06/05/25

Lecture - 30

27/11/20

Revanth Reddy Pannala
EBIT, Unibo
రేవంత్ రెడ్డి పన్నాల

→ The **Standard Deviation** is also called **Uncertainity!**

Q) Now, what relation there could be b/w the Standard Deviations of Two Operators over the same wave function?

Ans) offcourse the interestin case is in which the two operators donot commute

A operator, $\langle A \rangle$ ⇒ expectation value of the operator

Heisenberg Uncertainty Relation — I

- Given two Hermitian operators $\mathcal{A}$, $\mathcal{B}$, the covariance of the eigenvalues is given by

$$\langle (A - \langle A \rangle)(B - \langle B \rangle) \rangle = \langle AB - \langle A \rangle B - \langle B \rangle A + \langle A \rangle \langle B \rangle \rangle =$$
$$= \langle AB \rangle - \langle A \rangle \langle B \rangle .$$

- The operators $\mathcal{A}_0 = \mathcal{A} - \langle A \rangle$ and $\mathcal{B}_0 = \mathcal{B} - \langle B \rangle$ are also Hermitian; defining the complex functions $f \doteq \mathcal{A}_0 \psi$ and $g \doteq \mathcal{B}_0 \psi$, and introducing a real parameter λ, let $\sigma \doteq f + j\lambda g$. It is found:

Norm of 'σ' is by construction Non negative

$$\langle \sigma | \sigma \rangle \geq 0 \implies \int_\tau \left[f^* f + j\lambda (f^* g - g^* f) + \lambda^2 g^* g \right] \mathrm{d}\tau \geq 0 ,$$

$$\boxed{\int_\tau \left[\psi^* \mathcal{A}_0^2 \psi + j\lambda \psi^* (\mathcal{A}_0 \mathcal{B}_0 - \mathcal{B}_0 \mathcal{A}_0) \psi + \lambda^2 \psi^* \mathcal{B}_0^2 \psi \right] \mathrm{d}\tau \geq 0 .}$$

Expectation value of A_0^2

- The *commutator* of $\mathcal{A}_0$ and $\mathcal{B}_0$ is the operator $\mathcal{C}_0$ such that

$$j\mathcal{C}_0 = \mathcal{A}_0 \mathcal{B}_0 - \mathcal{B}_0 \mathcal{A}_0 .$$

- It is easily seen that, if $\mathcal{A}_0$ and $\mathcal{B}_0$ are Hermitian, then $\mathcal{C}_0$ is also Hermitian, whence its eigenvalues are real. From the above

$$\langle A_0^2 \rangle - \lambda \langle C_0 \rangle + \lambda^2 \langle B_0^2 \rangle \geq 0 .$$

→ We studied that the Eigen values of the Hermetian operators are real.

$$f(\lambda) = \langle A_0^2\rangle - \lambda\langle C_0\rangle + \lambda^2\langle B_0^2\rangle \geq 0$$

In conclusion, we have a 2nd order polynomial w.r.to 'λ' this polynomial has Real coefficients

$\langle A_0^2\rangle$ & $\langle B_0^2\rangle$ by construction are +ve

So now, we have to find the condition for which the polynomial is Non-negative.

for $f(\lambda)$ to be Non-negative the Roots of polynomial must be either complex conjugate (or) at most must be equal to each other

So, the parabola never touches Horizontal axis (or atleast touches tangentially.

∴ condition for which $f(\lambda)$ is +ve for any value of 'λ' is that the discriminants of the polynomial are either Negative (or '0'

for Quadratic eqn : $ax^2 + bx + c$

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$ → Discriminant

Heisenberg Uncertainty Relation — II

It has been found that $\langle A_0^2 \rangle - \lambda \langle C_0 \rangle + \lambda^2 \langle B_0^2 \rangle$ is a second-order polynomial with real coefficients; for it to be non negative, its discriminant must be non positive: $\langle C_0 \rangle^2 - 4 \langle A_0^2 \rangle \langle B_0^2 \rangle \le 0$. On the other hand, from the definitions it follows $\langle A_0^2 \rangle = (\Delta A)^2$, $\langle B_0^2 \rangle = (\Delta B)^2$, and $\langle C_0 \rangle = \langle C \rangle$, where the latter is the expectation value of the commutator $\mathcal{C} \doteq (\mathcal{AB} - \mathcal{BA})/j$. In conclusion:

$$\Delta A \, \Delta B \ge \frac{1}{2} \langle C \rangle .$$

Examples:

- If $\mathcal{A}$ and $\mathcal{B}$ commute, then $\mathcal{C} = 0$ and $\Delta A \, \Delta B \ge 0$, namely, there is no limit to the smallness of $\Delta A \, \Delta B$.
- If $\mathcal{A} = q_i$ and $\mathcal{B} = -j\hbar \, \partial / \partial q_i$, then $\mathcal{C} = \hbar \mathcal{I}$, $C = \hbar$, and

position operator $\Delta A \, \Delta B \ge \frac{\hbar}{2}$ momentum operator (Heisenberg relation).

Note: the derivation above embeds the proof of the Schwartz inequality $\int_\tau |f|^2 \, d\tau \times \int_\tau |g|^2 \, d\tau \ge |\int_\tau f^* g \, d\tau|^2$, $\forall f, g$.

Revanth Reddy Pannala
EBIT, Unibo
రేవంత్ రెడ్డి పన్నాల

Heisenberg Uncertainty Relation — III

- Given $\mathcal{A} = q_i$ and $\mathcal{B} = -j\hbar\,\partial/\partial q_i$, if ψ fulfills $\Delta A\,\Delta B = \hbar/2$, then ψ is called ***minimum uncertainty*** wavefunction. For this, it must be

$\int|\sigma|^2 d\tau = 0$ Here we impose $\delta^{2} = 0 \because \tau \neq 0$

$$\langle\sigma|\sigma\rangle = 0 \quad\Longrightarrow\quad \sigma = f + j\lambda g = (\mathcal{A}_0 + j\lambda\mathcal{B}_0)\,\psi = 0\,.$$

- Taking a one-dimensional case for simplicity, and letting $q_0 \doteq \langle A\rangle$, $p_0 \doteq \hbar k_0 \doteq \langle B\rangle$, the above yields

$$\lambda\hbar\frac{\mathrm{d}\psi}{\mathrm{d}q} = [j\lambda p_0 - (q-q_0)]\,\psi\,, \qquad \frac{\mathrm{d}\psi}{\psi} = \left[jk_0 - \frac{q-q_0}{\lambda\hbar}\right]\mathrm{d}q\,,$$

$$\psi(q) = \psi_0\,\exp\left[jk_0q - (q-q_0)^2/(2\lambda\hbar)\right],$$

where the normalization condition $\langle\psi|\psi\rangle = 1$ yields $\psi_0 = (\pi\lambda\hbar)^{-1/4}$. An expression for λ is found from $(\mathcal{A}_0 + j\lambda\mathcal{B}_0)\,\psi = 0$:

$$\mathcal{A}_0\psi = -j\lambda\mathcal{B}_0\psi \;\Rightarrow\; \langle\mathcal{A}_0^2\rangle = \lambda^2\langle\mathcal{B}_0^2\rangle \;\Rightarrow\; \lambda = \frac{\Delta A}{\Delta B} = \frac{(\Delta A)^2}{\hbar/2}\,.$$

Letting $\Delta q = \Delta A$ it follows (with Δq still arbitrary)

$$\psi(q) = \frac{1}{\sqrt[4]{2\pi}\sqrt{\Delta q}}\,\exp\left[jk_0q - \frac{(q-q_0)^2}{(2\Delta q)^2}\right].$$

A = position =

$\therefore \mathcal{A}_0 = \mathcal{A} - \langle A\rangle$

$\mathcal{B}_0 = \mathcal{B} - \langle B\rangle$

momentum

$\Rightarrow \mathcal{A}_0 = q - q_0$

$\mathcal{B}_0 = j\hbar\frac{d\psi}{dq} - p_0$

$\because (\mathcal{A}_0 + j\lambda\mathcal{B}_0)\psi = 0$

$\Rightarrow (q - q_0)\psi + j\lambda\left(-j\hbar\frac{d\psi}{dq} - p_0\psi\right) = 0$

$\Rightarrow (q-q_0)\psi + \lambda\hbar\frac{d\psi}{dq} - j\lambda p_0\psi = 0$

$\Rightarrow \boxed{\lambda\hbar\frac{d\psi}{dq} = \left(j\lambda p_0 - (q-q_0)\right)\psi}$

