3) Hermitian: the operator Â called Hermitian when it satisfies the following relation;

$$\int_{-\infty}^{\infty} \psi_n^* \hat{A} \psi_m \, d\tau = \int_{-\infty}^{\infty} \psi_m (\hat{A}\psi_n)^* \, d\tau \qquad \text{...........(2-14)}$$

Hermitian operator has two important properties that are;

i- Eigen values correspond to any Hermitian operator are real quantities. i.e. $a_n = a_n^*$

Proof:

From the eigen value equation we have;

$$\hat{A}\psi_n = a_n \psi_n \qquad \text{................(a)}$$

Multiply both sides by ψ_n^* we get;

$$\psi_n^* \hat{A} \psi_n = \psi_n^* a_n \psi_n$$

Integrating over all space one find;

$$\int_{-\infty}^{\infty} \psi_n^* \hat{A} \psi_n \, d\tau = \int_{-\infty}^{\infty} \psi_n^* a_n \psi_n \, d\tau \qquad \text{................ (b)}$$

Take the complex conjugate of equation (a) we have;

$$\hat{A}^* \psi_n^* = a_n^* \psi_n^* \qquad \text{.................(c)}$$

Multiply both sides of equation (c) by ψ_n we get;

$$\psi_n \hat{A}^* \psi_n^* = a_n^* \psi_n \psi_n^*$$

Integrating the last equation over all space one get;

$$\int_{-\infty}^{\infty} \psi_n \hat{A}^* \psi_n^* = \int_{-\infty}^{\infty} a_n^* \psi_n \psi_n^* \, d\tau \qquad \text{................ (d)}$$

Subtract equation (d) from (b) we find;

$$\int_{-\infty}^{\infty} \psi_n^* \hat{A} \psi_n \, d\tau - \int_{-\infty}^{\infty} \psi_n \hat{A}^* \psi_n^* \, d\tau = \int_{-\infty}^{\infty} \psi_n^* a_n \psi_n \, d\tau - \int_{-\infty}^{\infty} a_n^* \psi_n \psi_n^* \, d\tau$$

According to the definition of Hermitian operator, the left hand side of last equation vanishes. i.e.

$$\int_{-\infty}^{\infty} \psi_n^* \hat{A} \psi_n \, d\tau - \int_{-\infty}^{\infty} \psi_n \hat{A}^* \psi_n^* \, d\tau = 0$$

So;

$$0 = \left(a_n - a_n^*\right) \int_{-\infty}^{\infty} \psi_n^* \psi_n \, d\tau$$

From the normalization condition, we conclude that;

$$a_n = a_n^*$$

ii-Eigen functions correspond to different eigen values are orthogonal. i.e.

$$\int_{-\infty}^{\infty} \psi_n^* \psi_m \, d\tau = 0 \,.\, \int_{-\infty}^{\infty} \psi_m^* \psi_n \, d\tau = 0$$

Proof:

Assume that the two functions ψ_n and ψ_m are eign functions for the operator $\hat{A}$, so the following relations can be setup;

$$\hat{A}\psi_n = a_n \psi_n$$

$$\hat{A}\psi_m = a_m \psi_m$$

Multiply the first equation by ψ_m^*, taking the complex conjugate of the second equation and multiplying it by ψ_n, then integrating the results over all space we get;

$$\int_{-\infty}^{\infty} \psi_m^* \hat{A} \psi_n \, d\tau = a_n \int_{-\infty}^{\infty} \psi_m^* \psi_n \, d\tau \qquad \text{.................. (a)}$$

$$\int_{-\infty}^{\infty} \psi_n \hat{A}^* \psi_m^* = \int_{-\infty}^{\infty} a_m^* \psi_n \psi_m^* \, d\tau \qquad \text{.................. (b)}$$

Subtract equation (b) from (a) we find;

$$\int_{-\infty}^{\infty} \psi_m^* \hat{A} \psi_n \, d\tau - \int_{-\infty}^{\infty} \psi_n \hat{A}^* \psi_m^* \, d\tau = a_n \int_{-\infty}^{\infty} \psi_m^* \psi_n \, d\tau - a_m^* \int_{-\infty}^{\infty} \psi_n \psi_m^* \, d\tau$$

