Phys 521

Lectures 12-14

Postulates of quantum mechanics

Statement of postulates

1. Quantum state at $t_0 \longleftrightarrow$ normalized ket $|\psi(t_0)\rangle$

2. Measurable physical quantity $\mathcal{A} \longleftrightarrow$ observable (Hermitian operator) $\hat{A}$

Measurement: $\hat{A} = \sum_n a_n |a_n\rangle\langle a_n|$ is discrete nondegenerate for present

3. The result of a measurement of $\mathcal{A}$ is one of the eigenvalues of $\hat{A}$.

4. $\mathcal{P}(a_n) = |\langle a_n|\psi\rangle|^2$ (Born hypothesis)

5. Projection postulate: $|\psi\rangle \xrightarrow[a_n]{\text{measure}} |a_n\rangle$
(reduction of wave packet / collapse of wave function)

Time evolution:

6. $$i\hbar \frac{d|\psi(t)\rangle}{dt} = \hat{H}(t)|\psi(t)\rangle$$
$\hat{H}$ — Hamiltonian

Particle moving in 3 dimensions

States: $|\psi\rangle \leftrightarrow \langle\vec{r}|\psi\rangle$ square integrable

Observables: $\vec{r}$ $\quad \hat{\vec{r}} \quad \vec{R}$

Position $x, y, z \longleftrightarrow$ Observable $\hat{x}, \hat{y}, \hat{z}$ or X, Y, Z

Momentum $p_x, p_y, p_z \longleftrightarrow$ Observable $\hat{p}_x, \hat{p}_y, \hat{p}_z$ or P_x, P_y, P_z

$\vec{p} \quad \hat{\vec{p}} \quad \vec{P}$

$$[\hat{x}_i, \hat{p}_j] = [X_i, P_j] = i\hbar\,\delta_{ij}$$

Other observables:

$$a(\vec{r},\vec{p},t) \longrightarrow \hat{A} \equiv a(\hat{\vec{r}},\hat{\vec{p}},t)$$

Hamiltonian $\quad \mathcal{H}(\vec{r},\vec{p},t) = \frac{\vec{p}^{\,2}}{2m} + V(\vec{r})$

$$\longrightarrow \hat{H} = \mathcal{H}(\hat{\vec{r}},\hat{\vec{p}},t) = \frac{\hat{\vec{p}}^{\,2}}{2m} + V(\hat{\vec{r}})$$

HO in 1-d or in 3-d

Angular momentum: $\vec{\mathcal{L}} = \vec{r}\times\vec{p} \longrightarrow \hat{\vec{L}} = \hat{\vec{r}}\times\hat{\vec{p}}$

Note no ordering problems: Contrast $\vec{r}\cdot\vec{p}$

Measurement:

4. (a) Discrete nd: Use $|\varphi_n\rangle$ rep of 1-d HO — Eigenvalue problem, Born hypothesis

(b) Discrete d: Use energy eigenstates of 3-d HO, $|\varphi_{n_1 n_2 n_3}\rangle$, eigenvalue problem, Born hypothesis

$$\hat{A} = \sum_n a_n |a_n\rangle\langle a_n| = \sum_a a\hat{P}_a$$

$$\mathcal{P}(a) = \sum_{\{n|a_n=a\}} |\langle a_n|\psi\rangle|^2 = \langle\psi|\hat{P}_a|\psi\rangle$$

(c) Continuous nd: Use $\vec{r}$ and $\vec{p}$ as examples

$$\mathcal{P}(\vec{r})\, d^3r = |\langle\vec{r}|\psi\rangle|^2 d^3r$$

Eigenvalue problem
Born hypothesis
Integration over finite domain

Quantum statistics

$$\hat{A} = \sum_n a_n |u_n\rangle\langle u_n| = \sum_a a \hat{P}_a$$

Expectation value: $\langle \hat{A} \rangle = \sum_n a_n |\langle a_n|\psi\rangle|^2$

$$= \sum_n a \langle \psi | \hat{P}_a | \psi \rangle$$

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

Moments: $\langle \hat{A}^2 \rangle$

$\langle \hat{A}^k \rangle$

Functions: $\langle f(\hat{A}) \rangle = \langle \psi | f(\hat{A}) | \psi \rangle$

Uncertainties: $\overset{\text{Variance}}{(\Delta A)^2} \equiv \langle (\Delta \hat{A})^2 \rangle^{1/2} = \langle (\hat{A} - \langle \hat{A} \rangle)^2 \rangle^{1/2} = \langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2$

Uncertainty

ΔA

Schwarz inequality

Proof of up

Application to $\hat{x}$ and $\hat{p}$

5. Projection postulate

(a) Discrete nd: 1-d HO

(b) Discrete d:

$$|\psi\rangle \xrightarrow[a]{} \frac{\hat{P}_a |\psi\rangle}{\langle \psi | \hat{P}_a | \psi \rangle}$$ (Why?)

