Quantum Mechanics and Atomic Physics

Lecture 9:

The Uncertainty Principle and Commutators

http://www.physics.rutgers.edu/ugrad/361

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Announcement

- Quiz in next class (Oct. 5): will cover Reed Chapter 3 and 4 (up to today's lecture).
- Next HW due on Monday Oct. 10th

Summary of last time

- **Operators**: does something to a function and returns a result.

$$x_{op} = x$$

$$\vec{P}_{op} = -i\hbar\vec{\nabla}$$

$$E_{op} = i\hbar\frac{\partial}{\partial t}$$

$$KE_{op} = -\frac{\hbar^2}{2m}\nabla^2$$

$$PE_{op} = V(x)$$

$$H_{op} = -\frac{\hbar^2}{2m}\nabla^2 + V(x)$$

(Hamiltonian)

- In general:

$$\overline{f(x)} = \langle f(x) \rangle = \int \Psi^* \left[Q_{op}(f(x))\Psi \right] dx$$

$$= \langle \Psi | f(x) | \Psi \rangle$$

Summary: Hamiltonian

- Ψ both space and time dependent:

Ψ both space & time-dependent

$H_{op} = i\hbar \frac{\partial}{\partial t}$ Hamiltonian operator.

$H_{op} = -\frac{\hbar^2}{2m}\nabla^2 + V$ spatial form

- Hamilotonian operator is special, because it provides the Schroedinger equation

$$\underbrace{\left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)}_{H\text{: spatial}} \Psi(x,t) = \underbrace{i\hbar\frac{\partial}{\partial t}}_{H\text{: time}} \Psi(x,t)$$

Momentum expectation value for infinite square well

$$\bar{p} = \int_0^L \psi_n^* \left[(p_x)_{op} \psi_n \right] dx = \int_0^L \psi_n^* \left[-i\hbar \frac{d}{dx} \psi_n \right] dx$$

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

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

See appendix C in Reed for useful integrals

$$= -\frac{i\hbar}{L} \left[\sin^2 \frac{n\pi x}{L} \right]_0^L = 0 \quad !$$

- Again is not surprising.
- The well is symmetric so the particle should have no preference for traveling one way or the other.

Expectation value of Energy

$$\bar{E} = \int_0^L \Psi_n^* \left[H_{op} \Psi_n \right] dx = \int_0^L \Psi^* \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \Psi_n \right] dx$$

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

$$= \frac{\hbar^2}{m} \frac{n^2\pi^2}{L^3} \int_0^L \sin^2 \frac{n\pi x}{L} = \frac{\hbar^2 n^2 \pi^2}{mL^3} \left[\frac{x}{2} - \left(\sin \frac{2n\pi x}{L} \right) \frac{L}{4n\pi} \right]_0^L$$

$$= \frac{\hbar^2 n^2 \pi^2}{2mL^2} = E_n$$

As expected!

- The expectation value of the energy for the infinite square well state n is just the eigenvalue of that state!

Expectation value of p^2

- The need for this will become clear later (next time).

$$p_x^2 = (p_x)(p_x) = \left(-i\hbar\frac{\partial}{\partial x}\right)\left(-i\hbar\frac{\partial}{\partial x}\right)$$

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

Not a surprise.

So for infinite square well:

$$\overline{p^2} = 2m\,\overline{KE} = 2m\left(\frac{\hbar^2\pi^2 n^2}{2mL^2}\right) = \frac{\hbar^2\pi^2 n^2}{L^2}$$

Expectation value of x^2

- Again, this is something that we will find useful later.

$$\overline{x^2} = \int_0^L \psi_n^* \left[x^2 \psi_n\right] dx = \frac{2}{L}\int_0^L x^2 \sin^2 \frac{n\pi x}{L}\, dx$$

$$= \frac{2}{L}\left[\frac{x^3}{6} - \left(\frac{L}{4n\pi} - \frac{L^3}{8n^3\pi^3}\right)\sin\frac{2n\pi x}{L} - \frac{L^2}{4n^2\pi^2}\, x \cos\frac{2n\pi x}{L}\right]_0^L$$

$$= \frac{2}{L}\left[\frac{L^3}{6} - \frac{L^3}{4n^2\pi^2}\right] = \frac{L^2}{3}\left[1 - \frac{3}{2n^2\pi^2}\right]$$

