

Quantum Mechanics-Section17

Dr. Jayanta Das

Department of Physics, Maharaja College, Ara, Bihar-802301

1 Expectation Values

When the probability density $P(x, t)$ is known, the expectation values of any function $f(x)$ may be calculated as follows:

$$\langle f(x) \rangle = \int dx f(x) P(x, t) = \int dx \psi^*(x, t) f(x) \psi(x, t)$$

The integral is only defined under convergence. Also, we shall assume that the wavefunction $\psi(x)$ and all of their derivatives vanish sufficiently rapidly at infinity.

The momentum may be expressed in terms of x , this helps us to calculate the expectation value of momentum. As we know classically

$$p = mv = m \frac{dx}{dt}$$

We may write

$$\langle p \rangle = m \frac{d}{dt} \langle x \rangle = m \frac{d}{dt} \int dx \psi^*(x, t) x \psi(x, t)$$

This gives

$$\langle p \rangle = m \int_{-\infty}^{\infty} dx \left(\frac{\partial \psi^*}{\partial t} x \psi + \psi^* x \frac{\partial \psi}{\partial t} \right)$$

Note that there is no $\frac{dx}{dt}$ term under the integral sign. The only quantity that varies with time is $\psi(x, t)$, and it is this variation that gives rise to a change in $\langle x \rangle$ with time. As we know

$$i\hbar \frac{\partial \psi(x, t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x, t)}{\partial x^2}$$

using this equation we obtain:

$$\langle p \rangle = \frac{\hbar}{2i} \int_{-\infty}^{\infty} dx \left(\frac{\partial^2 \psi^*}{\partial x^2} x \psi - \psi^* x \frac{\partial^2 \psi}{\partial x^2} \right)$$

Now,

$$\begin{aligned} \frac{\partial^2 \psi^*}{\partial x^2} x \psi &= \frac{\partial}{\partial x} \left(\frac{\partial \psi^*}{\partial x} x \psi \right) - \frac{\partial \psi^*}{\partial x} \psi - \frac{\partial \psi^*}{\partial x} x \frac{\partial \psi}{\partial x} \\ \frac{\partial^2 \psi^*}{\partial x^2} x \psi &= \frac{\partial}{\partial x} \left(\frac{\partial \psi^*}{\partial x} x \psi \right) - \frac{\partial}{\partial x} (\psi^* \psi) + \psi^* \frac{\partial \psi}{\partial x} - \frac{\partial}{\partial x} \left(\psi^* x \frac{\partial \psi}{\partial x} \right) + \psi^* \frac{\partial \psi}{\partial x} + \psi^* x \frac{\partial^2 \psi}{\partial x^2} \end{aligned}$$

Hence the integrand has the form

$$\frac{\partial}{\partial x} \left(\frac{\partial \psi^*}{\partial x} x \psi - \psi^* x \frac{\partial \psi}{\partial x} - \psi^* \psi \right) + 2\psi^* \frac{\partial \psi}{\partial x}$$

The integral of the derivatives vanishes for square integrable functions, therefore the first term vanishes under integration. Hence,

$$\langle p \rangle = \int dx \psi^*(x, t) \frac{\hbar}{i} \frac{\partial}{\partial x} \psi(x, t)$$

This suggests that the momentum is represented by operator

$$p = \frac{\hbar}{i} \frac{\partial}{\partial x}$$

With the same logic

$$\langle p^2 \rangle = \int dx \psi^*(x,t) \left(-\hbar^2 \frac{\partial^2}{\partial x^2} \right) \psi(x,t)$$

References

- [1] Quantum Physics of Atoms, Molecules, Solids, Nuclei, and Particles, Authors: R. Eisberg, R. Resnick, Publisher: Wiley
- [2] Quantum Physics, Author: Stephen Gasiorowicz, Publisher: John Wiley and Sons
- [3] Quantum Mechanics: Theory and Applications, Authors: A. Ghatak, S. Lokanathan, Publisher: Trinity Press
- [4] Modern Quantum Mechanics, Author: J.J. Sakurai, Publisher: Benjamin/Cummings Publisher.
- [5] A textbook of Quantum Mechanics, Author: P M Mathews, K Venkatesan, Publisher: TMG

1

¹Figures are collected from online resources.