(c) Continuous spectra

6. Time evolution

SP: State $|\psi(t)\rangle$, Observable $\hat{A}(t) = a(\hat{\vec{r}}, \hat{\vec{p}}, t)$

$\uparrow$ explicit time dependence

Schrödinger equation: $i\hbar \dfrac{d|\psi(t)\rangle}{dt} = \hat{H}|\psi(t)\rangle$

(1) Position rep: if $\hat{H} = \dfrac{\hat{\vec{p}}^2}{2m} + V(\hat{\vec{r}})$, then

$$i\hbar \frac{\partial \langle \vec{r}|\psi(t)\rangle}{\partial t} = \langle \vec{r}|\hat{H}|\psi(t)\rangle = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right)\langle \vec{r}|\psi(t)\rangle$$

(2) Formal solution: $|\psi(t)\rangle = \underbrace{\exp\left(-\frac{i}{\hbar}\hat{H}t\right)}|\psi(0)\rangle$

(a) $i\hbar \dfrac{d\hat{U}(t,0)}{dt} = \hat{H}\hat{U}(t,0)$

$\equiv \hat{U}(t,0) = \left(\dfrac{\text{unitary evolution}}{\text{operator}}\right)$

(b) $\hat{U}(0,0) = \hat{1}$

Preserves normalization

(3) Energy basis: $\hat{H}|\varphi_n\rangle = E_n|\varphi_n\rangle$

$$\hat{U}(t,0)|\varphi_n\rangle = e^{-\frac{i}{\hbar}E_n t}|\varphi_n\rangle$$

(4) Observable $\hat{A}(t)$: $i\hbar \dfrac{d\langle\hat{A}\rangle_t}{dt} = \langle[\hat{A},\hat{H}]\rangle$ ... $\left(\begin{matrix}\text{explicit}\\ t\text{-d}\end{matrix}\right)$

Ehrenfest's theorem: classical motion

HP: $\langle\hat{A}\rangle_t = \langle\psi_S(t)|\hat{A}_S|\psi_S(t)\rangle = \langle\psi_S(0)|\underbrace{\hat{U}^\dagger(t,0)\hat{A}_S\hat{U}(t,0)}_{\hat{A}_H(t)}|\underbrace{\psi_S(0)\rangle}_{|\psi_H(t)\rangle}$

$$|\psi_H(t)\rangle = |\psi_S(0)\rangle = \hat{U}^\dagger(t,0)|\psi_S(t)\rangle$$

$$\hat{A}_H(t) = \hat{U}^\dagger(t,0)\,\hat{A}_S\,\hat{U}(t,0)$$

formal solution

Heisenberg equation: $i\hbar \dfrac{d\hat{A}_H(t)}{dt} = [\hat{A}_H, \hat{H}_H]$

Notice that $\hat{H}_H(t) = \hat{H}_S = \hat{H}_H(0)$

$$\langle \hat{A} \rangle_t = \langle \psi_H(t) | \hat{A}_H(t) | \psi_H(t) \rangle$$

Density operator

Suppose we know that a quantum system has probability p_j to be in the normalized state $|\chi_j\rangle$. The states need not be complete or orthogonal. Let $\hat{A} = \hat{A}^\dagger = \sum_{n\ell} a_n |\phi_{n\ell}\rangle\langle\phi_{n\ell}|$ be any observable. Then

a_n: eigenvalues; $|\phi_{n\ell}\rangle$: eigenstates

$$P(a_n) = \sum_j P(a_n|j)\, p_j$$

$$P(a_n|j) = \sum_\ell |\langle\phi_{n\ell}|\chi_j\rangle|^2 =$$

$$= \langle\chi_j| \underbrace{\left(\sum_\ell |\phi_{n\ell}\rangle\langle\phi_{n\ell}|\right)}_{\hat{P}_{a_n}} |\chi_j\rangle$$

$$= \langle\phi_j|\hat{P}_{a_n}|\phi_j\rangle$$

$\mathrm{tr}(\hat{O}) = \sum_m \underbrace{\langle\eta_m|\hat{O}|\eta_m\rangle}_{O_{mm}}$