- Note: $\langle x^2 \rangle$ is <u>not</u> equal to $\langle x \rangle^2$

Summary: expectation values for inf. Square well

For infinite square well:

$$\Psi_n(x,t) = \sqrt{\frac{2}{L}} \sin\frac{n\pi x}{L}\, e^{-iE_n t/\hbar}$$

$$\bar{x} = \langle x \rangle = \frac{L}{2}$$

$$\bar{p} = \langle p \rangle = 0$$

$$\bar{E} = \langle E \rangle = E_n = \frac{\hbar^2 n^2 \pi^2}{2mL^2}$$

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

$$\overline{x^2} = \langle x^2 \rangle = \frac{L^2}{3}\left[1 - \frac{3}{2n^2\pi^2}\right]$$

Dirac Notation

- It is easier to adapt a shorthand notation called **Dirac notation** or **Dirac bracket notation**:

Expectation value of $f(x)$:

$$\overline{f(x)} = \int \psi^*(x) \left[Q_{op}[f(x)]\, \psi(x) \right] dx$$

$$\equiv \langle \psi(x) \,|\, f(x) \,|\, \psi(x) \rangle$$; Error in the book

$Q_{op}[f(x)]$ is operator corresponding to $f(x)$

Further simplify:

$\langle f(x) \rangle$

- Overlap integral or inner product of Ψ_1 and Ψ_2:

$$\langle \Psi_1 | \Psi_2 \rangle = \int \Psi_1^*(x)\, \Psi_2(x)\, dx$$: called inner product

Error in the Roed book !

Example

- Reed, Problem 4-2:
  - Prove that for the infinite potential well wavefunctions:

$$\langle xp \rangle = -\langle px \rangle = i\hbar/2$$

$$\downarrow x \qquad\qquad \downarrow p$$

$$\langle xp \rangle = \overline{xp} = \int_0^L \sqrt{\frac{2}{L}} \sin\frac{n\pi x}{L}\, x \left[\sqrt{\frac{2}{L}} \left(-i\hbar \frac{\partial}{\partial x} \sin\frac{n\pi x}{L}\right)\right] dx$$

$$= \frac{-2i\hbar n\pi}{L^2} \int_0^L x \sin\frac{n\pi x}{L} \cos\frac{n\pi x}{L}\, dx$$

$$= \frac{-i\hbar n\pi}{L^2} \int_0^L x \sin\frac{2n\pi x}{L}\, dx = \frac{-i\hbar n\pi}{L^2} \left[\frac{\sin\frac{2n\pi x}{L} \cdot L^2}{4n^2\pi^2} - \frac{L}{2n\pi} x \cos\frac{2n\pi x}{L}\right]_0^L$$

$$= \frac{-i\hbar n\pi}{L^2}\left(-\frac{L^2}{2n\pi}\right) = \frac{i\hbar}{2}$$

$$\langle px \rangle = \overline{px} = -\frac{2i\hbar}{L}\int_0^L \sin\frac{n\pi x}{L}\left[\overset{p}{\downarrow}\frac{\partial}{\partial x}\left(\overset{x}{\downarrow}x \sin\frac{n\pi x}{L}\right)\right]dx$$

$$= -\frac{2i\hbar}{L}\left[\int_0^L \sin^2\frac{n\pi x}{L}\,dx + \frac{n\pi}{2L}\int_0^L x \sin\frac{2n\pi x}{L}\,dx\right]$$

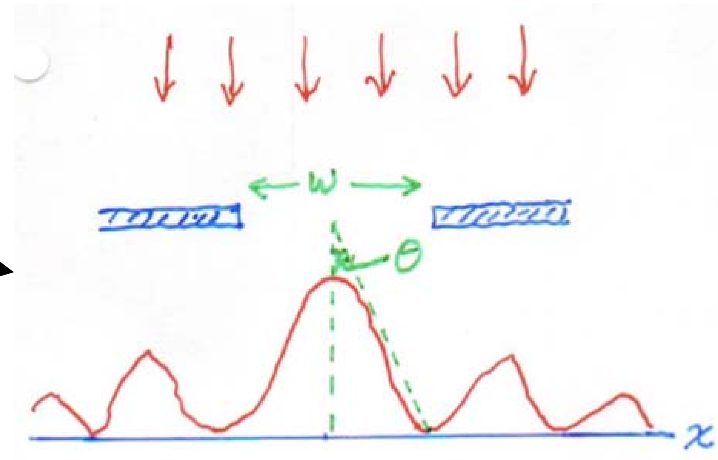
$$= \frac{-2i\hbar}{L}\left[\frac{L}{2} - \frac{L}{4}\right] = \frac{-i\hbar}{2}$$

