

Lecture 07

Postulates of Quantum Mechanics

Expectation values of p and p^2 for ground state of Infinite well



$$\begin{aligned}\langle p \rangle &= \int_0^L \left(\sqrt{\frac{2}{L}} \sin \frac{nX}{L} \right) \left(\frac{\hbar}{i} \frac{\partial}{\partial X} \right) \left(\sqrt{\frac{2}{L}} \sin \frac{nX}{L} \right) dx \\ &= \frac{\hbar}{i} \frac{2}{L} \frac{\pi}{L} \int_0^L \sin \frac{\pi X}{L} \cos \frac{\pi X}{L} dx = 0\end{aligned}$$

$$\begin{aligned}\frac{\hbar}{i} \frac{\partial}{\partial X} \left(\frac{\hbar}{i} \frac{\partial}{\partial X} \right) \psi &= -\hbar^2 \frac{\partial^2 \psi}{\partial X^2} = -\hbar^2 \left(-\frac{\pi^2}{L^2} \sqrt{\frac{2}{L}} \sin \frac{\pi X}{L} \right) \\ &= +\frac{\hbar^2 \pi^2}{L^2} \psi\end{aligned}$$

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



Postulate 1: State of a system

The state of any physical system is specified, at each time t , by a state vector $|\psi(t)\rangle$ in a Hilbert space \mathcal{H} ; $|\psi(t)\rangle$ contains (and serves as the basis to extract) all the needed information about the system. Any superposition of state vectors is also a state vector.

Schrodinger Formulation and Heisenberg Formulation



Postulate 2: Observables and operators

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.

Observable

Corresponding operator

$$\vec{r}$$

$$\hat{R}$$

$$\vec{p}$$

$$\hat{P} = -i\hbar \vec{\nabla}$$

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

$$\hat{T} = -\frac{\hbar^2}{2m} \nabla^2$$

$$E = \frac{p^2}{2m} + V(\vec{r}, t)$$

$$\hat{H} = -\frac{\hbar^2}{2m} \nabla^2 + \hat{V}(\hat{R}, t)$$

$$\vec{L} = \vec{r} \times \vec{p}$$

$$\hat{L} = -i\hbar \hat{R} \times \vec{\nabla}$$



Postulate 3: Measurements and eigenvalues of operators

The measurement of an observable A may be represented formally by the action of \hat{A} on a state vector $|\psi(t)\rangle$. The only possible result of such a measurement is one of the eigenvalues a_n (which are real) of the operator \hat{A} . If the result of a measurement of A on a state $|\psi(t)\rangle$ is a_n , the state of the system *immediately after* the measurement changes to $|\psi_n\rangle$:

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

where $a_n = \langle \psi_n | \psi(t) \rangle$. **Note:** a_n is the component of $|\psi(t)\rangle$ when projected¹ onto the eigenvector $|\psi_n\rangle$.



Postulate 4: Probabilistic outcome of measurements

- **Discrete spectra:** When measuring an observable A of a system in a state $|\psi\rangle$, the probability of obtaining one of the nondegenerate eigenvalues a_n of the corresponding operator \hat{A} is given by

$$P_n(a_n) = \frac{|\langle\psi_n|\psi\rangle|^2}{\langle\psi|\psi\rangle} = \frac{|a_n|^2}{\langle\psi|\psi\rangle},$$

where $|\psi_n\rangle$ is the eigenstate of \hat{A} with eigenvalue a_n . If the eigenvalue a_n is m -degenerate, P_n becomes

$$P_n(a_n) = \frac{\sum_{j=1}^m |\langle\psi_n^j|\psi\rangle|^2}{\langle\psi|\psi\rangle} = \frac{\sum_{j=1}^m |a_n^{(j)}|^2}{\langle\psi|\psi\rangle}.$$

The act of measurement changes the state of the system from $|\psi\rangle$ to $|\psi_n\rangle$. If the system is already in an eigenstate $|\psi_n\rangle$ of \hat{A} , a measurement of A yields with certainty the corresponding eigenvalue a_n : $\hat{A}|\psi_n\rangle = a_n|\psi_n\rangle$.

- **Continuous spectra:** The relation (3.2), which is valid for discrete spectra, can be extended to determine the probability density that a measurement of \hat{A} yields a value between a and $a + da$ on a system which is initially in a state $|\psi\rangle$:

$$\frac{dP(a)}{da} = \frac{|\psi(a)|^2}{\langle\psi|\psi\rangle} = \frac{|\psi(a)|^2}{\int_{-\infty}^{+\infty} |\psi(a')|^2 da'};$$

for instance, the probability density for finding a particle between x and $x + dx$ is given by $dP(x)/dx = |\psi(x)|^2/\langle\psi|\psi\rangle$.



Postulate 5: Time evolution of a system

The time evolution of the state vector $|\psi(t)\rangle$ of a system is governed by the time-dependent *Schrödinger equation*

$$i\hbar \frac{\partial |\psi(t)\rangle}{\partial t} = \hat{H} |\psi(t)\rangle,$$

where \hat{H} is the Hamiltonian operator corresponding to the total energy of the system.

