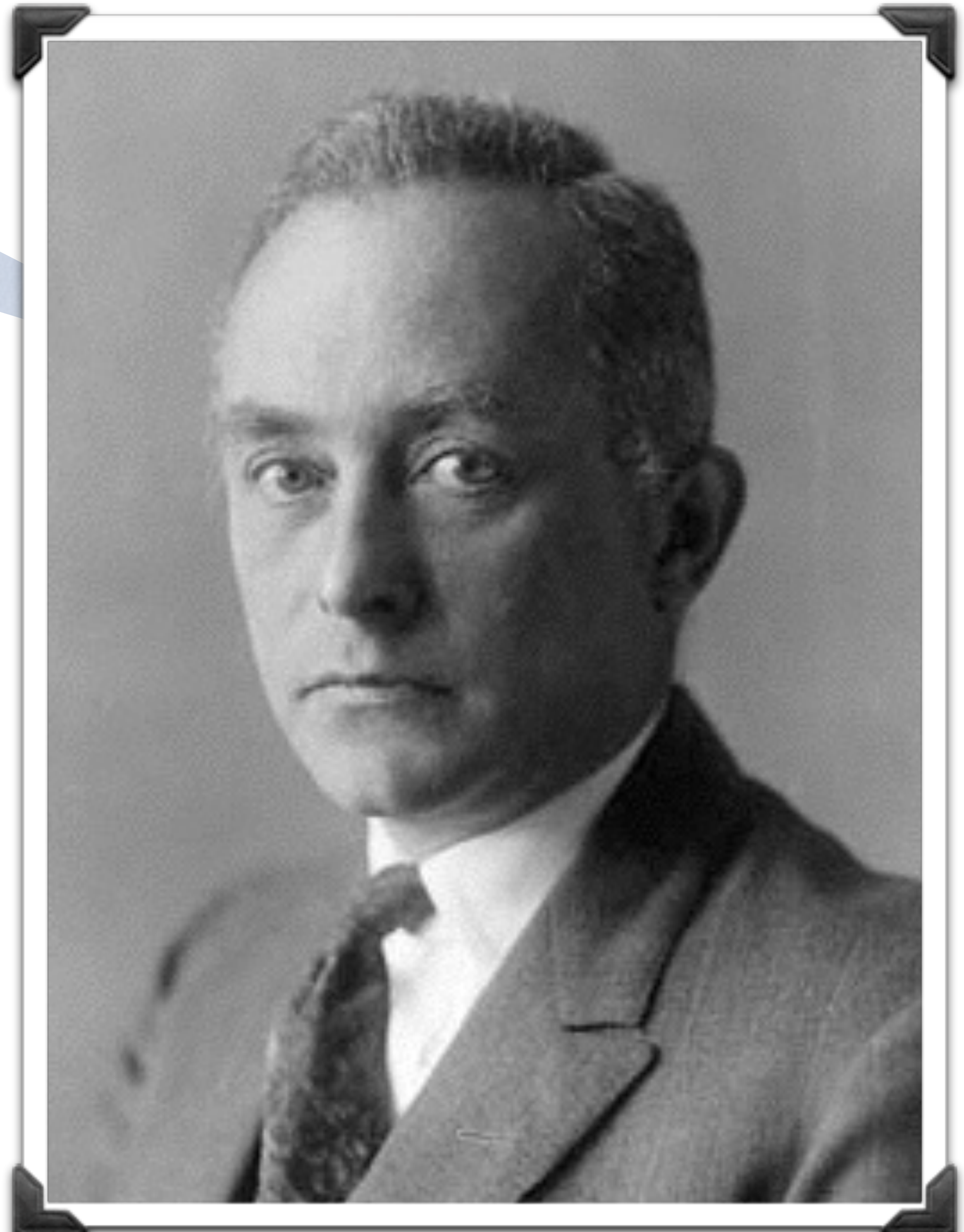
Welcome back to PHY 3305

Today's Lecture:

Expectation Values



Max Born

1882 - 1970

He is the one who figured out $P(x) = \psi^*\psi$ and got the 1954 Nobel prize for it.

Expectation Values:

How do we find the total probability of finding the particle somewhere in an experiment?

$$P = \int |\psi|^2 dx = 1$$

If we want to know the expectation of finding the particle around a given point x, then

$$\bar{x} \equiv \int_{all\ \ space} x|\psi(x)|^2 dx$$

This is the expectation value.

Beware! The expectation value is not an average value of the location of a particle. That suggests a particle has a position. This idea is contrary to the modern view of quantum mechanics.

