Hamiltonian operator:-

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

$$\hat{H} = \hat{T} + \hat{V}$$

$$= -\frac{\hbar^2}{2m}\nabla^2 + \hat{V}$$

$(\because p = -i\hbar\nabla)$

$$\hat{H}\psi = i\hbar\frac{\partial\psi}{\partial t}$$

$\Rightarrow -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = i\hbar\frac{\partial\psi}{\partial t}$

Parity operator:-

$$\hat{P} f(x) = f(-x)$$

$\rightarrow \hat{P}$ is parity operator.

a) Parity operator $\hat{P}$ is Hermitian:

$$\int \psi^*(\vec{r})\,\hat{P}\,\phi(\vec{r})\,d\vec{r}$$

$$= \int \psi^*(\vec{r})\,\phi(-\vec{r})\,d\vec{r} = \int \psi^*(-\vec{r})\,\phi(\vec{r})\,d\vec{r}$$

$$= \int [\hat{P}\,\psi(\vec{r})]^*\,\phi(\vec{r})\,d\vec{r}$$

(b) Eigen values of $\hat{P}$:-

$$\hat{P}\,\psi_\alpha(\vec{r}) = \alpha\,\psi_\alpha(\vec{r})$$

$\rightarrow \alpha$ is an eigen value.

$$\hat{P} f(-\vec{r}) = f(\vec{r})$$

$$\hat{P}[\hat{P} f(-\vec{r})] = \hat{P} f(\vec{r}) = f(-\vec{r}) = I f(-\vec{r})$$

$$\Rightarrow P^2 f(-\vec{r}) = \hat{I} f(-\vec{r})$$

$\Rightarrow P^2 = \hat{I} \rightarrow$ unit operator.

$$P^2\psi_\alpha(\vec{r}) = \alpha\, \hat{P}\psi_\alpha(\vec{r}) = \alpha^2\psi_\alpha(\vec{r}) \cancel{= \psi_\alpha(\vec{r})}$$
$$= \psi_\alpha(\vec{r})$$

$$\alpha^2 = 1$$
$$\therefore \alpha = \pm 1$$

If ψ_+ and ψ_- be the eigen function related to the eigenvalues +1 and -1 respectively.

$$\hat{P}\psi_+(\vec{r}) = \psi_+(\vec{r}) \quad , \quad \hat{P}\psi_-(\vec{r}) = -\psi_-(\vec{r})$$
$$\Rightarrow \psi_+(-\vec{r}) = \psi_+(\vec{r}) \quad , \quad \psi_-(-\vec{r}) = -\psi_-(\vec{r})$$

Thus $\psi_+(\vec{r})$ is an even function of $(\vec{r})$ and $\psi_-(\vec{r})$ is an odd function of $(\vec{r})$. The eigenfunctions ψ_+ are said to have <u>even parity</u> and ψ_- have <u>odd parity</u>.

$\psi(\vec{r})$ can be written as

$$\psi(\vec{r}) = \psi_+(\vec{r}) + \psi_-(\vec{r})$$

here, $\psi_+(\vec{r}) = \frac{1}{2}\left[\psi(\vec{r}) + \psi(-\vec{r})\right]$ has even parity

$\psi_-(\vec{r}) = \frac{1}{2}\left[\psi(\vec{r}) - \psi(-\vec{r})\right]$ has odd parity.

<u>Angular momentum operator:-</u>

$(\because L = r \times P)$

$$\hat{L} = \vec{r} \times (-i\hbar\nabla) = -i\hbar\,\vec{r}\times\nabla \qquad P = -i\hbar\frac{\partial}{\partial x}$$

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If L_x, L_y and L_z be the components $\vec{L}$ then,

$$\vec{L} = \hat{i}\hat{L}_x + \hat{j}\hat{L}_y + \hat{k}\hat{L}_z$$

$$= -i\hbar \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ x & y & z \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \end{vmatrix}$$

$$\hat{L}_x = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$$

$$\hat{L}_y = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)$$

$$\hat{L}_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$$

It is to be noted that L_x, L_y, L_z do not commute each other.

