and H. J. Ravindra *Engineering Physics.*

[4] R. Resnik, J. Walker and D. Halliday. *Fundamentals of Physics.*

[5] H. Young and R. Freedman. *University Physics.*

[6] D. J. Griffiths. *Introduction to Quantum mechanics.*

[7] B. H. Bransden and C. J. Joachain. *Quantum mechanics.*