

Physics 570A Lecture 7

Observables, operators, and expectation values

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

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

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

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

(assuming ψ is normalized.)

$$\text{e.g. } \langle x \rangle = \int dx \psi^*(x,t) x \psi(x,t) \quad |^2$$

$\langle x \rangle$ = the average value obtained after many measurements, or expectation value.

Similarly, the average value of any function of P_x can be obtained from the Fourier transform $\tilde{\psi}(k)$, $\rho(k) = |\tilde{\psi}(k)|^2$

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

$$\text{e.g. } \langle P_x \rangle = \int \frac{dk}{2\pi} \tilde{\psi}^*(k) \hbar k \tilde{\psi}(k).$$

Q^o What about functions of x & P_x ?

To answer this question, it is

useful to be able to write (3)

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

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

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

$$e^{-ikx} \frac{1}{\hbar k} \psi(x) = \frac{1}{i} \frac{\partial \psi}{\partial x} e^{-ikx} - \frac{1}{i} \frac{\partial}{\partial x} (\psi(x) e^{-ikx}) \quad \psi$$

$$\int_{-\infty}^{\infty} dx \frac{1}{\hbar k} \psi(x) e^{-ikx} = \int_{-\infty}^{\infty} dx \frac{1}{i} \frac{\partial \psi}{\partial x} e^{-ikx}$$

$$- \left. \frac{1}{i} \psi(x) e^{-ikx} \right]_{-\infty}^{\infty} \rightarrow 0$$

$$\langle P_x \rangle = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \int_{-\infty}^{\infty} dx' \psi^*(x') e^{ikx'} \int_{-\infty}^{\infty} dx \frac{1}{i} \frac{\partial \psi}{\partial x} e^{-ikx}$$

$$= \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dx' \psi^*(x') \frac{1}{i} \frac{\partial \psi}{\partial x} \underbrace{\int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ik(x'-x)}}_{\delta(x-x')}$$

$$\langle P_x \rangle = \int_{-\infty}^{\infty} dx \psi^*(x) \frac{1}{i} \frac{\partial \psi}{\partial x} \quad \text{Q.E.D.}$$

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

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

Example: Kinetic energy [6]

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

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

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?

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

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

$$iB = \frac{1}{2} (\langle E \rangle - \langle E \rangle^*) = i \text{Im} \langle E \rangle$$

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

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

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

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 (2)
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 mechanical operators, unlike classical variables, do not always commute. For example,

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

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

Define

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

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

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

Uncertainty

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

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

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

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

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

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