College of Science
Department of Physics
Fourth Class
Lecture 13

Quantum Mechanics

2023-2024

Lecture 13: Free particle in a box

Preparation

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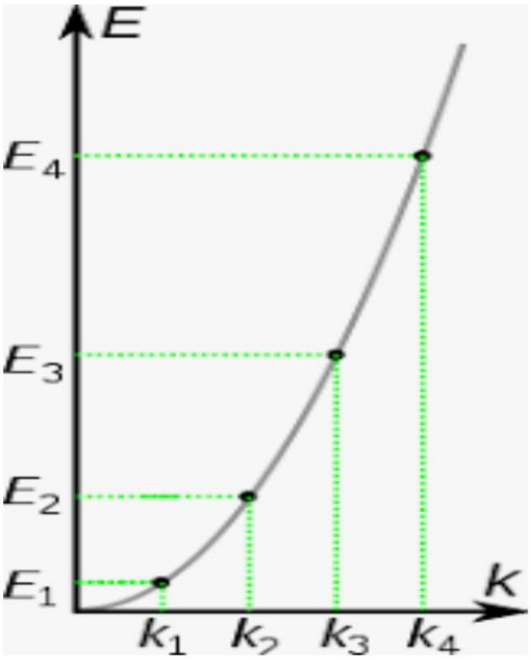
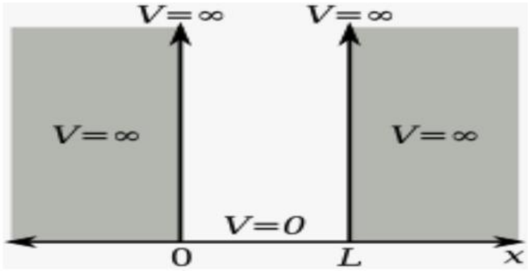
6.2 Free particle in a box

Let a single particle of mass "m" be confined within a rectangular potential box with edges parallel to X,Y & Z – axes of length l_x,l_y,l_z respectively. The particle can move freely within the region

$$0 < x < l_x \quad , \quad 0 < y < l_y \quad , \quad 0 < z < l_z$$





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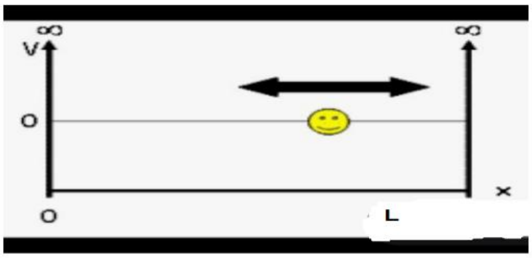


Wave Mechanics 4 -- Particle ...

i.e. inside the box, the potential function V(x,y,z) is equal zero, but it is ∞ ever where outside the box. Therefore, the particle will rebound when it will strike either of the boundaries.

The schrӧedinger eq. for the particle is

$$-\frac{\hbar^2}{2m}\nabla^2\Psi = E\Psi \qquad \rightarrow V = 0$$

Or $\nabla^2\Psi + \frac{2m}{\hbar^2}E\Psi = 0 \quad \rightarrow \quad V = 0$

E is total energy of the particle

m is mass of the particle

$$\frac{\partial^2\Psi}{\partial x^2} + \frac{\partial^2\Psi}{\partial y^2} + \frac{\partial^2\Psi}{\partial z^2} + \frac{2m}{\hbar^2}E\Psi = 0 --------8$$

This eq. solved by separation of variables.

Ψ(x,y,z)= X(x) Y(y) Z(z)

Substitute in eq.8 and divide by Ψ we get

$$\frac{1}{X}\frac{\partial^2 X(x)}{\partial x^2}+\frac{1}{Y}\frac{\partial^2 Y(y)}{\partial y^2}+\frac{1}{Z}\frac{\partial^2 Z(z)}{\partial z^2}+\frac{2m}{ħ^2}E=0$$

$$\frac{1}{X}\frac{\partial^2 X(x)}{\partial x^2}=-\frac{1}{Y}\frac{\partial^2 Y(y)}{\partial y^2}-\frac{1}{Z}\frac{\partial^2 Z(z)}{\partial z^2}-\frac{2m}{ħ^2}E$$

