Lecture-XXIV

Quantum Mechanics Expectation values and uncertainty

Expectation values

We are looking for expectation values of position and momentum knowing the state of the particle, i,e., the wave function $\psi(x,t)$.

Position expectation: $\langle x \rangle = \int_{-\infty}^{+\infty} x |\Psi(x, t)|^2 dx$. What exactly does this mean?

It does not mean that if one measures the position of one particle over and over again, the average of the results will be given by $\int x |\Psi|^2 dx$

On the contrary, the first measurement (whose outcome is indeterminate) will collapse the wave function to a spike at the value actually obtained, and the subsequent measurements (if they're performed quickly) will simply repeat that same result.

Rather, <x> is the average of measurements performed on particles all in the state ψ , which means that either you must find some way of returning the particle to its original state after each measurement, or else you prepare a whole ensemble of particles, each in the same state ψ , and measure the positions of all of them: <x> is the average of these results.

The position expectation may also be written as: $\langle x \rangle = \int_{-\infty}^{+\infty} x \psi^* \psi dx = \int_{-\infty}^{+\infty} \psi^* x \psi dx$

Momentum expectation:

Classically: $p = mv = m\frac{dx}{dt}$ Quantum mechanically, it is Let us try: $\langle p \rangle = m\frac{d}{dt} \langle x \rangle = m\frac{d}{dt} \int_{-\infty}^{\infty} dx \, \psi^*(x, t) x \psi(x, t) \begin{bmatrix} d < x > /dt & \text{is the velocity of the expectation value of } x, & \text{not the velocity of the particle.} \end{bmatrix}$

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

Note that there is no dx/dt 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. Use the Schrodinger equation and its complex conjugate to evaluate the above and we 102 100 2.1 have $\langle p$

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

Now

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

This means that the integrand has the form

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

Because the wave functions vanish at infinity, the first term does not contribute, and the integral gives $\sum_{n=1}^{\infty} (1-n)^{n}$

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

As the position expectation was represented by $\langle x \rangle = \int_{-\infty}^{+\infty} \psi^* x \psi dx$

This suggests that the momentum be represented by the differential operator

$$\hat{p} \to -i\hbar \frac{\partial}{\partial x}$$

and the position operator be represented by $\hat{x} \rightarrow x$

To calculate expectation values, operate the given operator on the wave function, have a product with the complex conjugate of the wave function and integrate.

$$\langle p \rangle = \int \psi^* \hat{p} \psi dx$$
 and $\langle x \rangle = \int \psi^* \hat{x} \psi dx$

What about other dynamical variables?

Expectation of other dynamical variables

To calculate the expectation value of any dynamical quantity, first express in terms of operators x and p, then insert the resulting operator between ψ^* and ψ , and integrate:

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

For example: Kinetic energy $T = \frac{1}{2}mv^2 = \frac{p^2}{2m} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$
Therefore, $\langle T \rangle = \frac{-\hbar^2}{2m}\int \Psi^* \frac{\partial^2 \Psi}{\partial x^2} dx$.
Hamiltonian: $H = K + V = \frac{p^2}{2m} + V(x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$

Hamiltonian: $H = K + V = \frac{p}{2m} + V(x) = -\frac{n}{2m}\frac{\partial}{\partial x^2} + V(x)$

Angular momentum : $\mathbf{L} = \mathbf{r} \times m\mathbf{v} = \mathbf{r} \times \mathbf{p}$

but does not occur for motion in one dimension.

Could the momentum expectation be imaginary?

The expectation value of p is always real. Let us calculate

$$\langle p \rangle - \langle p \rangle^* = \int_{-\infty}^{\infty} dx \left[\psi^* \left(\frac{\hbar}{i} \right) \frac{\partial \psi}{\partial x} - \psi \left(-\frac{\hbar}{i} \right) \frac{\partial \psi^*}{\partial x} \right]$$
$$= \frac{\hbar}{i} \int_{-\infty}^{\infty} dx \left[\psi^* \frac{\partial \psi}{\partial x} + \psi \frac{\partial \psi^*}{\partial x} \right] = \frac{\hbar}{i} \int_{-\infty}^{\infty} dx \frac{\partial}{\partial x} (\psi^* \psi) = 0$$

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The last step follows from the square integrability of the wave functions. Sometimes one has occasion to use functions that are not square integrable but that obey periodic boundary conditions, such as

$$\psi(x) = \psi(x+L)$$

Also, under these circumstances

$$\langle p \rangle - \langle p \rangle^* = \frac{\hbar}{i} \int_0^\infty dx \, \frac{\partial}{\partial x} (\psi^* \psi) = \frac{\hbar}{i} \left(|\psi(L)|^2 - |\psi(0)|^2 \right) = 0$$

An operator whose expectation value for all admissible wave functions is real is called a Hermitian operator. Therefore, the momentum operator is Hermitian.