$$[\hat{L}_x, \hat{L}_y] = i\hbar\hat{L}_z$$

$$[\hat{L}_y, \hat{L}_z] = i\hbar\hat{L}_x$$

$$[\hat{L}_z, \hat{L}_x] = i\hbar\hat{L}_y$$

The components $\hat{L}_x$, $\hat{L}_y$, $\hat{L}_z$ of $\hat{L}$ commute with the Hamiltonian of the system.

$$[\hat{H}, \hat{L}_x] = 0, \quad [\hat{H}, \hat{L}_y] = 0, \quad [\hat{H}, \hat{L}_z] = 0$$

In spherical polar co-ordinates

$$\hat{L}_x = i\hbar\left[\sin\phi\frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right]$$

$$\hat{L}_y = -i\hbar\left[\cos\phi\frac{\partial}{\partial\theta} - \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right]$$

& $\hat{L}_z = -i\hbar \frac{\partial}{\partial \phi}$

We can prove that,

$$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$$

$$= -\hbar^2 \left[\frac{1}{\sin\theta} \frac{\partial}{\partial \theta} \left(\sin\theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial \phi^2} \right]$$

Further $\hat{L}^2$ commute with each of $\hat{L}_x, \hat{L}_y, \hat{L}_z$

i.e $[\hat{L}^2, \hat{L}_x] = 0$

$[\hat{L}^2, \hat{L}_y] = 0$

& $[\hat{L}^2, \hat{L}_z] = 0$

(a) Ladder operator L_+ & L_-

$$\hat{L}_+ = \hat{L}_x + i\hat{L}_y$$

& $$\hat{L}_- = \hat{L}_x - i\hat{L}_y$$

Commutation of $\hat{L}_z$ with $\hat{L}_+$ & $\hat{L}_-$

$$[\hat{L}_z, \hat{L}_+] = [L_z, L_x + iL_y]$$

$$= [L_z, L_x] + i[L_z, L_y]$$

$$= i\hbar L_y + i(-i\hbar L_x)$$

$$= i\hbar L_y + \hbar L_x$$

$$= \hbar [L_x + iL_y]$$

$$= \hbar L_+$$

$$\boxed{\therefore [\hat{L}_z, \hat{L}_+] = \hbar L_+}$$

Similarly, we can show that

$$[\hat{L}_z, \hat{L}_-] = -\hbar \hat{L}_-$$

$$\& \quad [\hat{L}_+, \hat{L}_-] = 2\hbar \hat{L}_z$$

(b) Commutation of $\hat{L}_x, \hat{L}_y, \hat{L}_z$ with $\hat{x}, \hat{y}, \hat{z}$.

$$[\hat{L}_x, \hat{x}] = (\hat{L}_x \hat{x} - \hat{x}\hat{L}_x)$$

$$= \left[y\left(\frac{\hbar}{i}\frac{\partial}{\partial z}\right) - z\left(\frac{\hbar}{i}\frac{\partial}{\partial y}\right)\right]$$

$$- x\left[y\left(\frac{\hbar}{i}\frac{\partial}{\partial z}\right) - z\left(\frac{\hbar}{i}\frac{\partial}{\partial z}\right)\right]$$

If $\psi(x)$ is a function of x then

$$(\hat{L}_x\hat{x} - \hat{x}\hat{L}_x)\psi = \left[y\left(\frac{\hbar}{i}\frac{\partial}{\partial z}(x\psi)\right) - z\left(\frac{\hbar}{i}\frac{\partial}{\partial y}(x\psi)\right)\right]$$

$$- x\left[y\left(\frac{\hbar}{i}\frac{\partial \psi}{\partial z}\right) - z\left(\frac{\hbar}{i}\frac{\partial \psi}{\partial y}\right)\right]$$

$$= 0$$

$$\Rightarrow [\hat{L}_x, \hat{x}] = 0$$

Similarly, $[\hat{L}_x, \hat{y}] = i\hbar z$, $[\hat{L}_x, \hat{z}] = -i\hbar y$

$[\hat{L}_y, \hat{y}] = 0$, $[\hat{L}_y, \hat{z}] = i\hbar x$

$[\hat{L}_y, \hat{x}] = -i\hbar z$, $[\hat{L}_z, \hat{y}] = -i\hbar x$

$[\hat{L}_z, \hat{z}] = 0$, $[\hat{L}_z, \hat{x}] = i\hbar y$