PHYS 621 Lecture Notes 4

The Postulates of Quantum Mechanics

Classical Mechanics: Classical paths $q_i(t)$
momenta $p_i(t)$

State at time t given by $\{q_i, p_i\}$

Dynamics governed by a Hamiltonian $H(p_i, q_i, t)$

Hamilton's Equations
$$\dot{q}_i = \frac{\partial H}{\partial p_i}$$
$$\dot{p}_i = -\frac{\partial H}{\partial q_i}$$

Quantum Mechanics: No definite trajectories,
– probabilistic description

We need: states
observables w/ probabilities
Dynamics (i.e. time evolution)

Postulate 1:

At every time t, the state is given by a ket $|\psi\rangle$ in Hilbert space.

Postulate 2:

Classical observables A are replaced by corresponding Hermitian operators $\hat{A}$ acting on the states $|\psi\rangle$.

Ambiguity: operators need not commute

what operator corresponds to xp^2?

$$\hat{x}\hat{p}^2 \, ?$$

$$\hat{x}\hat{p}\hat{x} \, ?$$

etc.

Postulate 3: The only possible result of an ideal measurement of an observable $\hat{A}$ is an eigenvalue λ of $\hat{A}$.

A state of the system $|\psi_\lambda\rangle$ with that eigenvalue satisfies

$$\hat{A}|\psi_\lambda\rangle = \lambda|\psi_\lambda\rangle$$

and is called an eigenstate of $\hat{A}$.

- $\hat{A}$ Hermitian → eigenvalues are real.
  — we only measure real values of observables
- States can be written as linear combinations of eigenstates of $\hat{A}$!

$$\boxed{|\psi\rangle = \sum_n c_n |v_n\rangle}$$

$$\hat{A}|v_n\rangle = \lambda_n |v_n\rangle$$

- If other observables can also be measured, then $\hat{A}|v_{n,b}\rangle = \lambda_n |v_{n,b}\rangle$

labels some other observable

$$\hat{A}\left(\sum_b |v_{n,b}\rangle\right) = \lambda_n \left(\sum_b |v_{n,b}\rangle\right)$$

Arbitrary state $|\psi\rangle = \sum_{n,b} c_{n,b} |v_{n,b}\rangle$.

- If $|x\rangle$ is an eigenstate of the position operator $\hat{x}$ with eigenvalue x, define

$$\boxed{\psi(x) = \langle x|\psi\rangle}$$ the wave function

- Eigenvalues can be discrete → <u>quantum</u>

If there is a finite number of eigenvalues of observables in a system, then the Hilbert space is finite dimensional.

<u>Example</u>: spin-1/2 particle has spin eigenstates

$|\uparrow\rangle$ with $\hat{S}_z|\uparrow\rangle = \frac{\hbar}{2}|\uparrow\rangle$

and $|\downarrow\rangle$ with $\hat{S}_z|\downarrow\rangle = -\frac{\hbar}{2}|\downarrow\rangle$

→ 2-dimensional Hilbert space.

- Note that the spin observable has no classical counterparts but it still corresponds to a Hermitian operator.

- Set of eigenvalues of $\hat{A}$ is called the <u>spectrum</u> of $\hat{A}$

Postulate 4:

The probability of obtaining an eigenvalue λ_n corresponding to eigenstate $|v_n\rangle$ of observable $\hat{A}$ in a normalized state $|\psi\rangle$ with $\langle\psi|\psi\rangle = 1$, is

$$\boxed{P_n = |\langle v_n|\psi\rangle|^2}$$

The Born Rule

Choose $\{|v_n\rangle\}$ to be an orthonormal basis $\boxed{\langle v_i|v_j\rangle = \delta_{ij}}$

$$\boxed{|\psi\rangle = \sum_i c_i |v_i\rangle}$$

$$\rightarrow P_n = |\langle v_n|\psi\rangle|^2 = \left|\sum_i c_i \langle v_n|v_i\rangle\right|^2$$

$$= \left|\sum_i c_i \delta_{ni}\right|^2$$

$$\boxed{P_n = |c_n|^2}$$

Probabilities must sum to 1:

$$\boxed{\sum_i P_i = \sum_i |c_i|^2 = 1}$$

But $\langle\psi|\psi\rangle = \sum_{i,j} c_j^* c_i \langle v_j | v_i \rangle$

$$= \sum_i |c_i|^2 = 1$$

$$\Rightarrow \boxed{\langle\psi|\psi\rangle = 1}$$

— Physical states are normalizable.

