Modern Quantum Mechanics

Bo Zhao (赵博)
(Dated: June 28, 2024)

Blue: important for me.

FUNDAMENTAL POSTULATES OF QUANTUM MECHANICS

Background: Non-relativistic QM & closed system (not open system, Hamiltonian is Hermitian and it's eigenvalue is real (For $\mathcal{PT}$ symetric systems, Hamiltonian also can be real)).

Fundamental Postulates: **SOME IS**

P1 **State postulate**:

$$|\psi\rangle = (\langle\psi|)^\dagger, (|\psi\rangle \in \mathcal{H}). \tag{1}$$

P2 **Operator (Observable) postulate**: For observables, the operator is linear and Hermitian.

P3 **Measurement postulate**:

$$a.\ \hat{A}|\psi_n\rangle = A_n|\psi_n\rangle. \tag{2}$$

$$b.\ P(A_n) = |\langle\psi_n|\psi\rangle|^2. \tag{3}$$

$$c.\ |\psi\rangle \to |\psi_n\rangle\ (after\ measurement) \tag{4}$$

P4 **Evolution postulate**:

a. Schrödinger Picture:

$$i\hbar\frac{\mathrm{d}}{\mathrm{dt}}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle. \tag{5}$$

b. Heisenberge Picture:

$$\frac{\mathrm{d}\hat{F_H}}{\mathrm{dt}} = (\frac{\mathrm{d}\hat{F_S}}{\mathrm{dt}})_H + \frac{1}{i\hbar}[\hat{F_H}, \hat{H}]. \tag{6}$$

P5 **Identical particles & Symmetrization**:

a. Boson: S=0, 1, 2, $\cdots$ (Bose-Einstein statistics)

b. Fermion: S=$\frac{1}{2}$, $\frac{3}{2}$, $\frac{5}{2}$, $\cdots$ (Fermi-Dirac statistics)

HILBERT'S SPACE $\mathcal{H}$

Compared with Euclidean space $\mathcal{R}$, dimension of $\mathcal{H}$ is not limited.

Rules of $\mathcal{H}$

a. Linear space (vector space)

b. Inner product space

Rules of vector in $\mathcal{H}$ (not all):

a. $\forall|\psi\rangle \in \mathcal{H}$, $\exists(-|\psi\rangle)$, make $(-|\psi\rangle) + |\psi\rangle = 0$.

Adjoint (not all):

a. $(\hat{A}_1\hat{A}_2\cdots\hat{A}_n)^{-1} = \hat{A}_n^{-1}\cdots\hat{A}_2^{-1}\hat{A}_1^{-1}$

Three kinds of operators:

a. Hermitian operator

b. Unitary operator: $\hat{U}^\dagger = \hat{U}^{-1}$ & linearity

c. Anti-unitary operator: $\hat{U}^\dagger = \hat{U}^{-1}$ & anti-linearity

Linearity: $\langle\psi_1|(a|\psi_2\rangle + b|\psi_3\rangle) = a\langle\psi_1|\psi_2\rangle + b\langle\psi_1|\psi_3\rangle$

Anti-linearity: $(\langle\psi_2|a + \langle\psi_3|b)|\psi_1\rangle = a^*\langle\psi_2|\psi_1\rangle + b^*\langle\psi_3|\psi_1\rangle$

Duality/Trinity/Quaternity:

a. Hermitian

b. Unitary - Symmetry transformation

c. Involuntary: $\hat{A}^2 = \mathbb{I}$

d. Idempotent: $\hat{A}^2 = \hat{A}$

OPERATOR

Eigenvalue:

Hermitian operator: real

Unitary operator: $e^{i\theta}$ (from defination, easy to derive)

Hermitian & Unitary: ± 1

Wavefunction:

Orthonormal: $\langle\psi_n|\psi_m\rangle = \delta_{nm}$

Completeness: $\sum_n |\psi_n\rangle\langle\psi_n| = \mathbb{I}_n$

For continous basis, they are similar.