Expectation Value:

The expectation value of a particle is the value we would obtain if we were to

- begin with a particle in state A, find it,
- start again with a particle in state A, find it again,
- and so on

Repeat the experiment many times and average the locations.

The expectation value is a number, not a function.

The expectation value of the square of the position is given by

$$\bar{x^2} \equiv \int_{all\ space} x^2 |\psi(x)|^2 dx$$

With this definition in hand, we can now define the uncertainty.

$$\Delta x \equiv \sqrt{\int_{all\ space} (x - \bar{x})^2 |\psi(x)|^2 dx}$$

Keep in mind, this is a value not a function.

$$\Delta x \equiv \sqrt{\int_{all\ space} (x - \bar{x})^2 |\psi(x)|^2 dx}$$

1. This is the square root of the mean of the squares of the deviations of x from its expectation value -> rms deviation.
2. **IF AND ONLY IF** x never deviates from its expectation value is the quantity zero.
3. When the wave function is spread out over space, Δx also becomes broader and broader.

Let's expand this to a simpler form.

$$\Delta x \equiv \sqrt{\int_{all\ space} (x - \bar{x})^2 |\psi(x)|^2 dx}$$

$$(x - \bar{x})^2 = (x^2 - 2x\bar{x} + \bar{x}^2)$$

Keep in mind, this is a value not a function.

Write in terms of three integrals.

$$\Delta x \equiv \sqrt{\int_{all\ space} x^2 |\psi(x)|^2 dx - 2\bar{x} \int_{all\ space} x|\psi(x)|^2 dx + \bar{x}^2 \int_{all\ space} |\psi(x)|^2 dx}$$

this is just $\overline{x^2}$ this is just $\bar{x}$ this is 1 (normalization)

Thus,

$$\Delta x = \sqrt{\overline{x^2} - 2\bar{x}^2 + \bar{x}^2} = \sqrt{\overline{x^2} - \bar{x}^2}$$

average of the square square of the average

Note: we can insert any function of position and calculate its expectation value.

$$\overline{f(x)} \equiv \int_{all\ space} f(x)|\psi(x)|^2 dx$$

Expectation values are mathematical tools that allow us to connect the form of the wave functions of observable properties of a quantum system such as position or momentum.

operator

$$\bar{Q} = \int_{all\ space} \Psi^*(x,t)\hat{Q}\Psi(x,t)dx$$

An **operator** is a function that acts on the wave function. It represents the act of measuring a property, Q, or the system.

What does this mean schematically?

- $\hat{Q}\Psi(x,t)$ is the act of making the measurement which puts the wave function into some definite state.
- $\Psi^*(x,t)(\hat{Q}\ \Psi(x,t))$ is the probability of that outcome, given the original wave function.
- Integrating gives you the expectation value for that measurement.

What are some operators?

TABLE 5.2 Basic operators

Observable	Momentum	Position	Energy
Operator	$\hat{p} = -i\hbar\frac{\partial}{\partial x}$	$\hat{x} = x$	$\hat{E} = i\hbar\frac{\partial}{\partial t}$

Functions of an operator are also possible.

Example: Kinetic Energy

$$KE = \frac{p^2}{2m}$$

The operator for Kinetic Energy is then

$$\hat{KE} = \frac{1}{2m}\hat{p}^2 = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$$

EXAMPLE: PARTICLE IN AN INFINITE WELL

For a particle in the ground state of an infinite well, find Δx, Δp and $\Delta x \Delta p$.

To calculate the uncertainty, we need the expectation value and the square of the expectation value.

$$\Delta Q = \sqrt{\overline{Q^2} - \bar{Q}^2}$$

where Q = x

Step 1: Calculate $\overline{x}$.

$$\bar{x} = \int_{all\ \ space} \psi^*(x) x \psi(x) dx$$

$$\bar{x} = \int_{all\ \ space} \psi^*(x) x \psi(x) dx$$

Recall

$$\psi_1(x) = \sqrt{\frac{2}{L}} sin(\frac{\pi x}{L})$$

Substitute

$$\bar{x} = \int_0^L \sqrt{\frac{2}{L}} sin(\frac{\pi x}{L}) x \sqrt{\frac{2}{L}} sin(\frac{\pi x}{L}) dx$$

$$= \frac{2}{L} \int_0^L x sin^2(\frac{\pi x}{L}) dx$$

$$\bar{x} = \frac{1}{2} L$$

$$\Delta Q = \sqrt{\overline{Q^2} - \bar{Q}^2}$$

Step 2: Calculate $\overline{x^2}$.

$$\overline{x^2} = \int_0^L \sqrt{\frac{2}{L}} sin(\frac{\pi x}{L}) x^2 \sqrt{\frac{2}{L}} sin(\frac{\pi x}{L}) dx$$

$$= \frac{L}{2} \int_0^L x^2 sin^2(\frac{\pi x}{L}) dx$$

$$\overline{x^2} = L^2(\frac{1}{3} - \frac{1}{2\pi^2})$$

Step 3: Put it together.

$$\Delta x = \sqrt{\overline{x^2} - \bar{x}^2} = \sqrt{L^2(\frac{1}{3} - \frac{1}{2\pi^2}) - (\frac{1}{2}L)^2}$$

$$\Delta x = 0.181 L$$

To find momentum, we need to repeat steps 1 - 3, but this time using the momentum operator.

