Lecture 06

Expectation values and Operators

Introduction of Quantum Mechanics : Dr Prince A Ganai
Classical Domain

Different approaches \[ F = Ma \]

Lagrangian and Hamiltonian dynamics

Hamiltonian Approach \[ \dot{x} = \frac{\partial H}{\partial p_i}, \quad \dot{p} = -\frac{\partial H}{\partial x_i} \]

Concept of Phase Space and Dynamical variables \[ Q(x, p) \]

Momentum, Kinetic energy, Angular Momentum, etc
Classical Approach breaks down - Uncertainty Principle comes in

Wave Particle duality

Wave function and Schrodinger equation

\[ i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V\Psi = H\Psi \]

\[ P(x, t) \, dx = |\Psi(x, t)|^2 \, dx \]
How does Probability evolve with time

\[
\frac{d}{dt} \int_{-\infty}^{+\infty} |\Psi(x, t)|^2 \, dx = \int_{-\infty}^{+\infty} \frac{\partial}{\partial t} |\Psi(x, t)|^2 \, dx.
\]

\[
\frac{\partial}{\partial t} |\Psi|^2 = \frac{\partial}{\partial t} (\Psi^* \Psi) = \Psi^* \frac{\partial \Psi}{\partial t} + \frac{\partial \Psi^*}{\partial t} \Psi
\]

\[
\frac{\partial \Psi}{\partial t} = \frac{i\hbar}{2m} \frac{\partial^2 \Psi}{\partial x^2} - \frac{i}{\hbar} V \Psi, \quad \frac{\partial \Psi^*}{\partial t} = -\frac{i\hbar}{2m} \frac{\partial^2 \Psi^*}{\partial x^2} + \frac{i}{\hbar} V \Psi^*
\]

\[
\frac{\partial}{\partial t} |\Psi|^2 = \frac{i\hbar}{2m} \left( \Psi^* \frac{\partial^2 \Psi}{\partial x^2} - \frac{\partial^2 \Psi^*}{\partial x^2} \Psi \right)
\]

\[
= \frac{\partial}{\partial x} \left[ \frac{i\hbar}{2m} \left( \Psi^* \frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x} \Psi \right) \right]
\]

\[
J(x, t) \equiv \frac{i\hbar}{2m} \left( \Psi \frac{\partial \Psi^*}{\partial x} - \Psi^* \frac{\partial \Psi}{\partial x} \right)
\]
How does Probability evolve with time

\[
\frac{d}{dt} \int_{-\infty}^{+\infty} |\Psi(x, t)|^2 \, dx = \frac{i\hbar}{2m} \left( \Psi^* \frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x} \Psi \right) \bigg|_{-\infty}^{+\infty} = 0
\]

Thus Schrodinger equation guaranties if a wave function is normalised at \(t=0\), it will stay normalised for all time

\[
P_{ab}(t) = \int_{a}^{b} |\Psi(x, t)|^2 \, dx \quad \frac{dP_{ab}(t)}{dt} = \int_{a}^{b} \frac{\partial}{\partial t} |\Psi(x, t)|^2 \, dx
\]

\[
\frac{\partial}{\partial t} |\Psi(x, t)|^2 = \frac{i\hbar}{2m} \left( \Psi^* \frac{\partial^2 \Psi}{\partial x^2} - \Psi \frac{\partial^2 \Psi^*}{\partial x^2} \right)
\]

\[
= \frac{\partial}{\partial x} \left[ \frac{i\hbar}{2m} \left( \Psi^* \frac{\partial \Psi}{\partial x} - \Psi \frac{\partial \Psi^*}{\partial x} \right) \right]
\]

\[
\frac{\partial}{\partial t} P_{ab}(t) = - \int_{a}^{b} \frac{\partial}{\partial x} J(x, t) \, dx
\]
Measurements in Quantum Mechanics

\[ < x > = \int_{\infty}^{\infty} x |\Psi(x, t)|^2 dx \]

**Momentum expectation**

\[ p = mv = m \frac{dx}{dt} \]

\[ < p > = \frac{d < x >}{dt} \]

\[ < p > = \frac{d}{dt} \int_{\infty}^{\infty} \Psi(x, t)^* x \Psi(x, t) dx \]

\[ = m \int_{-\infty}^{\infty} dx \left( \frac{\partial \psi^*(x, t)}{\partial t} x \psi(x, t) + \psi^*(x, t) x \frac{\partial \psi(x, t)}{\partial t} \right) \]
Momentum expectation:

Classically:

Quantum mechanically, it is

Let us try:

\[ \frac{d}{dt} \langle x \rangle = \frac{\hbar}{2i} \int_{-\infty}^{\infty} dx \left( \frac{\partial^2 \psi^*}{\partial x^2} x \psi - \psi^* x \frac{\partial^2 \psi}{\partial x^2} \right) \]

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 Schrödinger equation and its complex conjugate to evaluate the above and we have

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

This means that the integrand has the form

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

What about other dynamical variables?