For degenerate case:

Orthonormal: $\langle\psi_n^i|\psi_m^{i'}\rangle = \delta_{nm}\delta_{ii'}$

Completeness: $\sum_n\sum_i |\psi_n^i\rangle\langle\psi_n^i| = \mathbb{I}_n$

Eigenspectrum - Set of eigenvalues.

Subspace:

$\mathcal{H}_n = |\psi_n^i\rangle, (i = 1, 2, \cdots, g_n)$, g_n denotes degeneracy. This subspace is consist of the wave functions of a degenerate eigenvalue.

Obviously, $\mathcal{H} = \biguplus_n \mathcal{H}_n = diag(\mathcal{H}_1, \mathcal{H}_2\cdots, \mathcal{H}_n)$.

About dimension, dim($\mathcal{H}_n$)=g_n, dim($\mathcal{H}$)=dim($\biguplus_n \mathcal{H}_n$) =$\sum_n g_n$. $\mathcal{H}_n \perp \mathcal{H}_m$.

Direct sum $\bigoplus$: for the same observable operator.

Tensor product $\bigotimes$: for different freedom (particle/observable).

Equivalence$\sim$: $|\psi\rangle \sim c|\psi\rangle \sim e^{i\theta}|\psi\rangle$ mean they denote same state.

Gram-Schmidt Orthogonalization: degenerate states are linearly independent but may not be orthogonal. Therefore, we use this method to make them orthogonal.

For $|\psi_n^i\rangle$

a. normalized $|\psi_n^1\rangle$: $|\psi_n^1\rangle \to |\varphi_n^1\rangle = \frac{|\psi_n^1\rangle}{\sqrt{\langle\psi_n^1|\psi_n^1\rangle}}$.

b. got orthogonal $|\chi_n^2\rangle$: $|\chi_n^2\rangle = |\psi_n^2\rangle - \langle\psi_n^1|\psi_n^2\rangle|\psi_n^1\rangle$ (the second term denotes the projection of $|\psi_n^2\rangle$ onto the direction of $|\varphi_n^1\rangle$).

c. normalized $|\chi_n^2\rangle$: $|\chi_n^2\rangle \to |\varphi_n^2\rangle = \frac{|\chi_n^2\rangle}{\sqrt{\langle\chi_n^2|\chi_n^2\rangle}}$.

$\cdots$

"Ray" space: the space consists of same state with different coefficient (same direction in $\mathcal{H}$).

TENSOR PRODUCTION

Origin: multi-freedom

a. multi particle

b. single particle, multi observables

c. single particle, single observable, multi components

Defination: $|\psi\rangle_1 \in \mathcal{H}_1$, $|\varphi\rangle_2 \in \mathcal{H}_2 \Longrightarrow \mathcal{H} = \mathcal{H}_1 \bigotimes \mathcal{H}_2$, $|\chi\rangle = |\psi\rangle_1 \bigotimes |\varphi\rangle_2$.

Properties of tensor product:

a. commutivity:

$$|\psi\rangle_1 \bigotimes |\varphi\rangle_2 = |\varphi\rangle_2 \bigotimes |\psi\rangle_1. \tag{7}$$

b. linearity:

$$a(|\psi\rangle_1 \bigotimes |\varphi\rangle_2) = (a|\psi\rangle_1) \bigotimes |\varphi\rangle_2 = |\psi\rangle_1 \bigotimes (a|\varphi\rangle_2). \tag{8}$$

c. distributivity:

$$(a|\psi_1\rangle_1 + b|\psi_2\rangle_1) \bigotimes |\varphi\rangle_2 = a|\psi_1\rangle_1 \bigotimes |\varphi\rangle_2 + b|\psi_2\rangle_1 \bigotimes |\varphi\rangle_2. \tag{9}$$

d. dimension:

$$dim(\mathcal{H}_1 \bigotimes \mathcal{H}_2) = dim(\mathcal{H}_1) \cdot dim(\mathcal{H}_2) \tag{10}$$

e. value:

$$A_{mn} \otimes B_{pq} = \begin{pmatrix} a(1,1)B & a(1,2)B & \cdots & a(1,n)B \\ a(2,1)B & a(2,2)B & \cdots & a(2,n)B \\ \vdots & \vdots & \ddots & \vdots \\ a(m,1)B & a(m,2)B & \cdots & a(m,n)B \end{pmatrix} \tag{11}$$

f. **entangled state**:

Considering two state $|\psi\rangle_1 = \sum_i c_i |u_i\rangle_1 \in \mathcal{H}_1 = \{|u_1\rangle_1, |u_2\rangle_1\}$, $|\varphi\rangle_2 = \sum_j d_j |v_j\rangle_2 \in \mathcal{H}_2 = \{|v_1\rangle_2, |v_2\rangle_2\}$, we have

$$\begin{aligned} |\psi\rangle_1 \bigotimes |\varphi\rangle_2 =& c_1 d_1 |u_1\rangle_1 \bigotimes |v_1\rangle_2 + c_1 d_2 |u_1\rangle_1 \bigotimes |v_2\rangle_2 \\ &+ c_2 d_1 |u_2\rangle_1 \bigotimes |v_1\rangle_2 + c_2 d_2 |u_2\rangle_1 \bigotimes |v_2\rangle_2, \end{aligned} \tag{12}$$

we can find that state $\chi = \frac{1}{\sqrt{2}}(|u_1\rangle_1 \otimes |v_1\rangle_2 + |u_2\rangle_1 \otimes |v_2\rangle_2)$ is not a **tensor product state**, because if we make $c_1 d_2 = c_2 d_1 = 0$, observably, $c_1 d_1$ and $c_2 d_2$ cannot be zero at the same time. And the state χ is called an entangled state.

Kinds of entangled state:

N=2 (number of particle/mode), only Bell-state (Bell basic, EPR state ,Schrödinger cat state)

$$: \frac{1}{\sqrt{2}}(|u_1\rangle_1 \bigotimes |v_1\rangle_2 + |u_2\rangle_1 \bigotimes |v_2\rangle_2). \tag{13}$$

N>2,

① Werner state(W-state): robust

② GHZ state: fragile

③ NOON state

g. inner product of tensor product:

$$({}_1\langle\psi_2| \bigotimes {}_2\langle\varphi_2|)(|\psi_1\rangle_1 \bigotimes |\varphi_1\rangle_2) = ({}_1\langle\psi_2|\psi_1\rangle_1) \cdot ({}_2\langle\varphi_2|\varphi_1\rangle_2), \tag{14}$$

for basis vector:

$$\begin{aligned} ({}_1\langle u_i| \bigotimes {}_2\langle v_j|)(|u_k\rangle_1 \bigotimes |v_l\rangle_2) &= ({}_1\langle u_i|u_k\rangle_1) \cdot ({}_2\langle v_j|v_l\rangle_2) \\ &= \delta_{ik}\delta_{jl}, \end{aligned} \tag{15}$$

for operator:

$$\begin{aligned} \hat{A}_1(|\psi\rangle_1 \bigotimes |\varphi\rangle_2) &= (\hat{A}_1 \bigotimes \mathbb{I}_2)(|\psi\rangle_1 \bigotimes |\varphi\rangle_2) \\ &= \hat{A}_1|\psi\rangle_1 \bigotimes |\varphi\rangle_2. \end{aligned} \tag{16}$$

COMPATIBILE OBSERVATION

Concepts

a. compatibile observation (commuting observation): $[\hat{A}, \hat{B}] = 0$, $\hat{A}$, $\hat{B}$ are compatibile observation.

b. common eigenvalues (simultaneous eigenvalues) CE

c. set of common eigenstates (set of simultaneous eigenstates) SCE

d. complete set of commuting observable CSCO

e. good quantum number (quantum number of conserved observable)

Theorem of compatibile observation

$$[\hat{A}, \hat{B}] = 0 \Leftrightarrow \textit{orthonormal}\ \text{SCE}. \tag{17}$$

REPRESENTATION & REPRESENTATION TRANSFORMATION

Representation⇔Basis, projection in a certain representation.