All quantum mechanical operators corresponding to physical observables are then Hermitian operators.

Product of operators:

Products of operators need careful definition, because the order in which they act is important.

Example :

$$xp\psi(x) = -i\hbar x \frac{d\psi(x)}{dx}$$
 whereas $px\psi(x) = -i\hbar \frac{d}{dx}(x\psi(x)) = -i\hbar x \frac{d\psi(x)}{dx} - i\hbar\psi(x)$

They are different. However, one can deduce

$$[p, x]\psi(x) \equiv (px - xp)\psi(x) = -i\hbar\psi(x)$$

Since this is true for all $\psi(x)$, we conclude that we have an operator relation, which reads

$$[p, x] = -i\hbar$$
 or $[x, p] = i\hbar$

This is a *commutation relation*, and it is interesting because it is a relation between operators, independent of what wave function this acts on. The difference between classical physics and quantum mechanics lies in that physical variables are described by operators and these do not necessarily commute.

In general one could show that: $[f(x), p] = i\hbar \frac{df}{dx}$

The Heisenberg Uncertainty Relations

The wave function $\psi(x)$ cannot describe a particle that is both well-localized in space and has a sharp momentum. The uncertainty in the measurement is given by

where
$$\Delta x \Delta p \ge \hbar/2$$

where $\Delta x = \left[\langle x^2 \rangle - \langle x \rangle^2 \right]^{1/2}$ and $\Delta p = \left[\langle p^2 \rangle - \langle p \rangle^2 \right]^{1/2}$

to be evaluated using position and momentum operators.

This is in great contrast to classical mechanics. What the relation states is that there is a quantitative limitation on the accuracy with which we can describe a system using our familiar, classical notions of position and momentum. Position and momentum are said to be *complementary* (*conjugate*) variables.

Example 1: A particle of mass *m* is in the state

$$\Psi(x,t) = Ae^{-a[(mx^2/\hbar)+it]},$$

where A and a are positive real constants. (a) Find A. (b) Calculate the expectation values of <x>, <x²>, , and <p²>. (d) Find σ_x and σ_p . Is their product consistent with the uncertainty principle?

(a)
$$1 = 2|A|^2 \int_0^\infty e^{-2amx^2/\hbar} dx = 2|A|^2 \frac{1}{2} \sqrt{\frac{\pi}{(2am/\hbar)}} = |A|^2 \sqrt{\frac{\pi\hbar}{2am}}; \quad A = \left(\frac{2am}{\pi\hbar}\right)^{1/4}.$$

(b)
$$\langle x \rangle = \int_{-\infty}^{\infty} x |\Psi|^2 dx = 0.$$
 [Odd integrand.]

$$\langle x^2 \rangle = 2|A|^2 \int_0^\infty x^2 e^{-2amx^2/\hbar} dx = 2|A|^2 \frac{1}{2^2(2am/\hbar)} \sqrt{\frac{\pi\hbar}{2am}} = \boxed{\frac{\hbar}{4am}}.$$

$$\langle p \rangle = m \frac{d\langle x \rangle}{dt} = \boxed{0.}$$

Remember:

$$\int_0^\infty e^{-ax^2} dx = \frac{1}{2} \left(\frac{\pi}{a}\right)^{\frac{1}{2}}$$
$$\int_0^\infty x^2 e^{-ax^2} dx = \frac{1}{4a} \left(\frac{\pi}{a}\right)^{\frac{1}{2}}$$

$$\begin{split} \langle p^2 \rangle &= \int \Psi^* \left(\frac{\hbar}{i} \frac{\partial}{\partial x} \right)^2 \Psi dx = -\hbar^2 \int \Psi^* \frac{\partial^2 \Psi}{\partial x^2} dx \\ &= -\hbar^2 \int \Psi^* \left[-\frac{2am}{\hbar} \left(1 - \frac{2amx^2}{\hbar} \right) \Psi \right] dx = 2am\hbar \left\{ \int |\Psi|^2 dx - \frac{2am}{\hbar} \int x^2 |\Psi|^2 dx \right\} \\ &= 2am\hbar \left(1 - \frac{2am}{\hbar} \langle x^2 \rangle \right) = 2am\hbar \left(1 - \frac{2am}{\hbar} \frac{\hbar}{4am} \right) = 2am\hbar \left(\frac{1}{2} \right) = \boxed{am\hbar.} \end{split}$$