According to the definition of Hermitian operator, the left hand side of last equation vanishes. Thus;

$$0 = (a_n - a_m^*) \int_{-\infty}^{\infty} \psi_m^* \psi_n \, d\tau$$

Which leads to;

$$\int_{-\infty}^{\infty} \psi_m^* \psi_n \, d\tau = 0$$

However, normalization and orthogonal conditions can be collected together by the following formula;

$$\int_{-\infty}^{\infty} \psi_m^* \psi_n \, d\tau = \delta_{mn}$$

Where (δ_{mn}) is the kroneker delta that have the following two values;

$$\delta_{mn} = 1 \quad \text{at} \quad \mathrm{m = n}$$

$$\delta_{mn} = 0 \quad \text{at} \quad \mathrm{m \neq n}$$

Example: Prove that p_x is a Hermitian operator.

Solution:

From the definition of Hermitian operator;

$$\int_{-\infty}^{\infty} \psi_n^* \hat{A} \psi_m \, d\tau = \int_{-\infty}^{\infty} \psi_m (\hat{A} \psi_n)^* \, d\tau$$

$$\int_{-\infty}^{\infty} \psi_n^* (-i\hbar \frac{\partial}{\partial x}) \, \psi_m \, dx = \quad -i\hbar \int_{-\infty}^{\infty} \psi_n^* \frac{\partial}{\partial x} \psi_m \, dx$$

Using the by part integration; $\int_{-\infty}^{\infty} \mathrm{u\,dv} = \mathrm{uv}\Big|_{-\infty}^{+\infty} - \int_{-\infty}^{\infty} \mathrm{v\,du}$, assuming that;

$\mathrm{dv} = \frac{\partial}{\partial x} \psi_m \, dx$ and $\mathrm{u} = \psi_n^*$. So, $\mathrm{v} = \psi_m$ and . However, $\mathrm{du} = \frac{\partial \psi_n^*}{\partial x} dx$

$$\int_{-\infty}^{\infty} \psi_n^* (-i\hbar \frac{\partial}{\partial x}) \, \psi_m \, dx = -i\hbar \psi_n^* \psi_m \Big|_{-\infty}^{+\infty} + i\hbar \int_{-\infty}^{\infty} \psi_m \frac{\partial \psi_n^*}{\partial x} \, dx$$

$$= i\hbar \int_{-\infty}^{\infty} \psi_m \frac{\partial \psi_n^*}{\partial x} \, dx = \int_{-\infty}^{\infty} \psi_m (i\hbar \frac{\partial \psi_n^*}{\partial x}) \, dx$$

$$= \int_{-\infty}^{\infty} \psi_m \, (-i\hbar \frac{\partial \psi_n}{\partial x})^* \, dx$$

$$= \int_{-\infty}^{\infty} \psi_m \, (\hat{p}_x \psi_n)^* \, dx$$

H.W: Verify wither the operator $\frac{\partial}{\partial x}$ is a Hermitian or not.

Example: Establish the following operator equation; $\frac{\partial}{\partial x} x^n = n\, x^{n-1} + x^n \frac{\partial}{\partial x}$ and then show that; $[\frac{\partial}{\partial x}, x^n] = n\, x^{n-1}$.

Solution:

For any function for (x), say $\psi(x)$ one can write;

$$(\frac{\partial}{\partial x} x^n)\psi(x) = \frac{\partial}{\partial x}(x^n \psi(x))$$

$$= n\, x^{n-1} \psi(x) + x^n \frac{\partial \psi(x)}{\partial x}$$

Since this equation must be valid for any function of (x) thus the operator equation is;

$$\frac{\partial}{\partial x} x^n = n\, x^{n-1} + x^n \frac{\partial}{\partial x}$$

Consequently;

$$[\frac{\partial}{\partial x}, x^n]\psi(x) = (\frac{\partial}{\partial x} x^n \psi(x)) - (x^n \frac{\partial}{\partial x})\, \psi(x)$$

$$= nx^{n-1}\psi(x) + x^n \frac{\partial \psi(x)}{\partial x} - x^n \frac{\partial \psi(x)}{\partial x}$$

$$= nx^{n-1}\psi(x)$$

Example: Evaluate the commutation relation; $[\frac{\partial}{\partial x}, \frac{\partial^n}{\partial x^n}]$.