This Diff. eq^n is seperable

$$\frac{d\psi}{\psi} = \left[jk_0 - \frac{(q-q_0)}{\hbar d} \right] dq$$

I OBS

$$\Rightarrow \ln\psi = jqk_0 - \frac{q^2 - 2qq_0}{2\hbar d} + \ln\psi_0 + \frac{(q_0^2)}{2\hbar d}$$

Integration constant

$$\Rightarrow \ln(\psi) = jqk_0 - \frac{q^2 - 2qq_0 + q_0^2}{2\hbar d} + \ln\psi_0$$

$$\Rightarrow \ln(\psi) - \ln(\psi_0) = jqk_0 - \frac{(q-q_0)^2}{2\hbar d}$$

$$\Rightarrow \ln\left(\frac{\psi}{\psi_0}\right) = jqk_0 - \frac{(q-q_0)^2}{2\hbar d}$$

$$\Rightarrow \frac{\psi}{\psi_0} = e^{\left(jqk_0 - \frac{(q-q_0)^2}{2\hbar d}\right)}$$

$$\Rightarrow \quad \boxed{\psi(q) = \psi_0 \, e^{\left(jqk_0 - \frac{(q-q_0)^2}{2\hbar\lambda}\right)}}$$

This is a Gaussian

$$\boxed{\psi(q) = \psi_0 \, e^{(jqk_0)} \cdot e^{-\frac{(q-q_0)^2}{2\hbar\lambda}}}$$

This function is Normalizable because Gaussian is Integrable and Square integrable

enforce ⇒

$$\langle \psi | \psi \rangle = 1 \quad \Rightarrow \quad \psi_0 = (\pi \lambda \hbar)^{-1/4}$$

where the normalization condition $\langle \psi | \psi \rangle = 1$ yields $\psi_0 = (\pi \lambda \hbar)^{-1/4}$. An expression for λ is found from $(\mathcal{A}_0 + j\lambda \mathcal{B}_0)\,\psi = 0$:

$$\mathcal{A}_0 \psi = -j\lambda \mathcal{B}_0 \psi \;\Rightarrow\; \langle A_0^2 \rangle = \lambda^2 \langle B_0^2 \rangle \;\Rightarrow\; \lambda = \frac{\Delta A}{\Delta B} = \frac{(\Delta A)^2}{\hbar/2}.$$

Letting $\Delta q = \Delta A$ it follows (with Δq still arbitrary)

$$\boxed{\psi(q) = \frac{1}{\sqrt[4]{2\pi}\sqrt{\Delta q}} \exp\left[jk_0 q - \frac{(q-q_0)^2}{(2\Delta q)^2} \right]}.$$

Gaussian

This is the expression for minimum Uncertainty wave packet

Revanth Reddy Pannala
EBIT, Unibo
రేవంత్ రెడ్డి పన్నాల

Time Derivative of the Expectation Value — I

- The time derivative of $\langle A \rangle = \langle \psi | \mathcal{A} | \psi \rangle$ is given by

$$\boxed{\frac{\mathrm{d}}{\mathrm{d}t}\int_\tau \psi^* \mathcal{A} \psi \, \mathrm{d}\tau} = \int_\tau \left(\frac{\partial \psi^*}{\partial t} \mathcal{A} \psi + \psi^* \frac{\partial \mathcal{A}}{\partial t} \psi + \psi^* \mathcal{A} \frac{\partial \psi}{\partial t} \right) \mathrm{d}\tau \, .$$

- From Schrödinger's equation it follows $\partial \psi / \partial t = -j \mathcal{H} \psi / \hbar$ and $\partial \psi^* / \partial t = j \mathcal{H} \psi^* / \hbar$, whence

Expectation value of the commutator

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle A \rangle = \frac{j}{\hbar} \int_\tau \psi^* (\mathcal{H}\mathcal{A} - \mathcal{A}\mathcal{H}) \psi \, \mathrm{d}\tau + \int_\tau \psi^* \frac{\partial \mathcal{A}}{\partial t} \psi \, \mathrm{d}\tau \, .$$