(c)
$$\sigma_x^2 = \langle x^2 \rangle - \langle x \rangle^2 = \frac{\hbar}{4am} \Longrightarrow \sigma_x = \sqrt{\frac{\hbar}{4am}}$$

$$\sigma_p^2 = \langle p^2 \rangle - \langle p \rangle^2 = am\hbar \Longrightarrow \sigma_p = \sqrt{am\hbar}.$$

$$\sigma_x \sigma_p = \sqrt{\frac{\hbar}{4am}} \sqrt{am\hbar} = \frac{\hbar}{2}.$$

This is consistent with the uncertainty principle.

Example 2: Consider a particle whose normalized wave function is

$$\psi(x) = 2\alpha \sqrt{\alpha} x e^{-\alpha x} \qquad x > 0$$
$$= 0 \qquad x < 0$$

(a) For what value of x does $P(x) = |\psi|^2$ peak? (b) Calculate $\langle x \rangle$, $\langle x^2 \rangle$ and $\langle p \rangle$, $\langle p^2 \rangle$. (c) Verify uncertainty relation.

(a) The peak in P(x) occurs when dP(x)/dx = 0 that is, when

$$\frac{d}{dx}(x^2e^{-2\alpha x}) = 2x(1-\alpha x)e^{-2\alpha x} = 0 \implies x = 1/\alpha.$$
(b) $\langle x \rangle = \int_0^\infty dx \, x(4\alpha^3 x^2 e^{-2\alpha x}) = \frac{1}{4\alpha} \int_0^\infty dy \, y^3 e^{-y} = \frac{3!}{4\alpha} = \frac{3}{2\alpha}$
 $\langle x^2 \rangle = \int_0^\infty dx \, x^2(4\alpha^3 x^2 e^{-2\alpha x}) = \frac{4!}{8\alpha^2} = \frac{3}{\alpha^2}$

Gamma functions: $\Gamma(n) = \int_{0}^{\infty} x^{n-1} e^{-x} dx$ for $n > 0, \Gamma(n+1) = n\Gamma(n)$; $\Gamma(n) = (n-1)!$ for *n* is pointive integer. $\Gamma(1) = 1$ and $\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}$

$$\langle p \rangle = -i\hbar (4\alpha^3) \int_0^\infty x e^{-\alpha x} \frac{\partial}{\partial x} (x e^{-\alpha x}) dx = 0 \quad \text{(Has to be real)}$$

$$\langle p^2 \rangle = -\hbar^2 (4\alpha^3) \int_0^\infty x e^{-\alpha x} \frac{\partial^2}{\partial x^2} (x e^{-\alpha x}) dx = -\hbar^2 (4\alpha^3) \left[-2\alpha \int_0^\infty x e^{-2\alpha x} dx + \alpha^2 \int_0^\infty x^2 e^{-2\alpha x} dx \right]$$

$$= -\hbar^2 \left[-\frac{2\alpha (4\alpha^3)}{(2\alpha)^2} \int_0^\infty y e^{-y} dy + \alpha^2 \left(4\alpha^3 \int_0^\infty x^2 e^{-2\alpha x} dx \right) \right] = -\hbar^2 \left[-2\alpha^2 + \alpha^2 \right] = \alpha^2 \hbar^2$$

(c)
$$\Delta x^{2} = \left\langle x^{2} \right\rangle - \left\langle x \right\rangle^{2} = \frac{3}{\alpha^{2}} - \left(\frac{3}{2\alpha}\right)^{2} = \frac{3}{4\alpha^{2}}; \ \Delta x = \frac{\sqrt{3}}{2\alpha},$$
$$\Delta p^{2} = \left\langle p^{2} \right\rangle - \left\langle p \right\rangle^{2} = \alpha^{2}\hbar^{2}; \ \Delta p = \alpha\hbar;$$
$$\Delta x \Delta p = \frac{\sqrt{3}}{2\alpha} \alpha\hbar = \frac{\sqrt{3}}{2}\hbar > \frac{\hbar}{2}$$