Introduction of Quantum Mechanics : Dr Prince A Ganai
Because the wave functions vanish at infinity, the first term does not contribute, and the integral gives
\[ \langle x \rangle = \int_{-\infty}^{+\infty} \psi^* x \psi \, dx. \]

This suggests that the momentum be represented by the differential operator
\[ \hat{p} \rightarrow -i\hbar \frac{\partial}{\partial x}. \]

As the position expectation was represented by
\[ \int \psi^* x \psi \, dx, \]

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:
\[ \langle Q(x, p) \rangle = \int \psi^* Q(x, \frac{i \hbar}{\partial x}) \psi \, dx. \]

For example: Kinetic energy
\[ T = \frac{1}{2} m v^2 = \frac{p^2}{2m} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}, \]

\[ \langle T \rangle = \frac{-\hbar^2}{2m} \int \psi^* \frac{\partial^2 \psi}{\partial x^2} \, dx. \]
\[
\dot{x}/dt = \tilde{\partial} H/\partial p \quad \text{and} \quad \dot{p}/dt = -\tilde{\partial} H/\partial x,
\]

To every physically measurable quantity \( A \), called an observable or dynamical variable, there corresponds a linear Hermitian operator \( \hat{A} \) whose eigenvectors form a complete basis.

\[
\hat{A}|\psi(t)\rangle = a_n|\psi_n\rangle,
\]

\[
f(\vec{r}, \vec{p}) \quad \longrightarrow \quad F(\hat{R}, \hat{P}) = f(\hat{R}, -i\hbar \nabla),
\]

\[
H = \frac{1}{2m} \vec{p}^2 + V(\vec{r}, t)
\]

\[
\hat{H} = -\frac{\hbar^2}{2m} \nabla^2 + V(\hat{R}, t),
\]
### Operators and expectation values

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Physical quantity</th>
<th>Operator</th>
</tr>
</thead>
<tbody>
<tr>
<td>$f(x)$</td>
<td>Any function of $x$—the position $x$, the potential energy $V(x)$, etc.</td>
<td>$f(x)$</td>
</tr>
<tr>
<td>$p_x$</td>
<td>$x$ component of momentum</td>
<td>$\frac{\hbar}{i} \frac{\partial}{\partial x}$</td>
</tr>
<tr>
<td>$p_y$</td>
<td>$y$ component of momentum</td>
<td>$\frac{\hbar}{i} \frac{\partial}{\partial y}$</td>
</tr>
<tr>
<td>$p_z$</td>
<td>$z$ component of momentum</td>
<td>$\frac{\hbar}{i} \frac{\partial}{\partial z}$</td>
</tr>
</tbody>
</table>
### Operators and expectation values

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Physical quantity</th>
<th>Operator</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E$</td>
<td>Hamiltonian (time independent)</td>
<td>$\frac{p_{\text{op}}^2}{2m} + V(x)$</td>
</tr>
<tr>
<td>$E$</td>
<td>Hamiltonian (time dependent)</td>
<td>$\hat{\hbar} \frac{\partial}{\partial t}$</td>
</tr>
<tr>
<td>$E_k$</td>
<td>Kinetic energy</td>
<td>$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$</td>
</tr>
<tr>
<td>$L_z$</td>
<td>$z$ component of angular momentum</td>
<td>$-i\hbar \frac{\partial}{\partial \phi}$</td>
</tr>
</tbody>
</table>
\[ \langle p \rangle = \int_0^L \left( \sqrt{\frac{2}{L}} \sin \frac{n x}{L} \right) \left( \frac{\hbar}{i} \frac{\partial}{\partial x} \right) \left( \sqrt{\frac{2}{L}} \sin \frac{n x}{L} \right) dx \]
\[ = \frac{\hbar}{i} \frac{2 \pi}{L} \int_0^L \sin \frac{\pi x}{L} \cos \frac{\pi x}{L} dx = 0 \]

\[ \frac{\hbar}{i} \frac{\partial}{\partial x} \left( \frac{\hbar}{i} \frac{\partial}{\partial x} \right) \psi = -\hbar^2 \frac{\partial^2 \psi}{\partial x^2} = -\hbar^2 \left( -\frac{\pi^2}{L^2} \sqrt{\frac{2}{L}} \sin \frac{\pi x}{L} \right) \]
\[ = + \frac{\hbar^2 \pi^2}{L^2} \psi \]

\[ \langle p^2 \rangle = \frac{\hbar^2 \pi^2}{L^2} \int_0^L \psi^* \psi dx = \frac{\hbar^2 \pi^2}{L^2} \]

"Introduction of Quantum Mechanics : Dr Prince A Ganai"
Curiosity Kills the Cat

Lecture 06
Concluded