- If states are degenerate, i.e.

$$\hat{A}|v_{n,b}\rangle = \lambda_n |v_{n,b}\rangle$$

indexed by b,

then $|\psi\rangle = \sum_{n,b} c_{n,b} |v_{n,b}\rangle$

with $\langle v_{i,a} | v_{j,b}\rangle = \delta_{ij}\delta_{ab}$

then the probability of measuring λ_n is

$$\sum_b |c_{n,b}|^2$$

Define the projection operator onto the space of states w/ eigenvalue λ_n:

$$\mathbb{P}_{V_n} |\psi\rangle = \sum_b c_{n,b} |v_{n,b}\rangle$$

n fixed

probability $P_n = \langle\psi| \mathbb{P}_{V_n} |\psi\rangle$

$$= \left(\sum_{m,a} c^*_{m,a} \langle v_{m,a}|\right) \left(\sum_b c_{n,b} |v_{n,b}\rangle\right)$$

$$= \sum_{m,a,b} c^*_{m,a} c_{n,b} \langle v_{m,a}|v_{n,b}\rangle$$

$$= \sum_b |c_{n,b}|^2$$

$\mathbb{P}_{V_n}$ satisfies $\mathbb{P}_{V_n}^2 = \mathbb{P}_{V_n}$ (project twice = project once)

$\mathbb{P}_{V_n}^\dagger = \mathbb{P}_{V_n}$ $\left(\langle\psi| \mathbb{P}_{V_n} = \sum_b c^*_{n,b} \langle v_{n,b}|\right)$

· Continuous spectrum

Example: $\langle x|\hat{x}|x'\rangle = x\,\delta(x-x')$

$\langle x|\hat{p}|x'\rangle = -i\hbar\,\delta'(x-x')$

$\hat{x}|x\rangle = x|x\rangle$

Completeness relation: $\int dx\,|x\rangle\langle x| = \hat{\mathbb{1}}$

Suppose $\hat{A}|\psi\rangle = \lambda|\psi\rangle$

Then $\int dx'\,\underbrace{\langle x|\hat{A}|x'\rangle}_{A_{xx'}}\underbrace{\langle x'|\psi\rangle}_{\psi(x')} = \lambda\underbrace{\langle x|\psi\rangle}_{\psi(x)}$

$$\Rightarrow \boxed{\int dx'\,A_{xx'}\,\psi(x') = \lambda\,\psi(x)}$$

Example : $\hat{P}$ Momentum operator

Suppose $\hat{P}|\psi\rangle = p|\psi\rangle$

$$\int dx' \langle x|\hat{P}|x'\rangle\langle x'|\psi\rangle = p\langle x|\psi\rangle$$

$$\int dx' \left(-i\hbar\,\delta'(x-x')\right)\psi(x') = p\,\psi(x)$$

$$\int dx' \left(i\hbar\,\delta(x-x')\,\psi'(x')\right) = p\,\psi(x)$$

Note $\delta'(x-x') = -\delta'(x'-x)$

$$\Rightarrow \boxed{-i\hbar\frac{d\psi}{dx} = p\,\psi(x)}$$

- Suppose a system has eigenvalues for more than one observable.

Then the Hilbert space is a tensor product of the individual Hilbert spaces $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$.

$$\hat{A}_{(1)}|a_1, b_2\rangle = a_1|a_1, b_2\rangle$$

$$\hat{B}_{(2)}|a_1, b_2\rangle = b_2|a_1, b_2\rangle$$

$$\hat{A}_{(1)} = \hat{A}\otimes\hat{\mathbb{1}}, \quad \hat{B}_{(2)} = \hat{\mathbb{1}}\otimes\hat{B}$$

$$\hat{A}_{(1)} \hat{B}_{(2)} |a_1, b_2\rangle = a_1 b_2 \, |a_1, b_2\rangle$$

$$\hat{B}_{(2)} \hat{A}_{(1)} |a_1, b_2\rangle = a_1 b_2 \, |a_1, b_2\rangle$$

The eigenstates $|a_1, b_2\rangle$ form a basis of the Hilbert space.