Let $\frac{1}{X}\frac{\partial^2 X(x)}{\partial x^2}= k_x^2 \qquad k_x - const. \ -----9$

$$k_x^2=-\frac{1}{Y}\frac{\partial^2 Y(y)}{\partial y^2}-\frac{1}{Z}\frac{\partial^2 Z(z)}{\partial z^2}-\frac{2m}{ħ^2}E$$

$$\frac{1}{Y}\frac{\partial^2 Y(y)}{\partial y^2}=-k_x^2-\frac{1}{Z}\frac{\partial^2 Z(z)}{\partial z^2}-\frac{2m}{ħ^2}E$$

Let $\frac{1}{Y}\frac{\partial^2 Y(y)}{\partial y^2}=k_y^2$ ---------10

$$-k_x^2-\frac{1}{Z}\frac{\partial^2 Z(z)}{\partial z^2}-\frac{2m}{ħ^2}E=k_y^2$$

This eq. may be written as

$$\frac{1}{Z}\frac{\partial^2 Z(z)}{\partial z^2}=k_z^2 \ -----11$$

$$=-k_x^2-k_y^2-\frac{2m}{ħ^2}\ E$$

$$k_x^2+k_y^2+k_z^2=-\frac{2m}{ħ^2}\ E$$

$$k_x^2=-\frac{2m}{ħ^2}\ E_x \quad , \quad k_y^2=-\frac{2m}{ħ^2}\ E_y \ , \qquad k_z^2=-\frac{2m}{ħ^2}\ E_z$$

The eqs.(9,10,11) may be written as

$$\frac{\partial^2 X(x)}{\partial x^2}+\frac{2m}{ħ^2}\ E_x X=0 \quad ----a$$

$$\frac{\partial^2 Y(y)}{\partial y^2}+\frac{2m}{ħ^2}\ E_y Y=0 \ -----b$$

&

$$\frac{\partial^2 Z(z)}{\partial z^2} + \frac{2m}{\hbar^2} E_z Z = 0 \; - - - - c \quad 12$$

The general solution of eq. 12a will be sine function of arbitrary amplitude, frequency, and phase, i.e.

X(x)= A sin (Bx + C) -----------13

Where A, B & C are constants to be determined from consideration of the boundary conditions as

$|\Psi|^2$ represent the probability of finding the particle at any point within the box.

$|X(x)|^2$ is the probability of finding the particle at any point along x-axis

As the pot. → ∞ "Very high" at the walls of the box, the probability of finding the particle at walls will be zero, i.e.

$|X(x)|^2$ =0 when x=0 & $x=l_x$

Or X(x)=0 when x=0 & $x=l_x$

Using these boundary condition, eq.13 gives

X(x) = A sin (Bx +C) = 0

sin C=0 when x=0 and sin (Bl_x +C) =0 when $x= l_x$

which yield C=0 & sin Bl_x =0

or $Bl_x=n_x \pi$ n_x= 1,2,3,------+ve integer

$$B = \frac{n_x \pi}{l_x}$$

Substituting values of B & C in eq. 13

X(x)= A sin$\frac{n_x \pi x}{l_x}$ --------14

For simplicity we assume A to be a real number, then using the condition of normalize

$$\int_0^{l_x} |X(x)|^2 dx = 1$$

We have $\int_0^{l_x} \left|A\, sin\frac{n_x \pi x}{l_x}\right|^2 dx = 1$

Or $A^2 \int_0^{l_x} sin^2 \frac{n_x \pi x}{l_x} dx = 1$

$$A^2 \frac{l_x}{2} = 1 \qquad \rightarrow \qquad A = \sqrt{\frac{2}{l_x}}$$

Substituting the value of A in eq.14, the normalized function X(x) is given by

$$X(x) = \sqrt{\frac{2}{l_x}} \sin\frac{n_x \pi x}{l_x} \ -------- 15$$

$$\frac{\partial^2 X}{\partial x^2} = -\left(\frac{n_x \pi}{l_x}\right)^2 X(x) \ ------ 16$$

Sub.15 & 16 in to eq.12a , we get

$$\frac{\partial^2 X(x)}{\partial x^2} + \frac{2m}{ħ^2} E_x X = 0$$

$$-\left(\frac{n_x \pi}{l_x}\right)^2 X(x) + \frac{2m}{ħ^2} E_x\, X(x) = 0$$

Or $\boxed{E_x = \frac{1}{2m}\left(\frac{n_x \pi ħ}{l_x}\right)^2 = \frac{n_x^2 h^2}{8 m l_x^2}}$ $--17$ when ħ=$\frac{h}{2\pi}$, n=1,2,3 ---