Solution:

$$[\frac{\partial}{\partial x}, \frac{\partial^n}{\partial x^n}]\psi(x) = (\frac{\partial}{\partial x} \frac{\partial^n}{\partial x^n})\, \psi(x) - (\frac{\partial^n}{\partial x^n} \frac{\partial}{\partial x})\psi(x)$$

$$= \frac{\partial}{\partial x}(\frac{\partial^n \psi(x)}{\partial x^n}) - \frac{\partial^n}{\partial x^n}(\frac{\partial \psi(x)}{\partial x})$$

$$= \frac{\partial^{n+1}\psi(x)}{\partial x^{n+1}} - \frac{\partial^{n+1}\psi(x)}{\partial x^{n+1}}$$

$$= 0$$

The tow operators $\frac{\partial}{\partial x}$ and $\frac{\partial^n}{\partial x^n}$ are not commute

Example: Verify the operator equation

1. $(\frac{d}{dy} - y)(\frac{d}{dy} + y) = \frac{d^2}{dy^2} - y^2 + 1$
2. $(\frac{d}{dy} + y)(\frac{d}{dy} - y) = \frac{d^2}{dy^2} - y^2 - 1$ **(H.W.)**

Solution:

1.

$$(\frac{d}{dy} - y)(\frac{d}{dy} + y)\ \psi_n(y)$$

$$= (\frac{d}{dy} - y)\{(\frac{d}{dy} + y)\ \psi_n(y)\}$$

$$= (\frac{d}{dy} - y)\{\frac{d\psi_n(y)}{dy} + y\psi_n(y)\}$$

$$= \frac{d}{dy}\{\frac{d\psi_n(y)}{dy} + y\psi_n(y)\} - y\{\frac{d\psi_n(y)}{dy} + y\psi_n(y)\}$$

$$= \frac{d^2\psi_n(y)}{dy^2} + \frac{d}{dy} y\psi_n(y) - y\frac{d\psi_n(y)}{dy} - y^2\psi_n(y)$$

$$= \frac{d^2\psi_n(y)}{dy^2} + \psi_n(y) + y\frac{d\psi_n(y)}{dy} - y\frac{d\psi_n(y)}{dy} - y^2\psi_n(y)$$

$$\frac{d^2\psi_n(y)}{dy^2} - y^2\psi_n(y) + \psi_n(y) = (\frac{d^2}{dy^2} - y^2 + 1)\ \psi_n(y)$$

Since $\psi(y)$ is an arbitrary function of *y*, so we can write the operator equation as:

$$(\frac{d}{dy} - y)(\frac{d}{dy} + y) = \frac{d^2}{dy^2} - y^2 + 1$$

Example: Show that $\psi(x)=e^{-\frac{1}{2}x^2}$ is an eigen function of the operator $\frac{\partial^2}{\partial x^2}-x^2$ and find the corresponding eigen value.

Solution:

$$\hat{A}\psi_n(x)=a_n\,\psi_n(x)$$
$$=\left(\frac{\partial^2}{\partial x^2}-x^2\right)e^{-\frac{1}{2}x^2}$$
$$=\frac{\partial^2}{\partial x^2}e^{-\frac{1}{2}x^2}-x^2e^{-\frac{1}{2}x^2}$$
$$=\frac{\partial}{\partial x}\left(-x\,e^{-\frac{1}{2}x^2}\right)-x^2\,e^{-\frac{1}{2}x^2}$$
$$=-e^{-\frac{1}{2}x^2}+x^2\,e^{-\frac{1}{2}x^2}-x^2\,e^{-\frac{1}{2}x^2}$$
$$=-e^{-\frac{1}{2}x^2}$$
$$=-\psi_n(x)$$

Since the function $\psi(x)=e^{-\frac{1}{2}x^2}$ remained unaltered under the operator, thus, it is an eigen function of $\hat{A}$ and its corresponding eigen value is $a_n=-1$.

2.8 Observables and Operators

Observable define as that physical quantity (dynamical variable) which in principle can be measured, such as the energy, momentum, position, angular momentum, …. etc. In quantum mechanics observables represented, generally, by a correspondence Hermitian operator, see the table below.

