2- Time independent Schrödinger equation (TISE)

We can separate the variable in Eqn. (9) [$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi + V(r,t)\,\Psi(r,t)$] and obtain two equations, one depending on the variable (t) and the other on the variable (r). We can write $\Psi(r,t)$ as the product of two functions $\Psi(r)$ and $\phi(t)$. Where $\Psi(r)$ a function of space is coordinates only and $\phi(t)$ is a function of time only.

$$\therefore \Psi(r,t) = \Psi(r)\,\phi(t) \qquad \ldots\ldots\ldots\ldots\ldots\ldots (10)$$

In one – dimension

$$\Psi(x,t) = A\, e^{\frac{i}{\hbar}(p_x x - Et)}$$

$$\Psi(x,t) = A\; e^{\left(\frac{i\,p_x}{\hbar}\right)x} . e^{-\left(\frac{i\,E}{\hbar}\right)t} = \Psi\, e^{-\left(\frac{i\,E}{\hbar}\right)t}$$

Where $\Psi = A\; e^{\left(\frac{i\,p_x}{\hbar}\right)x}$

Substituting this value in Eqn. (8) [$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V(x,t)\Psi(x,t)$]

we obtain:

$$i\hbar\, \frac{\partial}{\partial t}\left(\Psi e^{-\left(\frac{i\,E}{\hbar}\right)t}\right) = -\frac{\hbar^2}{2m}\, \frac{\partial^2}{\partial\, x^2}\left(\Psi\, e^{-\left(\frac{i\,E}{\hbar}\right)t}\right) + V\,\Psi\, e^{-\left(\frac{i\,E}{\hbar}\right)t}$$

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

$$E\,\Psi\, e^{-\left(\frac{i\,E}{\hbar}\right)t} = -\frac{\hbar^2}{2m}\, \frac{\partial^2}{\partial\, x^2}\left(\Psi\, e^{-\left(\frac{i\,E}{\hbar}\right)t}\right) + V\,\Psi\, e^{-\left(\frac{i\,E}{\hbar}\right)t}$$

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

بحذف العامل المشترك $e^{-\left(\frac{iE}{\hbar}\right)t}$ من طرفي المعادلة اعلاه نحصل على :

$$E\,\Psi = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\,\Psi$$

Or $$E\,\Psi + \frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} - V\,\Psi = 0$$

Or $$\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + (E - V)\Psi = 0$$

بضرب طرفي المعادلة اعلاه ب $\frac{2m}{\hbar^2}$ نحصل على:

$$\frac{2m}{\hbar^2} * \frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + \frac{2m}{\hbar^2}(E - V)\Psi = 0$$

$$\frac{\partial^2\Psi}{\partial x^2} + \frac{2m}{\hbar^2}(E - V)\Psi = 0$$ In 1- dimension ……………... (11)

$$\frac{\partial^2\Psi}{\partial x^2} + \frac{\partial^2\Psi}{\partial y^2} + \frac{\partial^2\Psi}{\partial z^2} + \frac{2m}{\hbar^2}(E - V)\Psi = 0$$ In 3- dimension

Or $$\nabla^2\,\Psi + \frac{2m}{\hbar^2}(E - V)\Psi = 0$$ ……………… (12)

Where $$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

-Expectation Values

In quantum mechanics, physical quantities are not described by definite values as in classical physics; instead, they are described by a wave function ψ(x ,t) that contains all the possible information about the physical system. When a measurement of a given physical quantity is performed repeatedly on an identical system, the results may differ from one measurement to another.

However, it is possible to define an average value of these results, which is known as the expectation value. This quantity represents the statistical mean of the measurement outcomes and provides a direct link between the mathematical description of the wave function and experimentally observable physical quantities.

في ميكانيكا الكم لا تُوصَف الكميات الفيزيائية بقيم محددة وثابتة كما في الفيزياء الكلاسيكية بل تُوصَف بدالة موجية $\psi(x,t)$ تحتوي على جميع المعلومات الممكنة عن النظام الفيزيائي .وعند إجراء قياس لكمية فيزيائية معيّنة بشكل متكرر على نظام متماثل تمامًا في كل مرة، قد تختلف النتائج من قياس إلى آخر.

ومع ذلك، من الممكن تعريف قيمة متوسطة لهذه النتائج تُعرَف باسم القيمة المتوقعة (Expectation Value) تمثل هذه الكمية المتوسط الإحصائي لنتائج القياسات، وتوفّر رابطًا مباشرًا بين الوصف الرياضي للدالة الموجية والكميات الفيزيائية التي يمكن ملاحظتها تجريبيًا.

-Expectation Values of Basic Physical Quantities

1- Expectation Value of Position

The position operator is defined as: $x = \hat{x}$

The expectation value of the position is given by:

$$< x >= \int \psi^*(x,t)\, x\, \psi(x,t)\, dx$$

This quantity represents the average position of the particle obtained from a large number of measurements.

2- Expectation Value of Momentum

In one dimension, the momentum operator is defined as:

$$\hat{p} = -i\hbar \frac{d}{dx}$$

The expectation value of the momentum is given by:

$$< p >= \int \psi(x,t) \left(-i\hbar \frac{d}{dx}\right) \psi^*(x,t)\, dx$$

This expression gives the average momentum of the particle over many measurements.

3- Expectation Value of Energy

The energy operator (Hamiltonian) is defined as:

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

The expectation value of the energy is given by:

$$< E >= \int dx\, \psi(x,t)\ \widehat{H}\ \psi^*(x,t)$$

This value represents the average energy of the quantum system.

-Example:

A particle limited to the x - axis has the wave function $\psi = ax$ between $x = 0$ and $x = 1$; $\psi = 0$ elsewhere.

(a) Find the probability that the particle can be found between $(x = 0.45)$ and $(x = 0.55)$.

(b) Find the expectation value ⟨x ⟩ of the particle's position.

Solution:

(a) The probability is

$\int_{x1}^{x2} |\psi|^2 \, dx = \int_{x1}^{x2} \psi^* \, \psi \, dx = \int_{0.45}^{0.55} (\mathrm{ax})(\mathrm{ax}) \, dx$

$$\therefore \int_{0.45}^{0.55} (\mathrm{ax})(\mathrm{ax}) \, dx = a^2 \int_{0.45}^{0.55} x^2 \, dx$$

$$= a^2 \left[\frac{x^3}{3}\right]_{0.45}^{0.55}$$

$\therefore a^2 \left[\frac{x^3}{3}\right]_{0.45}^{0.55} = a^2 \left\{\frac{0.55^3}{3} - \frac{0.45^3}{3}\right\} = 0.025 \, a^2$

(b) Find the expectation value

$$< x >= \int_0^1 \psi^*(x,t) \, x \, \psi(\mathrm{x,t}) \, dx$$

$$< x >= \int_0^1 \mathrm{x} \, (\mathrm{ax})(ax) \, dx$$

$$= a^2 \int_0^1 x^3 \, dx = a^2 \left[\frac{x^4}{4}\right]_0^1$$

$$= a^2 \left\{\frac{1^4}{4} - \frac{0^4}{4}\right\} = \frac{a^2}{4}$$