Phys 521 Fall 2024

Lecture 4 - Postulates

(1) Dynamical system represented by ray in Hilbert space (norm of ray not physical). Call this ray the quantum state ("$|\psi\rangle$").

overall phase of state not physical.
properly normalized state, $\langle\psi|\psi\rangle = 1$.

Note: it is convenient to also use the non-normalizable plane wave state, in position basis,

$$|p\rangle \doteq \langle x|p\rangle = \phi_p(x) = \frac{1}{\sqrt{2\pi\hbar}} \exp\left(\frac{ipx}{\hbar}\right)$$

$$\langle p'|p\rangle = \int_{-\infty}^{\infty} dx \, \langle p'|x\rangle \langle x|p\rangle$$

$$= \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dx \, \exp\left(\frac{i(p-p')x}{\hbar}\right)$$

$p = \hbar k$

$$= \frac{1}{2\pi} \int dx \, \exp\left(-i(k'-k)x\right) = \delta(p'-p)$$

plane wave normalization

(2) Unitary time evolution operator defined as

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

$$U^{\dagger}(t,t_0)U(t,t_0) = \hat{I} \; ; \; \langle\psi(t)|\psi(t)\rangle = \langle\psi(t_0)|\psi(t_0)\rangle$$

For infinitessimal time dt,

$$\hat{U}(t+dt, t) = \hat{I} - \frac{i}{\hbar} H \, dt \xrightarrow[dt \to 0]{} \hat{I}$$

$\hat{H}$ has dimentions of energy, is called the Hamiltonian operator. Note, in classical mechanic's H generates translations in time, (see Shankar).

<u>$\hat{U}(t)$ evolution equation</u>. We must be careful because we might have $H(t)$ and perhaps even

$$[\hat{H}(t_1), \hat{H}(t_2)] \neq 0$$

Composition property $t_2 > t_1 > t_0$

$$U(t_2, t_0) = U(t_2, t_1)U(t_1, t_0)$$

Thus, for small Δt, $t+\Delta t > t > t_0$

$$U(t+\Delta t, t_0) = U(t+\Delta t, t)\, U(t, t_0)$$

$$= \left(I - \frac{i}{\hbar} H \Delta t\right) U(t, t_0)$$

$$\frac{U(t+\Delta t, t_0) - U(t, t_0)}{\Delta t} = \frac{-i}{\hbar} H\, U(t, t_0)$$

define ratio in limit $\Delta t \to 0$ as $\frac{\partial U(t,t_0)}{\partial t}$

$$\boxed{i\hbar \frac{\partial}{\partial t} U(t, t_0) = H\, U(t, t_0)}$$

true very generally for any H. Therefore state evolves as

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

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

general Schrödinger equation.

Suppose H has no explicit time dependence. Then we can integrate time evolution equation

$$\hat{U}(t) = \lim_{N \to \infty} \left[1 - \frac{i}{\hbar} H \frac{t}{N}\right]^N = e^{-i\hat{H}t/\hbar}$$

Suppose $H(t)$ but $[H(t_1), H(t_2)] = 0$, then

$$U(t,t_0) = \exp\left[\frac{-i}{\hbar}\int_{t_0}^{t} dt' H(t')\right]$$

You prove (recitation #3) that satisfies time evolution equation with boundary condition

$$\lim_{t \to t_0} U(t,t_0) = I$$

Most generally, $[H(t_1), H(t_2)] \neq 0$, then solution is Dyson series

$$U(t,t_0) = I + \sum_{n=1}^{\infty} \left(\frac{-i}{\hbar}\right)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \cdots$$

$$\cdots \int_{t_0}^{t_{n-1}} dt_n \, H(t_1) H(t_2) \cdots H(t_n)$$

See Sakurai

Comment on sign in U,

$$U(t+dt,t) \cong 1 - \frac{i}{\hbar} H\,dt$$

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

Then for free particle you show (recitation #2)

$$\frac{d}{dt}\langle x\rangle = \frac{1}{m}\langle p\rangle$$

proving U exponential has correct sign.