$$\rightarrow \boxed{[\hat{A}_{(1)}, \hat{B}_{(2)}] = \hat{A}_{(1)} \hat{B}_{(2)} - \hat{B}_{(2)} \hat{A}_{(1)} = 0}$$

- Consider the <u>expectation value</u> of an observable

$$\langle \hat{A} \rangle = \sum_n P_n a_n = \sum_n |c_n|^2 a_n$$

$$= \sum_{n,m} c_m^* c_n \underbrace{\langle v_m | \hat{A} | v_n \rangle}$$

$$= a_n \langle v_m | v_n \rangle$$

$$= a_n \delta_{mn}$$

$$= \langle \psi | \hat{A} | \psi \rangle$$

$$\Rightarrow \boxed{\langle \hat{A} \rangle = \langle \psi | \hat{A} | \psi \rangle}$$

Postulate 5

After a measurement of an observable $\hat{A}$, the state of the system is described by the ket $|v_n\rangle$ with eigenvalue λ_n corresponding to the measured value of the observable.

- For a degenerate initial state, the state after measurement is the projection onto the subspace of $\mathcal{H}$ with eigenvalue λ_n:

$$\mathbb{P}_{v_n} |\psi\rangle$$

- Question: what is a measurement? How does it "collapse the wavefunction" like this?

☆ Do we really need a separate postulate for what happens during a measurement?

Postulate 6

Time evolution of a state is determined by the Schrödinger Equation:

$$\boxed{i\hbar \frac{d|\psi\rangle}{dt} = \hat{H}|\psi(t)\rangle}$$

where $\hat{H}(\hat{q}_i, \hat{p}_i)$ is the Hamiltonian for the system.

- Suppose we describe the time evolution in terms of a time-evolution operator $\hat{U}(t,t_0)$ such that

$$\boxed{|\psi(t)\rangle = \hat{U}(t,t_0)|\psi(t_0)\rangle.}$$

Then $\langle\psi(t)|\psi(t)\rangle = 1 = \langle\psi(t_0)|\psi(t_0)\rangle$

$$= \langle\psi(t_0)|\underbrace{\hat{U}(t,t_0)^\dagger\,\hat{U}(t,t_0)}_{=\mathbb{1}}|\psi(t_0)\rangle$$

$\Rightarrow \hat{U}(t,t_0)$ is unitary

To determine $\hat{U}(t, t_0)$ for a given Hamiltonian, consider a complete set of energy eigenstates $|E\rangle$, with

$$\boxed{\hat{H}|E\rangle = E|E\rangle}.$$ Time-independent Schrodinger Eq.

$$|\psi(t)\rangle = \sum_E |E\rangle \underbrace{\langle E|\psi(t)\rangle}_{\psi_E(t)}$$

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

$$= \sum_E E|E\rangle \psi_E(t)$$

$$= i\hbar \sum_E |E\rangle \frac{d}{dt}\psi_E(t)$$

$$\rightarrow \sum_E \left(i\hbar \frac{d}{dt}\psi_E(t) - E\psi_E(t)\right)|E\rangle = 0$$

Solution: $$\boxed{\psi_E(t) = e^{-iE(t-t_0)/\hbar}\psi_E(t_0)}$$

Then, $|\psi(t)\rangle = \sum_E e^{-iE(t-t_0)/\hbar} \psi_E(t_0)\,|E\rangle$

$$= \hat{U}(t,t_0)\,|\psi(t_0)\rangle$$

$$\Rightarrow \boxed{\hat{U}(t,t_0) = \sum_E e^{-iE(t-t_0)} |E\rangle\langle E|}$$

- For a degenerate energy spectrum,

$$|\psi(t)\rangle = \sum_{E,\alpha} e^{-iE(t-t_0)/\hbar} \psi_{E,\alpha}(t_0)\,|E\alpha\rangle$$

$$\hat{U}(t,t_0) = \sum_{E,\alpha} |E,\alpha\rangle\langle E\alpha|\, e^{-iE(t-t_0)/\hbar}$$