Step 1: Calculate $\overline{p}$.

$$\bar{p} = \int_{\text{all space}} \psi^*(x)\,\hat{p}\,\psi(x)dx$$

Substitute in the wave equation and momentum operator.

$$\bar{p} = \int_0^L \left(\sqrt{\frac{2}{L}}\,\sin\frac{\pi x}{L}\right)\left(-i\hbar\frac{\partial}{\partial x}\right)\left(\sqrt{\frac{2}{L}}\,\sin\frac{\pi x}{L}\right)dx$$

Can I rewrite this as follows?

$$\bar{p} = \frac{L}{2}\int_0^L \frac{\partial}{\partial x}(sin^2(\frac{\pi x}{L}))dx$$

You must 'operate' on ψ first.

$$\bar{p} = \int_0^L \left(\sqrt{\frac{2}{L}}\sin\frac{\pi x}{L}\right)(-i\hbar)\frac{\pi}{L}\left(\sqrt{\frac{2}{L}}\cos\frac{\pi x}{L}\right)dx$$

$$\bar{p} = -i\hbar\frac{2\pi}{L^2}\int_0^L \sin\left(\frac{\pi x}{L}\right)\cos\left(\frac{\pi x}{L}\right)dx$$

$$\bar{p} = 0$$

Step 2: Calculate $\overline{p^2}$.

$$\overline{p^2} = \int_{\text{all space}} \psi^*(x)\,\hat{p}^2\psi(x)dx$$

Substitute in the wave equation and momentum operator.

$$\overline{p^2} = \int_0^L \left(\sqrt{\frac{2}{L}}\,\sin\,\frac{\pi x}{L}\right)\left(-\hbar^2\frac{\partial^2}{\partial x^2}\right)\left(\sqrt{\frac{2}{L}}\,\sin\frac{\pi x}{L}\right)dx$$

$$= \int_0^L \left(\sqrt{\frac{2}{L}}\,\sin\,\frac{\pi x}{L}\right)\left(-\hbar^2\right)\left(\frac{-\pi^2}{L^2}\right)\left(\sqrt{\frac{2}{L}}\,\sin\frac{\pi x}{L}\right)dx$$

$$= \frac{\pi^2\hbar^2}{L^2}\int_0^L \left(\sqrt{\frac{2}{L}}\,\sin\,\frac{\pi x}{L}\right)^2 dx$$

$$\overline{p^2} = \frac{\pi^2\hbar^2}{L^2}$$

$$\Delta Q = \sqrt{\overline{Q^2} - \bar{Q}^2}$$

Step 3: Put it together.

$$\Delta p = \sqrt{\overline{p^2} - \bar{p}^2}$$

$$= \sqrt{\frac{\pi^2\hbar^2}{L^2} - 0}$$

$$\Delta p = \frac{\pi\hbar}{L}$$

Considering that the average of p is zero, is it reasonable that uncertainty p is non-zero?

Yes, the particle may at least be found moving in different directions, which demands a nonzero momentum uncertainty.

Finally, we calculate the product of the uncertainties.

$$\Delta x \Delta p = 0.181 L \frac{\pi \hbar}{L}$$

$$\Delta x \Delta p = 0.568 \hbar$$

Note: According to the uncertainty principle,

$$\Delta x \Delta p \geq \frac{\hbar}{2}$$

which agrees with our answer.

SWE in Operator Form

$$KE = \frac{p^2}{2m} \longrightarrow \hat{KE} = \frac{1}{2m}\hat{p}^2$$

$$= \frac{1}{2m}(-i\hbar\frac{\partial}{\partial x})(-i\hbar\frac{\partial}{\partial x})$$

$$\hat{KE} = \frac{-\hbar^2}{2m}(\frac{\partial^2}{\partial x^2})$$

Using this we can rewrite

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

$$\hat{KE}\Psi(x,t) + \hat{U}(x)\Psi(x,t) = \hat{E}(x,t)$$

THE END
(FOR TODAY)