**Modern Physics**

### ***Normalization of wave function***

We know that $\psi(\vec{r},t)$ gives the probability amplitude of finding the particle at the position $\vec{r}$ , at the time instant $t$. Thus $\psi^*\psi d\tau$ gives the probability of obtaining the particle in the volume $d\tau$ in the time instant t and hence we get,

$$\iiint_V \psi^*\psi d\tau = 1$$

if the particle exists. This is known as Normalization of wave function. To ensure the existence of the particle anywhere in the universe we need the normalization of the wave function.

### ***Expectation Value***

The expectation value of an operator is the average of a large number of measurements or it is the mathematical expectation for the result of a single measurement which is equal to the average of the results of the large number of measurements on an independent system. If $\psi$ is the wave function that describes a particle, then the expectation value

$$<\chi>=\frac{\iiint \psi^*\hat{\chi}\psi d\tau}{\iiint \psi^*\psi d\tau}$$

### ***Operators in Quantum Mechanics***

It is to be noted that all physically observable quantities in quantum mechanics can be represented by operators.

$$<p_x>=\int \psi^*(-i\hbar\frac{\partial}{\partial x})\psi dx$$

$$<p_y>=\int \psi^*(-i\hbar\frac{\partial}{\partial y})\psi dy$$

$$<p_z>=\int \psi^*(-i\hbar\frac{\partial}{\partial z})\psi dz$$

These above three equations are equivalent to the single equation

$$<\vec{p}>=\int \psi^*(-i\hbar\vec{\nabla})\psi dr$$

Therefore, momentum operator

$$\vec{p}=-i\hbar\vec{\nabla}$$

The total energy of a particle moving in a potential $V$ , $E = \frac{p^2}{2m} + V$ to which is associated the Hamiltonian operator,

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

Thus,

$$< E >=< \frac{p^2}{2m} > + < V >$$

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

Therefore, energy operator

$$E = i\hbar\frac{\partial}{\partial t}$$

It is to be noted that energy, momentum etc. all these physically observable quantities are represented by operators and these operators must be Hermitian. If an operator $\hat{A}$ satisfies the condition,

$$\int \psi^* \hat{A}\psi dr = \int (\hat{A}\psi)^* \psi dr$$

then the operator $\hat{A}$ associated with the dynamical quantity must be hermitian. For example let us check, $\hat{A} = \frac{d}{dx}$ is it hermitian or not?

$$\int_{-\infty}^{+\infty} (\frac{d\psi}{dx})^* \psi dx = [\psi\psi^*]_{-\infty}^{+\infty} - \int_{-\infty}^{+\infty} \frac{d\psi}{dx}\psi^* dx$$

As $|\psi| \to 0$ when $|x| \to \infty$ . Therefore we get,

$$\int_{-\infty}^{+\infty} (\frac{d\psi}{dx})^* \psi dx = \int_{-\infty}^{+\infty} \psi^*(-\frac{d}{dx})\psi dx$$

and thus $\hat{A} = \frac{d}{dx}$ is not an hermitian operator.

By considering another example, a particle moving in an one dimension, described by the wave function $\psi(x, t)$ , normalised to unity and suppose we wish to check whether the operator $xp_x$ is hermitian or not.

$$\int_{-\infty}^{+\infty} \psi^* x(-i\hbar\frac{\partial}{\partial x})\psi dx$$

Integrating by parts we have,

$$= [-i\hbar x\psi^*\psi]_{-\infty}^{+\infty} + i\hbar\int_{-\infty}^{+\infty} \psi\frac{\partial}{\partial x}(x\psi^*)dx$$

The integrated part vanishes as $|\psi| \to 0$ when $|x| \to \infty$ . Thus,

$$\int_{-\infty}^{+\infty} \psi^* x(-i\hbar \frac{\partial}{\partial x})\psi dx = i\hbar \int_{-\infty}^{+\infty} \psi x(\frac{\partial \psi}{\partial x})^* dx + i\hbar \int_{-\infty}^{+\infty} \psi^* \psi dx$$

Since the second term on the right side is non zero, and therefore the operator $xp_x$ is not hermitian.

It is important to say that in contrast to classical mechanics, where all quantities obey ordinary algebra, we are dealing in quantum mechanics with operators, which in general do not commute with each other. That is, if $A$ and $B$ are two operators, the product $AB$ is not necessarily equal to the product $BA$ . The commutator of two operators $A$ and $B$ is defined as the difference $AB - BA$ and is denoted by the symbol $[A, B]$

$$[A, B] = AB - BA$$

If their commutators vanishes, then the two operators $A$ and $B$ commute, i.e.

$$AB = BA$$

For an example of operators which do not commute, let us consider the two operators $x$ and $p_x = -i\hbar \frac{\partial}{\partial x}$ . For any wave function $\psi(x, t)$ , we have

$$[x, p_x]\psi = (xp_x - p_x x)\psi$$

$$= -i\hbar[x\frac{\partial \psi}{\partial x} - \frac{\partial}{\partial x}(x, \psi)]$$

$$= i\hbar\psi$$

so that we may write the relation as,

$$[x, p_x] = i\hbar$$

More generally we can write,

$$[x, p_x] = [y, p_y] = [z, p_z] = i\hbar$$