College of Science
Department of Physics
Fourth Class
Lecture 12

Quantum Mechanics

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Lecture 12: Particles under the influence of a constant potential and particle in a box

Preparation

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Unit 6

Particles under the influence of a constant potential and particle in a box

6.1 The free particle

A free particle is one for which the potential energy V is quite independent of positions, and it may be set equal to zero, so that the schrӧedinger equation for a free particle become

$\hat{H}\Psi = E\Psi$ $\quad\quad\quad$ $\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V$

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

$$\nabla^2\Psi(x,y,z) + \frac{2m}{\hbar^2}E\Psi = 0$$

Or $\quad \frac{\partial^2\Psi}{\partial x^2} + \frac{\partial^2\Psi}{\partial y^2} + \frac{\partial^2\Psi}{\partial z^2} + \frac{2m}{\hbar^2}E\Psi = 0 ------1$

This is a partial differential equation in 3- independent variables x, y & z and may be solved by the method of separation of variables.

Ψ is finite everywhere in space since the particle is free to move anywhere in space, so that we may write the solution of eq.1 in the form

$\Psi(x,y,z) = X(x)\,Y(y)\,Z(z)$

Where X(x) , Y(y) & Z(z) are functions of their respective coordinates alone. Substituting this in eq.1 and dividing by X(x) Y(y) Z(z), we get

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

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

In this eq. L.H.S. is a function of x alone while R.H.S. is a function of y &z and is independent of x. It is, therefore, necessary that the value of the quantity to which each side is equal must be independent of x,y &z , i.e. Both sides must be equal to a constant k_x^2 ,so that

$\frac{1}{X}\frac{\partial^2 X(x)}{\partial x^2} = k_x^2$ -------------------2

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

$$\frac{1}{Y}\frac{\partial^2 Y(y)}{\partial y^2} = -k_x^2 - \frac{1}{Z}\frac{\partial^2 Z(z)}{\partial z^2} - \frac{2m}{\hbar^2}E - - - - - - - - - - 3$$

In this eq. L.H.S. is independent of z which R.H.S. is independent of y.

Therefore, the above equation is to be satisfied both sides must be equal to constant k_y^2 ,so that

$$\frac{1}{Y}\frac{\partial^2 Y(y)}{\partial y^2} = k_y^2 - - - - - - - 4$$

From eq.6 &4

$$-k_x^2 - \frac{1}{Z}\frac{\partial^2 Z(z)}{\partial z^2} - \frac{2m}{\hbar^2}E = k_y^2 \;\; - - - - - 5$$

Eq.5 may be written as

$$\frac{1}{Z}\frac{\partial^2 Z(z)}{\partial z^2} = -k_x^2 - \frac{2m}{\hbar^2}E - k_y^2 \;\; - - - - - 6$$

In this equation R.H.S. is constant.

Let this constant be k_z^2 , so that we may write

$$\frac{1}{Z}\frac{\partial^2 Z(z)}{\partial z^2} = k_z^2 = -k_x^2 - k_y^2 - \frac{2m}{\hbar^2}\; E - - - - 7$$

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

For convenience let substitute

$$k_x^2 = -\frac{2m}{\hbar^2}\; E_x$$

Then the differential equation in x from eq.2 may be written as

$$\frac{1}{X}\frac{\partial^2 X(x)}{\partial x^2} = k_x^2 \;\; \rightarrow \;\; \frac{1}{X}\frac{\partial^2 X(x)}{\partial x^2} = -\frac{2m}{\hbar^2}\, E_x$$

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

The general solution of this eq. can be written as

$$X(x) = N_x \sin\frac{\sqrt{2mE_x}}{\hbar}\, (x - x_o)$$

Where $N_x and\ x_o$ are arbitrary constants.

Similarly, we may obtain the differential equation in y & z by substituting

$$k_y^2 = -\frac{2m}{\hbar^2}\, E_y \;\; \& \;\;\; k_z^2 = -\frac{2m}{\hbar^2}\, E_z$$

In eqs. 4 &7

$$\frac{\partial^2 Y(y)}{\partial y^2} + \frac{2m}{\hbar^2}\, E_y Y = 0$$

&

$$\frac{\partial^2 Z(z)}{\partial z^2} + \frac{2m}{\hbar^2}\, E_z Z = 0$$

The general solution of these eqs.

$$Y(y) = N_y \sin\frac{\sqrt{2mE_y}}{\hbar}\, (y - y_o)$$

$$Z(z) = N_z \sin\frac{\sqrt{2mE_z}}{\hbar}\, (z - z_o)$$

E = $E_x + E_y + E_z$ $\qquad\qquad \Psi = X.Y.Z$

$$\Psi = N_x \sin\frac{\sqrt{2mE_x}}{\hbar}\, (x - x_o) N_y \sin\frac{\sqrt{2mE_y}}{\hbar}\, (y - y_o) N_z \sin\frac{\sqrt{2mE_z}}{\hbar}\, (z - z_o)$$

Where N= $N_x N_y N_z$

$$\boxed{\Psi = N\, sin\frac{\sqrt{2mE_x}}{\hbar}\, (x - x_o)\, sin\frac{\sqrt{2mE_y}}{\hbar}\, (y - y_o)\, sin\frac{\sqrt{2mE_z}}{\hbar}\, (z - z_o)}$$

The complete wave functions with the time factor can be written as follows

$$\Psi(x,y,z,t)=N \sin\frac{\sqrt{2mE_x}}{\hbar}\,(x-x_o)e^{-i\frac{E_xt}{\hbar}}\ \sin\frac{\sqrt{2mE_y}}{\hbar}\,(y-y_o)e^{-i\frac{E_yt}{\hbar}}\sin\frac{\sqrt{2mE_z}}{\hbar}\,(z-z_o)e^{-i\frac{E_zt}{\hbar}}$$

$$\Psi(x,y,z,t)=N \sin\frac{\sqrt{2mE_x}}{\hbar}\,(x-x_o)\sin\frac{\sqrt{2mE_y}}{\hbar}(y-y_o)\sin\frac{\sqrt{2mE_z}}{\hbar}(z-z_o)e^{-i\frac{(E_x+E_y+E_z)t}{\hbar}}$$

$$\boxed{\Psi(x,y,z,t)=N\ sin\frac{\sqrt{2mE_x}}{\hbar}\,(x-x_o)\ \ sin\frac{\sqrt{2mE_y}}{\hbar}\,(y-y_o)\,sin\frac{\sqrt{2mE_z}}{\hbar}\,(z-z_o)e^{-i\frac{Et}{\hbar}}}$$

Example H.W.

A particle with mass (m) and with zero energy has a time independent waves function $\varphi(x)=AXe^{-\frac{x^2}{L^2}}$ where A and L are constant. Determine the potential energy V(x) of the particle.