Observable	C.M.R	Q.M.R
Position	x	$\hat{x}$
Momentum	$p_x=m\dot{x}$	$\hat{p}_x=-i\hbar\frac{\partial}{\partial x}$
Total energy	$E=T+V(x)$	$\hat{H}=\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)$ Or $\hat{E}=i\hbar\frac{\partial}{\partial t}$

For each observable A represented by the quantum mechanical operator $\widehat{A}$ it is possible to setup an eign value equation as follows;

$$\hat{A}\psi_n(x) = a_n \psi_n(x)$$

The physical interpretation of the eigen value equation is that; the operator $\widehat{A}$ make a correspondence measurement for the observable A for the system in state n which describe by the wave function ψ_n. The possible result of the measurement process is the eigen value a_n .

$$\hat{A}\psi_n(x) = a_n \psi_n(x)$$

make a measurement ($\hat{A}$) — measurement result (a_n)

on a system in state n ($\psi_n(x)$)

Accordingly, when the momentum operator $\hat{p}$ operate on a system in state n and this system described by the wave function ψ_n it will measure the momentum of the system in that state n . i.e.

$$\hat{p}\,\psi_n = p_n\psi_n$$

And so,

$$\left.\begin{aligned} \widehat{p^2}\,\psi_n &= p_n^2\psi_n \\ \widehat{H}\,\psi_n &= E_n\psi_n \\ \hat{r}\,\psi_n &= r_n\psi_n \end{aligned}\right\} \qquad \text{............ (2-15)}$$

Recall equations (2-4), (2-5), (2-6) and (2-10) one can directly realize the following;

$$-i\hbar\frac{\partial\psi(x,t)}{\partial x} = p_x\,\psi(x,t) \qquad \text{............(2-4)}$$

$$-\hbar^2\frac{\partial^2\psi(x,t)}{\partial x^2} = p_x^2\,\psi(x,t) \qquad \text{............(2-5)}$$

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = E\,\psi(x,t) \qquad \text{............(2-6)}$$

$$\left[\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi(x) = E\,\psi(x) \qquad \text{............(2-10)}$$

$$\hat{p}_x = -i\hbar\frac{\partial}{\partial x}$$

$$\left.\begin{aligned}\hat{p}_x^2 &= -\hbar^2 \frac{\partial^2}{\partial x^2} \\ \hat{H}\psi_n &= i\hbar \frac{\partial}{\partial t} = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(\hat{x})\end{aligned}\right\} \quad \ldots\ldots\ldots\ldots (2\text{-}16a)$$

Similarly;

$$\hat{x}\psi_n = x_n\psi_n$$

In three dimensions the last four equations become;

$$\left.\begin{aligned}\hat{p} &= -i\hbar\nabla \\ \hat{p}^2 &= -\hbar^2\nabla^2 \\ \hat{H}\psi_n &= i\hbar\frac{\partial}{\partial t} = \frac{-\hbar^2}{2m}\nabla^2 + V(\hat{r}) \\ \hat{r}\psi_n &= r_n\psi_n\end{aligned}\right\} \quad \ldots\ldots\ldots\ldots (2\text{-}16b)$$

By this procedure, however, we can build up the quantum mechanical representation corresponds to any classical mechanic's observable or relation. For example;

$$E = H = T + V$$

$$H = \frac{p^2}{2m} + V(r)$$

$$i\hbar\frac{\partial}{\partial t} = \frac{-\hbar^2}{2m}\nabla^2 + V(\hat{r})$$

$$i\hbar\frac{\partial}{\partial t}\psi = \frac{-\hbar^2}{2m}\nabla^2\psi + V(\hat{r})\psi$$

Which is the T.D.S.E. When ψ is time independent function the L.H.S. of last equation can be replaced by; $E\psi$ and then one can get the T.I.D.S.E. as follows;

$$E\psi = \frac{-\hbar^2}{2m}\nabla^2\psi + V(\hat{r})\psi$$

H.W:

1. By using the classical relation $p_x = m\dot{x}$ find the mathematical formula of the velocity operator.
2. By using the classical relation $\vec{L} = \vec{r} \times \vec{p}$ show that;

$$L_x = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right),\ L_y = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) \text{ and } L_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$$