③ Observables correspond to Hermitian operators.
Let $\hat{\theta}$ be Hermitian, then basis of orthonormal eigenvectors $|\theta_i\rangle$,

$$\hat{\theta}|\theta_i\rangle = \theta_i|\theta_i\rangle \qquad \theta_i \text{ real eigenvalue}$$

then

$$|\psi\rangle = \sum_i |\theta_i\rangle\langle\theta_i|\psi\rangle$$

measurement of $\hat{\theta}$ gives θ_i with probability,

$$P_i = |\langle\theta_i|\psi\rangle|^2$$

<u>Born Rule</u> ; Following measurement of $\hat{O}$, state collapses to eigenstate $|O_i\rangle$ that gave observed eigenvalue O_i.
<u>collapse postulate</u>

$$|\psi\rangle \xrightarrow{\hat{O}} |O_i\rangle \text{ with probability } |\langle O_i|\psi\rangle|^2$$

Any given measurement will yield a particular eigenvalue O_i. Only by repeated measurements on <u>ensemble</u> of identically prepared $|\psi\rangle$ can we measure probabilities $|\langle O_i|\psi\rangle|^2$.

<u>note:</u> 1. $|\psi\rangle \xrightarrow{\hat{O}} |O_i\rangle$ is a non-unitary evolution of $|\psi\rangle$. Hence, problematic.

2. Subsequent measurements after collapse will give eigenvalue O_i with unit probability

Repeated measurements on ensemble of identically prepared states, can measure expectation value $\langle \hat{O} \rangle$ and variance $(\Delta O)^2$.

$$\langle \hat{O} \rangle \equiv \langle \psi | \hat{O} | \psi \rangle \quad \text{expectation value}$$

$$= \sum_{i,j} \langle \psi | O_i \rangle \langle O_i | \hat{O} | O_j \rangle \langle O_j | \psi \rangle$$

$$= \sum_i O_i \left| \langle O_i | \psi \rangle \right|^2 \quad \text{classical expectation}$$

value given $P_i = |\langle O_i | \psi \rangle|^2$.

Similarly for variance, $(\Delta O)^2$ is classical variance given P_i. It is the P_i that are quantum.

Commuting observables. If $[\hat{A}, \hat{B}] = 0$, they are said to be compatible. They can be simultaneously diagonalized!

$$\hat{A} |a,b\rangle = a |a,b\rangle$$
$$\hat{B} |a,b\rangle = b |a,b\rangle$$

$$[A,B] |a,b\rangle = (AB - BA) |a,b\rangle = (ab - ba) |a,b\rangle = 0$$

moreover, order of measurement does not matter

$$|\psi\rangle = \sum |a,b\rangle\langle a,b|\psi\rangle$$

$$P(a,b) = |\langle a,b|\psi\rangle|^2 = P(b,a)$$

Subtlety arises in case of degeneracy, 2 or more eigenvalues are the same. (See Shankar)

Consider A, B with 3 eigenvalues but $b_1 = b_2$.
The basis is
$|a_1,b_1\rangle$, $|a_2,b_1\rangle$, $|a_3,b_3\rangle$
general superposition state

$$|\psi\rangle = \lambda_1|a_1 b_1\rangle + \lambda_2|a_2 b_1\rangle + \lambda_3|a_3 b_3\rangle$$

where $\sum_{i=1}^{3} |\lambda_i|^2 = 1$

First measure A then B. Suppose A gives eigenvalue a_1.

$$A|\psi\rangle \xrightarrow{A} |\psi'\rangle = |a_1, b_1\rangle \quad \text{Prob } |\lambda_1|^2$$

Now measure B, must get eigenvalue b_1 with probability 1. Total probability is $P(B,A) = |\lambda_1|^2$.