$\psi(\vec{x}) = \langle\vec{x}|\psi\rangle$ - wavefunction in $\vec{x}$-representation.

Obviously, $\varphi_p = \int \mathrm{d}^3\vec{x}\ \psi(\vec{x})\psi_p^*(\vec{x})$, where $\psi_p(\vec{x}) = \langle\vec{x}|\vec{p}\rangle = Ne^{i\vec{p}\vec{x}/\hbar}$ (proof in future). Here, $N = (\frac{1}{2\pi\hbar})^{\frac{3}{2}}$ denotes normalization factor. $\psi_x(\vec{p}) = \langle\vec{p}|\vec{x}\rangle = Ne^{-i\vec{x}\vec{p}/\hbar}$.

Representation transformation of wavefunction:

$$\begin{aligned}|\psi\rangle &= \int \mathrm{d}^3\vec{x}\ |\vec{x}\rangle\psi(\vec{x}) \\ &= \sum_n |n\rangle C_n \\ &= \sum_n (\int \mathrm{d}^3\vec{x}\ |\vec{x}\rangle\langle\vec{x}|n\rangle C_n) \\ &= \int \mathrm{d}^3\vec{x}\ |\vec{x}\rangle \sum_n u_n(\vec{x})C_n \\ \Rightarrow \psi(\vec{x}) &= \sum_n C_n u_n(\vec{x}). \end{aligned} \tag{18}$$

Here, $\psi_{\vec{x}}$ and C_n are wavefunctions in the $\vec{x}$-representation and n-representation, respectively. $u_n(\vec{x}) = \langle\vec{x}|n\rangle$ is **trnasformation** function. In the last formula, we transform the wavefunction from the Hilbert space $\mathcal{H}_n$ to another Hilbert space $\mathcal{H}_x$ (my personal understanding).

Remark: t (time) is not an observable! It is a parameter! (At least in non-relativistic quantum mechanics, this statement is certain correct.)

Therefore, $\psi(x,t) = \langle\vec{x}|\psi(t)\rangle$. So $\underbrace{i\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi(x,t)\rangle = [\frac{\hat{\vec{p}}^2}{2m} + V(\vec{x})]|\psi(x,t)\rangle}_{\text{wrong}}$ is wrong, the correct form is $\underbrace{i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\langle\vec{x}|\psi(t)\rangle = [\frac{\hat{\vec{p}}^2}{2m} + V(\vec{x})]\langle\vec{x}|\psi(t)\rangle}_{\text{correct}}$

MATRIX MECHANICS

Some interesting proof:

a. wavefunction is column vector:

$$|\psi\rangle = \mathbb{I}|\psi\rangle = (\sum_n |u_n\rangle\langle u_n|)|\psi\rangle = \sum_n C_n|u_n\rangle. \tag{19}$$

b. observable is matrix:

$$\begin{aligned}\hat{A} &= \mathbb{I}\hat{A}\mathbb{I} \\ &= \left(\sum_n |u_n\rangle\langle u_n|\right)\hat{A}\left(\sum_m |u_m\rangle\langle u_m|\right) \\ &= \sum_{n,m} A_{n,m}|u_n\rangle\langle u_m|, \end{aligned} \tag{20}$$

where $A_{n,m} = \langle u_n|\hat{A}|u_m\rangle$.

