Physics 371 Lecture 5

Observables, operators, and expectation values

The wavefunction ψ, being complex, is evidently not directly observable. What is its connection to measureable quantities?

$$\rho(x,t) = \psi^*(x,t)\,\psi(x,t)$$

$$\langle f(x,t)\rangle = \int dx\, f(x,t)\,\rho(x,t)$$

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

(assuming ψ is normalized.)

e.g. $\langle x \rangle = \int dx\, \Psi^*(x,t)\, x\, \Psi(x,t)$.

- $\langle x \rangle$ = the average value obtained after many measurements, or <u>expectation value</u>.

Similarly, the average value of any function of p_x can be obtained from the Fourier

- transform $\tilde{\Psi}(k)$, $\rho(k) = |\tilde{\Psi}(k)|^2$

$$\langle g(p_x) \rangle = \langle g(\hbar k) \rangle = \int \frac{dk}{2\pi}\, g(\hbar k)\cdot \rho(k)$$

e.g. $\langle p_x \rangle = \int \frac{dk}{2\pi}\, \tilde{\Psi}^*(k)\, \hbar k\, \tilde{\Psi}(k)$.

Q: What about functions of x & p_x?

- To answer this question, it is

useful to be able to write

- $\langle p_x \rangle$ in terms of $\psi(x)$:

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

Proof: $\langle p_x \rangle = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \tilde{\psi}^*(k)\, \hbar k\, \tilde{\psi}(k)$

- use $\tilde{\psi}(k) = \int_{-\infty}^{\infty} dx\, \psi(x) e^{-ikx}$

$$\tilde{\psi}^*(k) = \int_{-\infty}^{\infty} dx'\, \psi^*(x')\, e^{ikx'}$$

$$\langle p_x \rangle = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \int_{-\infty}^{\infty} dx'\, \psi^*(x') e^{ikx'} \int_{-\infty}^{\infty} dx\, \psi(x) e^{-ikx}\, \hbar k$$

- Now, $\frac{\partial}{\partial x}\left(\psi(x) e^{-ikx}\right) = \frac{\partial \psi}{\partial x} e^{-ikx} - ik\, \psi(x) e^{-ikx}$

$$e^{-ikx}\hbar k\,\psi(x) = \frac{\hbar}{i}\frac{\partial\psi}{\partial x}e^{-ikx} - \frac{\hbar}{i}\frac{\partial}{\partial x}\left(\psi(x)e^{-ikx}\right)$$

$$\int_{-\infty}^{\infty} dx\ \hbar k\,\psi(x)e^{-ikx} = \int_{-\infty}^{\infty} dx\ \frac{\hbar}{i}\frac{\partial\psi}{\partial x}e^{-ikx}$$

$$- \frac{\hbar}{i}\psi(x)\,e^{-ikx}\Big]_{-\infty}^{\infty} \to 0$$

$$\langle p_x\rangle = \int_{-\infty}^{\infty}\frac{dk}{2\pi}\int_{-\infty}^{\infty}dx'\,\psi^*(x')e^{ikx'}\int_{-\infty}^{\infty}dx\ \frac{\hbar}{i}\frac{\partial\psi}{\partial x}e^{-ikx}$$

$$= \int_{-\infty}^{\infty}dx\int_{-\infty}^{\infty}dx'\ \psi^*(x')\,\frac{\hbar}{i}\frac{\partial\psi}{\partial x}\underbrace{\int_{-\infty}^{\infty}\frac{dk}{2\pi}e^{ik(x'-x)}}_{\delta(x-x')}$$

$$\langle p_x\rangle = \int_{-\infty}^{\infty}dx\ \psi^*(x)\,\frac{\hbar}{i}\frac{\partial\psi}{\partial x} \qquad \text{Q.E.D.}$$

- If we identify

$$\hat{p}_x = \frac{\hbar}{i}\frac{\partial}{\partial x} \quad \text{(momentum operator)},$$

then we have

$$\langle p_x \rangle = \int dx\, \psi^*(x)\, \hat{p}_x\, \psi(x)$$

Correspondence principle

- For any function $f(x, p_x, t)$, the quantum mechanical expectation value is

$$\boxed{\langle f(x, p_x, t) \rangle = \int dx\, \psi^*(x,t)\, f\left(x, \frac{\hbar}{i}\frac{\partial}{\partial x}, t\right) \psi(x,t)}$$

Example: Kinetic energy

- $$\hat{T} = \frac{\hat{p}_x^2}{2m} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} \quad \text{(in 1D)}$$

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

Energy: $$\hat{H} = \frac{\hat{p}_x^2}{2m} + V(x,t)$$

- $$\langle E(t) \rangle = \langle \hat{H} \rangle = \int dx\, \psi^*(x,t)\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)\right)\psi(x,t)$$

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

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

- Q: Can $\langle E \rangle$ be complex?

$$\langle E \rangle = A + iB$$

$$\langle E \rangle^* = A - iB$$

$$iB = \frac{1}{2}\left(\langle E \rangle - \langle E \rangle^* \right) = i\,\mathrm{Im}\langle E \rangle$$

$$\langle E \rangle - \langle E \rangle^* = i\hbar \int_{-\infty}^{\infty} dx \left(\psi^* \frac{\partial \psi}{\partial t} + \psi \frac{\partial \psi^*}{\partial t} \right)$$

$$= i\hbar \frac{d}{dt} \int_{-\infty}^{\infty} dx \; \psi^* \psi$$

$$= i\hbar \frac{dP}{dt} = 0,$$

provided particles are not entering or leaving the system at $x = \pm\infty$. $\langle E \rangle$ must be real for a closed system.

- The same holds true for any observable $f(x, p_x, t)$

$$\text{Im}\langle f(x, p_x, t)\rangle = 0.$$

Operator ordering

- One ambiguity in the application of the correspondence principle is that quantum mechanics operators, unlike classical variables, do not always commute. For example,

$$\hat{x}\hat{p}_x \psi(x) = x\frac{\hbar}{i}\psi'(x)$$

- but $\hat{p}_x \hat{x}\psi(x) = \frac{\hbar}{i}\frac{\partial}{\partial x}\left(x\psi(x)\right) = \frac{\hbar}{i}\psi(x) + x\frac{\hbar}{i}\psi'(x)$

Define

$$[\hat{x}, \hat{p}_x] \equiv \hat{x}\hat{p}_x - \hat{p}_x\hat{x}$$

$$(\hat{x}\hat{p}_x - \hat{p}_x\hat{x})\psi(x) = i\hbar\psi(x)$$

$$\Rightarrow [\hat{x}, \hat{p}_x] = i\hbar$$

Uncertainty

$$\langle x \rangle = \int dx\, \psi^* x \psi$$

$$\langle x^2 \rangle = \int dx\, \psi^* x^2 \psi$$

$$\Delta x = \sqrt{\langle (x - \langle x \rangle)^2 \rangle} = \text{standard deviation}$$

$$= \sqrt{\langle x^2 - 2x\langle x \rangle + \langle x \rangle^2 \rangle}$$

$$= \sqrt{\langle x^2 \rangle - 2\langle x \rangle\langle x \rangle + \langle x \rangle^2}$$

$$= \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$$