Connecting Quantum to Classical Mechanics



Poisson Brackets and Commutators

$$\{A, B\} = \sum_j \left(\frac{\partial A}{\partial q_j} \frac{\partial B}{\partial p_j} - \frac{\partial A}{\partial p_j} \frac{\partial B}{\partial q_j} \right).$$

$$\frac{\partial q_j}{\partial p_k} = 0, \quad \frac{\partial p_j}{\partial q_k} = 0;$$

$$\{q_j, q_k\} = \{p_j, p_k\} = 0, \quad \{q_j, p_k\} = \delta_{jk}.$$

$$\{A, B\} = -\{B, A\}$$

$$\{A, \alpha B + \beta C + \gamma D + \dots\} = \alpha\{A, B\} + \beta\{A, C\} + \gamma\{A, D\} + \dots$$

$$\{A, B\}^* = \{A^*, B^*\}$$

$$\{A, BC\} = \{A, B\}C + B\{A, C\},$$

$$\{A, \{B, C\}\} + \{B, \{C, A\}\} + \{C, \{A, B\}\} = 0$$

$$\{A, B^n\} = nB^{n-1}\{A, B\}, \quad \{A^n, B\} = nA^{n-1}\{A, B\}$$

The total time derivative of a dynamical variable A is given by

$$\frac{dA}{dt} = \sum_j \left(\frac{\partial A}{\partial q_j} \frac{\partial q_j}{\partial t} + \frac{\partial A}{\partial p_j} \frac{\partial p_j}{\partial t} \right) + \frac{\partial A}{\partial t} = \sum_j \left(\frac{\partial A}{\partial q_j} \frac{\partial H}{\partial p_j} - \frac{\partial A}{\partial p_j} \frac{\partial H}{\partial q_j} \right) + \frac{\partial A}{\partial t};$$

$$\frac{dq_j}{dt} = \frac{\partial H}{\partial p_j}, \quad \frac{dp_j}{dt} = -\frac{\partial H}{\partial q_j},$$

$$\frac{dA}{dt} = \{A, H\} + \frac{\partial A}{\partial t}.$$



Time Evolution of Expectation Values



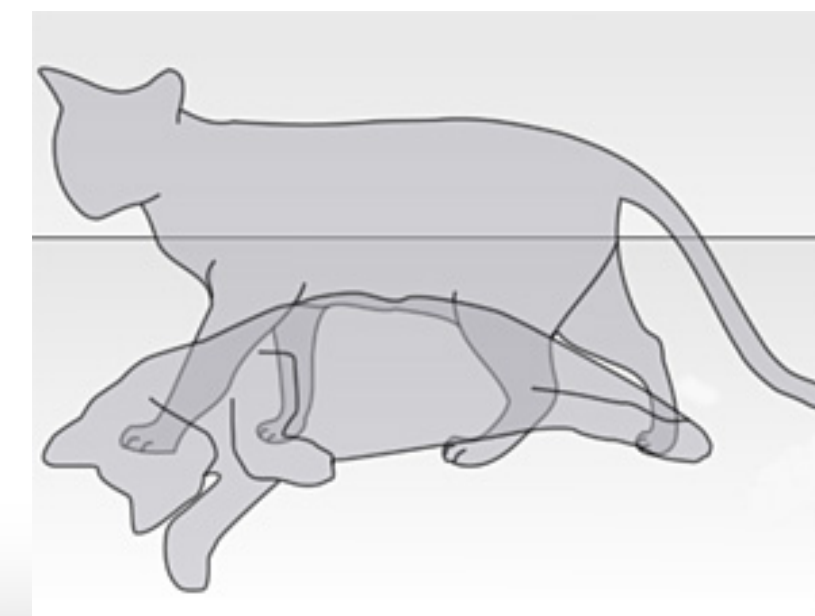
$$\langle \hat{A} \rangle = \langle \Psi(t) | \hat{A} | \Psi(t) \rangle.$$

$$\frac{d}{dt} \langle \hat{A} \rangle = \frac{1}{i\hbar} \langle \Psi(t) | \hat{A} \hat{H} - \hat{H} \hat{A} | \Psi(t) \rangle + \langle \Psi(t) | \frac{\partial \hat{A}}{\partial t} | \Psi(t) \rangle$$

$$\frac{d}{dt} \langle \hat{A} \rangle = \frac{1}{i\hbar} \langle [\hat{A}, \hat{H}] \rangle + \langle \frac{\partial \hat{A}}{\partial t} \rangle.$$

$$\text{If } [\hat{H}, \hat{A}] = 0 \text{ and } \frac{\partial \hat{A}}{\partial t} = 0 \implies \frac{d\langle \hat{A} \rangle}{dt} = 0 \implies \langle \hat{A} \rangle = \text{constant.}$$

$$\frac{1}{i\hbar} [\hat{A}, \hat{B}] \longrightarrow \{A, B\}_{\text{classical}}.$$



Curiosity Kills the Cat

Lecture 06
Concluded