- As a consequence, if $\mathcal{A}$ does not depend on t and commutes with $\mathcal{H}$, then $\langle A \rangle$ is conserved. Taking $\mathcal{H} = -\hbar^2/(2m)\nabla^2 + V$, an important example is $\mathcal{A} = x$:

$$(\mathcal{H}x - x\mathcal{H})\,\psi = \frac{\hbar^2}{2m}\left(x \frac{\partial^2 \psi}{\partial x^2} - \frac{\partial^2 x \psi}{\partial x^2} \right) = \frac{\hbar^2}{2m}\left(-2 \frac{\partial \psi}{\partial x} \right) ,$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle x \rangle = \frac{j}{\hbar} \int_\tau \psi^* \frac{\hbar^2}{2m}\left(-2 \frac{\partial \psi}{\partial x} \right) \mathrm{d}\tau = \frac{1}{m} \langle \psi | \hat{p}_x | \psi \rangle = \frac{\langle p_x \rangle}{m} \, .$$

In conclusion, the expectation values provide the relation $\mathrm{d}\langle x \rangle / \mathrm{d}t = \langle p_x \rangle / m$, which is formally identical to the classical one.

$$\frac{d}{dt}\langle A \rangle = \frac{j}{\hbar} \underbrace{\int_\tau \psi^* (\mathcal{H}A - A\mathcal{H}) \psi \, d\tau}_{\text{if 'A' commutes with 'H'} \; = 0} + \int_\tau \psi^* \frac{\partial A}{\partial t} \psi \, d\tau$$

* if commutes $\Rightarrow$ $HA = AH$

Then the term would be equal to zero

$$\Rightarrow \boxed{\int_\tau \psi^* \frac{\partial A}{\partial t} \psi \, d\tau = 0} \Rightarrow \frac{d}{dt}\langle A\rangle = 0$$

$\langle A\rangle$ Expectation value is conserved in Time

→ The property that $\langle A\rangle$ is conserved is equivalent to saying operator commutes with Hamiltonian

expectation of an operator

ex: Assuming the case of a free particle and

A : Momentum operator

$$H = -\frac{\hbar^2}{2m}\nabla^2$$ (potential for free particle is zero)

in this case the Hamiltonian (H) commutes with momentum operator (A) and it implies that

$$\boxed{\frac{d}{dt}\langle A\rangle = 0}$$ (Momentum is conserved which is equivalent to situation w.r.t. classical mechanics for a free particle)

→ Obviously, interesting cases are those in which operator A Does not Commute with the Hamiltonian $\mathcal{H}$

$$\boxed{\mathcal{H} = -\frac{\hbar^2}{2m}\nabla^2 + V \quad , \quad A = x}$$

$$\Rightarrow \quad (\mathcal{H}x - x\mathcal{H})\,\psi = \frac{\hbar^2}{2m}\left(x\frac{\partial^2\psi}{\partial x^2} - \frac{\partial^2 x\psi}{\partial x^2}\right) = \frac{\hbar^2}{2m}\left(-2\frac{\partial\psi}{\partial x}\right),$$

$$\frac{d}{dt}\langle A\rangle = \frac{\mathrm{d}}{\mathrm{d}t}\langle x\rangle = \frac{j}{\hbar}\int_\tau \psi^* \frac{\hbar^2}{2m}\left(-2\frac{\partial\psi}{\partial x}\right)\mathrm{d}\tau = \frac{1}{m}\langle\psi|\hat{p}_x|\psi\rangle = \frac{\langle p_x\rangle}{m}.$$

In conclusion, the expectation values provide the relation $\mathrm{d}\langle x\rangle/\mathrm{d}t = \langle p_x\rangle/m$, which is formally identical to the classical one.

$$\frac{d}{dt}\langle x\rangle = \frac{\langle P_x\rangle}{m}$$

$$\Rightarrow \quad \boxed{\langle P_x\rangle = m\frac{d}{dt}\langle x\rangle}$$

This is like a classical expression

$$P = mV$$

Revanth Reddy Pannala
EBIT, Unibo
రేవంత్ రెడ్డి పన్నాల

Time Derivative of the Expectation Value — II

- Here we will choose 'A' as a Momentum operator

- Still with $\mathcal{H} = -\hbar^2/(2m)\nabla^2 + V$, another important example is $\mathcal{A} = \hat{p}_x = -j\hbar\,\partial/\partial x$: Momentum operator