Next, consider reverse order. Measure B and get eigenvalue b_1.

$$|\psi\rangle \xrightarrow{B} |\psi'\rangle = \text{const}\left(\lambda_1 |a_1 b_1\rangle + \lambda_2 |a_2 b_1\rangle\right)$$

Probability is $|\lambda_1|^2 + |\lambda_2|^2$, normalization constant is

$$\text{const} = \left(|\lambda_1|^2 + |\lambda_2|^2\right)^{-1/2}$$

Now measure A and get a_1. Probability is $\dfrac{|\lambda_1|^2}{|\lambda_1|^2 + |\lambda_2|^2}$. $|\psi'\rangle \xrightarrow{A} |\psi''\rangle = |a_1 b_1\rangle$

multiplying probabilities

$$P(A,B) = \frac{|\lambda_1|^2}{|\lambda_1|^2 + |\lambda_2|^2} \times \left(|\lambda_1|^2 + |\lambda_2|^2\right) = |\lambda_1|^2$$

So $P(A,B) = P(B,A)$

We see crucial role of maintaining a normalized state.

Generally we can find a complete set of simultaneously commuting operators, "CSCO".

Set of observables $\{\Omega_i\}$, $i=1,N$ with

$[\Omega_i, \Omega_j]=0$ and eigenstate $|\omega_1, \ldots \omega_N\rangle$

$\Omega_1 |\omega_1, \omega_2 \ldots \omega_n\rangle = \omega_1 |\omega_1, \omega_2 \ldots \omega_n\rangle$, etc form a basis. measuring all Ω_i is all we can know about system.

Example: Hydrogen atom without spin.

Complete set is $\{H, \hat{L}^2, L_z\}$

$\hat{H}\, |n, l, m\rangle = E_n |n, l, m\rangle$

$E_n = -\frac{1}{n^2} \frac{\alpha^2 \mu c^2}{2}$ μ reduced mass ≈ m_e

$\alpha = \frac{e^2}{\hbar c} = \frac{1}{137.035\ldots}$ dimensionless fine structure constant

$\hat{L}^2 |n l m\rangle = \hbar^2 l(l+1) |n l m\rangle$ $l = 0, \ldots, n-1$

$\hat{L}_z |n l m\rangle = \hbar m |n l m\rangle$ $-l \le m \le l$

Energy degeneracy n^2.

Time dependence of expectation values

$$\langle A \rangle = \langle \psi(t) | A | \psi(t) \rangle$$

$$\frac{\partial}{\partial t} |\psi(t)\rangle = \frac{1}{i\hbar} H |\psi(t)\rangle$$

then total time derivative,

$$\frac{d}{dt}\langle A \rangle = \left(\frac{\partial}{\partial t}\langle \psi(t)|\right) A |\psi(t)\rangle$$

$$+ \langle \psi(t) | A \frac{\partial}{\partial t} | \psi(t) \rangle + \left\langle \frac{\partial A}{\partial t} \right\rangle$$

$$= \frac{i}{\hbar} \langle \psi(t) | HA - AH | \psi(t) \rangle + \left\langle \frac{\partial A}{\partial t} \right\rangle$$

$$= \frac{i}{\hbar} \langle [H, A] \rangle + \left\langle \frac{\partial A}{\partial t} \right\rangle$$

Time dependence in state is referred to as "Schrodinger picture". We could equally well put time dependence in operator, "Heisenberg picture".

$$A_H(t) = U^+ A U$$

$$\frac{\partial}{\partial t} U(t,0) = \frac{1}{i\hbar} H U(t,0)$$ and get operator equation

$$\frac{d}{dt} A_H(t) = \left(\frac{\partial}{\partial t} U^+\right) A U + U^+ A \frac{\partial U}{\partial t}$$ assume A time independent

$$= \frac{i}{\hbar}\left(U^+ H \underset{\uparrow UU^+}{} A U - U^+ A \underset{\uparrow UU^+}{} H U\right)$$

with $U^+ H U = H$ and $U^+ A U = A_H(t)$ get

$$\frac{dA^H}{dt} = \frac{i}{\hbar}[H, A^H]$$

with state $|\psi(0)\rangle$ time independent