① Basis independence

② $\mathrm{tr}(\hat{N}\hat{O}) = \mathrm{tr}(\hat{O}\hat{N})$

$\Rightarrow \mathrm{tr}(\hat{M}\hat{N}\hat{O}) = \mathrm{tr}(\hat{O}\hat{M}\hat{N})$ cyclic property

$$\Longrightarrow \quad P(a_n) = \sum_j p_j \langle\chi_j|\hat{P}_{a_n}|\chi_j\rangle$$

m-rep

$$= \sum_{j,m} p_j \langle\chi_j|\hat{P}_{a_n}|\eta_m\rangle\langle\eta_m|\chi_j\rangle$$

$$= \sum_m \langle\eta_m| \underbrace{\left(\sum_j p_j |\chi_j\rangle\langle\chi_j|\right)}_{\equiv\, \hat{\rho} \,=\, \hat{\rho}^\dagger} \hat{P}_{a_n} |\eta_m\rangle$$

$$= \mathrm{tr}(\hat{\rho}\hat{P}_{a_n})$$

$$\hat{\rho} = \sum_j p_j |\chi_j\rangle\langle\chi_j| = \hat{\rho}^\dagger = \begin{pmatrix}\text{density}\\ \text{operator}\end{pmatrix} \qquad \text{Matrix rep?}$$

Compact description of a quantum state, but nothing new.

Kinematics: $\hat{A} = \sum_{n,k} a_n |\phi_{nk}\rangle\langle\phi_{nk}| = \sum_n a_n \hat{P}_{a_n}$

$$\mathcal{P}(a_n) = \mathrm{tr}(\hat{\rho}\hat{P}_{a_n}) = \mathrm{tr}(\hat{P}_{a_n}\hat{\rho}) = \sum_m \langle\eta_m|\hat{\rho}\hat{P}_{a_n}|\eta_m\rangle$$

$$\underset{\substack{\uparrow\\ \text{nondegenerate}}}{=} \langle\phi_n|\hat{\rho}|\phi_n\rangle$$

$$\langle\hat{A}\rangle = \sum_n a_n \mathcal{P}(a_n) = \mathrm{tr}(\hat{A}\hat{\rho}) \leftarrow \text{replaces } \langle\psi|\hat{A}|\psi\rangle$$

Properties:

1. $\hat{\rho} = \hat{\rho}^\dagger$
2. $\langle\psi|\hat{\rho}|\psi\rangle \geq 0, \ \forall\, |\psi\rangle$
3. $\mathrm{tr}(\hat{\rho}) = \sum_j p_j = 1$

Spectral decomposition:

$$\hat{\rho} = \sum_k \lambda_k \underset{\substack{\uparrow\\ \text{orthonormal}}}{|\psi_k\rangle}\langle\psi_k|$$

$0 \leq \lambda_k \leq 1$

$\sum_k \lambda_k = 1$

4. $\mathrm{tr}(\hat{\rho}^2) = \sum_k \lambda_k^2 \leq \mathrm{tr}(\hat{\rho}) = 1$

Equality $\Longleftrightarrow$ $\hat{\rho} = |\psi\rangle\langle\psi|$ for some $|\psi\rangle$

Pure state vs. mixed state

Density matrix?

Dynamics: von Neuman equation

$$i\hbar \frac{d\hat{\rho}}{dt} = [\hat{H}, \hat{\rho}] \qquad (SP)$$

Solution: $\hat{\rho}(t) = \hat{U}(t,0)\,\hat{\rho}(0)\,\hat{U}^{\dagger}(t,0)$

HP: $\hat{\rho}_H(t) = \hat{\rho}_H(0)$

Thermal density operator:

Probability $P(E_r) = \frac{1}{Z} e^{-E_r/kT}$ to have energy E_r,

where $Z = \sum_r e^{-E_r/kT} = \begin{pmatrix}\text{partition}\\ \text{function}\end{pmatrix}$.

$$\hat{\rho} = \sum_r P(E_r)\,|E_r\rangle\langle E_r| = \frac{1}{Z} e^{-\hat{H}/kT}$$

$$Z = \mathrm{tr}\left(e^{-\hat{H}/kT}\right)$$

$$\langle \hat{H} \rangle = -\frac{1}{Z}\frac{\partial Z}{\partial \beta}, \quad \beta = 1/kT$$

Ex: SHO

$$P_n = \frac{1}{Z} e^{-\hbar\omega n/kT} = \frac{1}{1+\langle \hat{n}\rangle}\left(\frac{\langle \hat{n}\rangle}{1+\langle \hat{n}\rangle}\right)^n$$

$$Z = \frac{1}{1-e^{-\hbar\omega/kT}} = 1 + \langle \hat{n} \rangle$$

$$\langle \hat{n} \rangle = \frac{1}{e^{\hbar\omega/kT} - 1}$$

$$\langle \hat{n}^2 \rangle = 2\langle \hat{n}\rangle^2 + \langle \hat{n} \rangle$$

$$\langle (\Delta \hat{n})^2 \rangle = \langle \hat{n}\rangle^2 + \langle \hat{n} \rangle$$