So,

$$\langle xp \rangle = -\langle px \rangle = \frac{i\hbar}{2}$$

Heisenberg Uncertainty Principle

- Werner Heisenberg (1927) *Gedanken* (thought) experiments.
- Single-slit diffraction of electrons, of wavelength λ
- w= slit spacing
- Diffraction first minimum θ at (w sinθ =λ)
- Uncertainty in position Δx=w
- Uncertainty in p_x ≈ momentum needed to send electron to first minimum.



$$\text{So } \Delta p_x \geq p \cdot \sin\theta = \left(\frac{h}{\lambda}\right)\left(\frac{\lambda}{w}\right) = \frac{h}{w} = \frac{h}{\Delta x}$$

$$\Rightarrow \Delta p_x \cdot \Delta x \geq h$$

More sophisticated analysis:

$$\Delta p_x \cdot \Delta x \geq \frac{h}{4\pi}$$

$$\text{Define: } \hbar = \frac{h}{2\pi} \text{ then } \Delta p_x \cdot \Delta x \geq \frac{\hbar}{2}$$

Protons and neutrons in nuclei have minimum kinetic energies of a few MeV. So nuclear binding energies have to exceed few MeV.

The Uncertainty Principle

- In QM, is it possible to specify the positions of particles precisely?
  - **No, particles possess a wave nature!**
  - **Heisenberg's Uncertainty principle:**

$$\Delta x \Delta p \geq \hbar / 2$$

  - If we measure the particle's position more and more precisely, that comes with the expense of the particle's momentum becoming less and less well known.
  - And vice-versa.

Commutators

- How can we know if two observable quantities will obey the uncertainty relation?
  - Generalized uncertainty relation: see the reference in Reed for the proof:

$$(\Delta A)(\Delta B) \geq \frac{1}{2}\sqrt{-[A,B]^2}$$

$$[A,B] = A_{op}B_{op} - B_{op}A_{op}.$$

  - [A,B] is an operator and is known as the **commutator** of operators A and B
  - If a wavefunction is an eigenfunction of both A and B, then the order does not matter and [A,B]=0, and eigenvalues of A and B will be measurable simultaneously.

Let's verify the uncertainy principle

Verify w/ $x_{op} = x$ and $P_{op} = -i\hbar \frac{d}{dx}$

$$[x_{op}, P_{op}]\psi = (x_{op} P_{op} - P_{op} x_{op})\psi$$
$$= x\left(-i\hbar \frac{d}{dx}\psi\right) + i\hbar \frac{d}{dx}(x\psi)$$
$$= i\hbar\left(\cancel{-x\frac{d\psi}{dx}} + \psi + \cancel{x\frac{d\psi}{dx}}\right)$$
$$= i\hbar\psi$$

So,

$$\boxed{[x_{op}, P_{op}] = i\hbar}$$

$$\Rightarrow (\Delta x)(\Delta P) \geq \frac{1}{2}\sqrt{-(i\hbar)^2}$$
$$(\Delta x)(\Delta P) \geq \frac{1}{2}\hbar$$

✓

Example

- In an atomic nucleus, a proton is confined to $\Delta x \approx 10^{-15}$m. Find its minimum kinetic energy. (m_p=938MeV/c^2)

$$\Delta P_x \geq \frac{\hbar}{2\Delta x} \approx 100 \frac{MeV}{c} \quad \text{for } \Delta x = 10^{-15} m$$

$$\text{So} \quad P_{min} \approx 100 \frac{MeV}{c}$$

$$\text{So,} \quad E_{min} = \sqrt{(100)^2 + (938)^2}$$
$$= \underline{943 MeV}$$

$$\text{So} \quad K_{min} = E_{min} - E_0 = 943 - 938 = \underline{\underline{5 MeV}}$$

- So nuclear binding energies must be at least 5 MeV! Recall hydrogen atom's binding energy is 13.6 eV.