Commutator
$$(\mathcal{H}\hat{p}_x - \hat{p}_x\mathcal{H})\,\psi = -j\hbar\left(V\frac{\partial\psi}{\partial x} - \frac{\partial V\psi}{\partial x}\right) = j\hbar\psi\frac{\partial V}{\partial x},$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle p_x\rangle = \frac{j}{\hbar}\int_\tau \psi^* j\hbar\psi\frac{\partial V}{\partial x}\,\mathrm{d}\tau = -\langle\psi|\partial V/\partial x|\psi\rangle = \langle F_x\rangle\,.$$

- Also in this case the expectation values reproduce the classical relation. If $\partial V/\partial x$ depends weakly on position in the region where ψ is significant, then (*Ehrenfest theorem*)

$$\boxed{\frac{\mathrm{d}}{\mathrm{d}t}\langle p_x\rangle \simeq -\frac{\partial V}{\partial x}\int_\tau \psi^*\psi\,\mathrm{d}\tau = -\frac{\partial V}{\partial x} = F_x\,.}$$

- If, on the contrary, $\partial V/\partial x$ depends strongly on position (e.g., steps, barriers), then essential differences between the classical and quantum cases are to be expected.

****

Commutator : $(\mathcal{H}\hat{P}_x - \hat{P}_x\mathcal{H})\psi$

$$\Rightarrow \underbrace{\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}\left(-j\hbar\frac{\partial}{\partial x}\psi\right) - \left(-j\hbar\frac{\partial}{\partial x}\psi\right)\frac{\partial^2}{\partial x^2}\right)}_{=0} +$$

$$\left(-j\hbar\, V\frac{\partial\psi}{\partial x} - \left(-j\hbar\frac{\partial}{\partial x}V\psi\right)\right)$$

$$\Rightarrow -j\hbar v \frac{\partial \psi}{\partial x} + \left(j\hbar \frac{\partial}{\partial x}(v\psi) \right)$$

$$\Rightarrow -j\hbar v \frac{\partial \psi}{\partial x} + \left(j\hbar \left(v \frac{\partial}{\partial x}\psi - \psi \frac{\partial}{\partial x} v \right) \right)$$

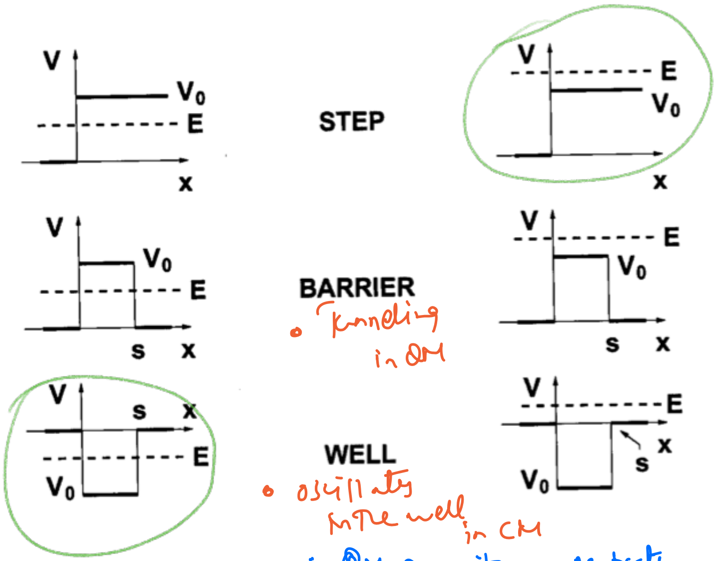
$$\Rightarrow \cancel{-j\hbar v \frac{\partial \psi}{\partial x}} + \cancel{j\hbar v \frac{\partial \psi}{\partial x}} - j\hbar \psi \frac{\partial v}{\partial x}$$

$$(H\hat{p}_x - \hat{p}_x H)\psi = -j\hbar \psi \frac{\partial v}{\partial x}$$

** Not part of the Exam from Now until further Notice **

Note; We have concluded above that the cases in which CM is very different from QM is when there are Rapid variations in SPACE w.r.to PE (V)

We are now going to consider set of cases which are easy to analyze Analytically.



T. 14.1: Gradino, barriera e buca di energia potenziale.

- Tunneling in QM
- oscillates in the well in CM
- In QM can it may penetrate but wavefunction can be Normalizable.

Revanth Reddy Pannala
EBIT, Unibo
రేవంత్ రెడ్డి పన్నాల