Note :1- energy is quantized E1, E2,E3,------

2- $E_{min} = E_1 \neq 0$

Similarly, we may solve eqs.12b &12c and obtain

$$Y(y) = \sqrt{\frac{2}{l_y}} \sin\frac{n_y \pi y}{l_y} \qquad , n_y = 1,2,3, -----$$

$$Z(z) = \sqrt{\frac{2}{l_z}} \sin\frac{n_z \pi z}{l_z} \quad , \qquad n_z = 1,2,3,----$$

$$\boxed{E_y = \frac{n_y^2 h^2}{8ml_y^2}} ------18 \qquad \boxed{E_z = \frac{n_z^2 h^2}{8ml_z^2}} ----19$$

Having

$$k_x^2 + k_y^2 + k_z^2 = -\frac{2m}{\hbar^2} E$$

And

$$k_x^2 = -\frac{2m}{\hbar^2} E_x \quad , \quad k_y^2 = -\frac{2m}{\hbar^2} E_y \ , \qquad k_z^2 = -\frac{2m}{\hbar^2} E_z$$

$E = E_x + E_y + E_z$

Eqs. 17,18,19 give the allowed values of energy levels along X, Y & Z axes respectively.

The allowed values of total energy are given by

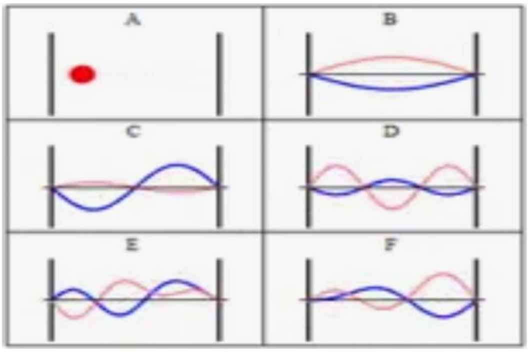
$E = E_x + E_y + E_z = \frac{h^2}{8m}\left[\frac{n_x^2}{l_x^2} + \frac{n_y^2}{l_y^2} + \frac{n_z^2}{l_z^2}\right]$

Where n_x, n_y, n_z denote any set of three positive numbers.

The complete wave – function Ψ_{n_x,n_y,n_z} has the form, for various values of the values of the quantum numbers n_x, n_y & n_z .

$$\Psi_{n_x,n_y,n_z}(x,y,z) = X(x)Y(y)Z(z)$$

$$=2\sqrt{\frac{2}{l_x l_y l_z}} \sin\frac{n_x \pi x}{l_x}\ sin\frac{n_y \pi y}{l_y}\ sin\frac{n_z \pi z}{l_z}$$



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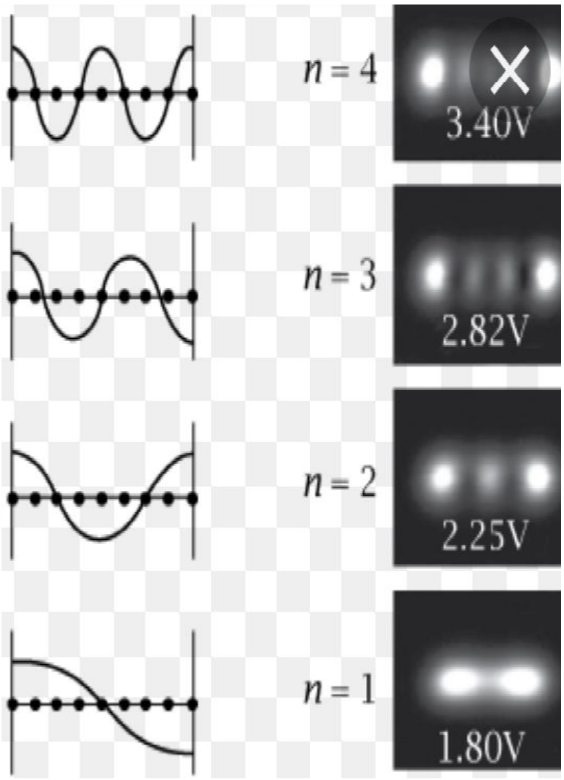

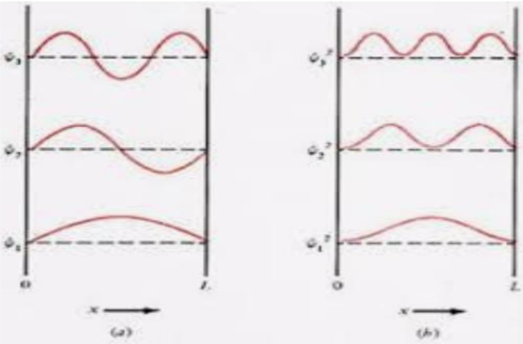

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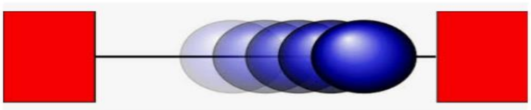