Example, con't

- Now suppose there were electrons in nuclei…

$\Delta p_x \gtrsim 100 \frac{MeV}{c}$ as above

$p_{min} = 100 \frac{MeV}{c}$ as above

<u>But</u> $E_{min} = \sqrt{(100)^2 + (0.511)^2} \approx 100 MeV$

<u>and</u> $K_{min} = E_{min} - E_0 = 100 - 0.511$

$\approx \underline{100 MeV}$

Uncertainty Principle

- Uncertainty in x and p are the *standard deviations*:

$$\Delta x^2 = \frac{1}{N}\sum_i (x_i - \bar{x})^2 = \frac{1}{N}\sum (x_i^2 - 2\bar{x}x_i + \bar{x}^2)$$

$$= \overline{x^2} - 2\bar{x}\frac{1}{N}\sum x_i + \frac{1}{N}\sum \bar{x}^2$$

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

$$\Delta x^2 = \overline{x^2} - \bar{x}^2 = \langle x^2\rangle - \langle x\rangle^2$$

or

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

$$\Delta p = \sqrt{\langle p^2\rangle - \langle p\rangle^2}$$

For infinite square well

- Let's use the expectation values we already evaluated …

$$\Delta x = \sqrt{\frac{L^2}{3}\left(1 - \frac{3}{2n^2\pi^2}\right) - \frac{L^2}{4}}$$

$$= L\sqrt{\frac{1}{12} - \frac{1}{2n^2\pi^2}}$$

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

$$\Delta x \, \Delta p = \sqrt{\frac{n^2\pi^2}{12} - \frac{1}{2}}\;\hbar$$

Infinite square well, con't

- The minimum value is for n=1:

For $n=1$ (min value):

$$\Delta x\, \Delta p = \sqrt{\frac{\pi^2}{12} - \frac{1}{2}}\ \hbar$$

$$= 0.568\hbar$$

$$\gtrsim 0.5\,\hbar \quad ! \quad ✓$$

How about $n \to \infty$?

$$\Delta x \Delta p \approx \frac{n\pi}{\sqrt{12}} \approx 0.907\, n\hbar$$

The potential that gives the minimum possible value of $\Delta x\ \Delta p$ is for a simple harmonic oscillator.

More on this next time.

But now an example …

Example: Harmonic Oscillator

- The potential for a harmonic oscillator (*like the motion of a spring*!):

$$V(x) = \frac{kx^2}{2} \qquad -\infty \leq x \leq \infty$$

$V(x)$ is symmetric about 0 so

$$\langle x \rangle = \langle p \rangle = 0$$

$$E = \frac{p^2}{2m} + V(x) = \frac{p^2}{2m} + \frac{kx^2}{2}$$

$$\langle E \rangle = \frac{\langle p^2 \rangle}{2m} + \frac{k}{2}\langle x^2 \rangle$$

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

$$\Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} = \sqrt{\langle p^2 \rangle}$$

$$\Rightarrow \langle E \rangle = \frac{(\Delta p)^2}{2m} + \frac{k}{2} (\Delta x)^2$$

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

$$\Rightarrow \langle E \rangle \geq \frac{\hbar^2}{8m(\Delta x)^2} + \frac{k}{2} (\Delta x)^2$$

$$\frac{d\langle E \rangle}{d(\Delta x)} = 0 = -\frac{\hbar^2}{4m} \frac{1}{(\Delta x)^3} + k(\Delta x)$$

$$(\Delta x)^4 = \frac{\hbar^2}{4mk}$$

$$\Rightarrow \langle E \rangle_{min} = \frac{\hbar}{4}\sqrt{\frac{k}{m}} + \frac{\hbar}{4}\sqrt{\frac{k}{m}}$$

$$\langle E \rangle_{min} = \frac{\hbar}{2}\sqrt{\frac{k}{m}} = \frac{\hbar\omega}{2}$$

where $\omega \equiv \sqrt{\frac{k}{m}}$

ω is angular frequency of the oscillator

Summary/Announcements

- Uncertainty principle $\Delta x \Delta p \geq \hbar / 2$
- Next Time: Orthogonality, superposition, and time dependent wave functions plus Ehrenfest and Virial theorems
- Quiz in next class (Oct. 5): covers Reed Chapter 3 and 4 (up to today's lecture).
- Next HW due on Monday Oct. 10^{th}