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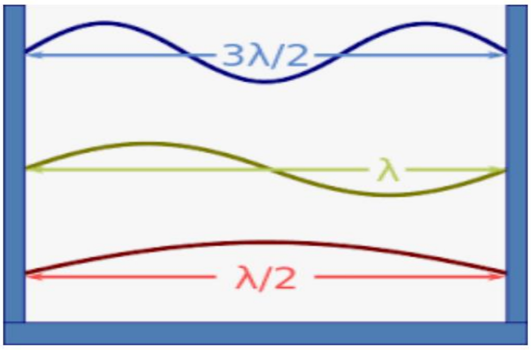

Problem 1:

Prove that the wave functions of a particle in one dimensioinal box($l_x = a$) are orthogonal.

Solution:

$$\Psi(x) = \sqrt{\frac{2}{l_x}}\ \sin\frac{n_x\pi x}{l_x}$$

$$\Psi_n(x) = \sqrt{\frac{2}{a}}\ \sin\frac{n_x\pi x}{a} \qquad when\ l_x\ = a$$

The orthogonal condition is

$$\int_{-\infty}^{\infty}\Psi_n^*\Psi_l\ dx = 0 \qquad n \neq l$$

In free particle wave function in a box

$$\frac{2}{a}\int_0^a \sin\frac{n\pi x}{a}\quad \sin\frac{l\pi x}{a}\quad dx = \frac{1}{a}\int_0^a 2\ \sin\frac{n\pi x}{a}\quad \sin\frac{l\pi x}{a}\quad dx$$

$=\frac{1}{a}\int_0^a(cos\frac{(n-l)\pi x}{a} - cos\frac{(n+l)\pi x}{a})dx$

$$= \frac{1}{a}\left[\frac{a}{(n-l)\pi}sin\frac{(n-l)\pi x}{a} - \frac{a}{(n+l)\pi}sin\frac{(n+l)\pi x}{a}\right]_0^a = 0$$

Because $n - l\ \rightarrow integer\ \ \& n + l\ \rightarrow integer$

So sin 0=0

$\sin(n-l)\pi = 0 \quad \& \quad \sin(n+l)\,\pi = 0$

$$\frac{2}{a}\int_0^a \sin\frac{n\pi x}{a}\quad \sin\frac{l\pi x}{a}\quad dx =\ zero$$

The wave functions are orthogonal

Problem 2:

a- Verify that a travelling wave solution of the schrӧedinger eq. for a free particle
Ψ(x,t)= $A\ expi(k_x\, x - \omega t)$ is also an eigen function of linear momentum

b- Evaluate the probability density for the same travelling wave solution and show that both results are consistent with Heisenberg uncertainty principle.

Solution:

a- $\Psi(x,t) = A\ expi(k_x x - \omega t)$

$$= A \exp(ik_x x) \exp\left(-i\frac{Et}{\hbar}\right)$$

Where E is the energy eigen value and

$$k_x = \frac{\sqrt{2mE_x}}{\hbar}$$

$\hat{P}\Psi$(x,t)=$\frac{\hbar}{i}\frac{\partial}{\partial x}\Psi(x,t)$= $\frac{\hbar}{i}\frac{\partial}{\partial x}A exp(ik_x x)$exp $(\frac{-iEt}{\hbar})$

$$=\hbar k_x \Psi(x,t)$$

$\hbar k_x$ is eigen value of linear momentum $P = \hbar k_x = \sqrt{2mE_x}$

thus, for a fixed energy the linear momentum is uniquely defined.

b- The prob.density= $\Psi^*(x,t)\Psi(x,t) = A^* A$
i.e. This is independent of X and thus the X-coordinate is completely unknown
i.e. As the momentum is uniquely defined, the position cannot be known ($\Delta P = 0$, $\Delta x = \infty$).

Problem: H.W

1- A crystalline chip in a cell phone has a side length of (0.2nm). Calculate the minimum speed of an electron move inside it.
2- Calculate the maximum speed of a particle has mass (1gm) inside the box a side length (1 cm). calculate the A- particle's energy if the velocity is (3 cm/s). B- n to that energy level.