Trace:

$$\begin{aligned}\mathrm{Tr}\hat{A} = \mathrm{Tr}(\mathbb{I}\hat{A}\mathbb{I}) &= \sum_{n,m} A_{n,m}\underbrace{\mathrm{Tr}(|u_n\rangle\langle u_m|)}_{\delta_{nm}}, \\ &= \sum_n A_{nn} \\ &= \int \mathrm{d}n\ A(n,n)\ (for\ continuous\ spectrum) \end{aligned} \tag{21}$$

Here, we considering that $|u_n\rangle$ can be chose as **standard basis vector**.

Properties of the Trace:

a. $\mathrm{Tr}(|\psi\rangle\langle\varphi|) = \mathrm{Tr}(\langle\varphi|\psi\rangle)$

b. $\mathrm{Tr}(\hat{A}\hat{B}) = \mathrm{Tr}(\hat{B}\hat{A})$

c. $\mathrm{Tr}(\hat{A}_1\hat{A}_2\cdots\hat{A}_n) = \mathrm{Tr}(A_{\sigma(1)}A_{\sigma(2)}\cdots A_{\sigma(n)})$, $\sigma : \{1,2,\cdots,n\} \to \{1,2,\cdots,n\}$)

Representation transformation of wavefunction (another view) and observable:

we have two basis: $|\psi\rangle = \sum_n C_n|u_n\rangle$, $|\psi\rangle = \sum_m D_m|v_m\rangle$, where $C_n = \langle u_n|\psi\rangle$, $D_m = \langle v_m|\psi\rangle$ are wavefunctions.

$$\begin{aligned}D_m &= \langle v_m|\sum_n C_n|u_n\rangle \\ &= \sum_n \langle v_m|u_n\rangle C_n \\ &= \sum_n S_{mn}C_n \\ \Rightarrow D &= SC. \end{aligned} \tag{22}$$

Here, S_{mn} is **overlap matrix** that can transform wavefunction C_n to D_m. $S_{nm} = S^*_{mn} = (S^\top)^*_{mn} = (S^\dagger)_{nm}$, therefore, $S = S^\dagger$. Moreover, $D = SC = SS^\dagger D \Rightarrow SS^\dagger = \mathbb{I}$, S is a trinity matrix.

Similarly, for observable, we have: $\hat{A} = \sum_{n,n'} A_{nn'}|u_n\rangle\langle u_{n'}|$, $\hat{A} = \sum_{m,m'} A_{mm'}|v_m\rangle\langle v_{m'}|$, where $A_{nn'} = \langle u_n|\hat{A}|u_{n'}\rangle$, $A_{mm'} = \langle v_m|\hat{A}|v_{m'}\rangle$.

$$\begin{aligned}A_{mm'} &= \langle v_m|\sum_{n,n'} A_{nn'}|u_n\rangle\langle u_{n'}|v_{m'}\rangle \\ &= \sum_{n,n'}\langle v_m|u_n\rangle A_{nn'}\langle u_{n'}|v_{m'}\rangle \\ &= \sum_{n,n'} S_{mn}A_{nn'}S_{n'm'} \\ \Rightarrow A^{'} &= SAS^\dagger = SAS^{-1}. \end{aligned} \tag{23}$$

Projection operator (projector):

$\hat{P}_\psi = |\psi\rangle\langle\psi|$

Properties:

a. $\hat{P}^2_\psi = \hat{P}_\psi$ (assume $|\psi\rangle$ has normalized)

b. $\hat{P}^\dagger_\psi = \hat{P}_\psi$

Eigenvalue: $\hat{P}_\psi|\psi\rangle = 0\ or 1|\psi\rangle$. The corresponding eigenstates are $|\lambda_\perp\rangle$ (perpendicular state) and $|\lambda_\|\rangle$ (parallel state), respectively.

For degenerate case, $\hat{A}|u^i_n\rangle = A_n|u^i_m\rangle$, projector of subspace n is $\hat{P}_n = \sum_{i=1}^{g_n}|u^i_n\rangle\langle u^i_n|$ (discrete)) $\hat{P}_{\Delta a} = \int_a^{a+\Delta a}\mathrm{d}a\ \sum_{r=1}^{g(r)}|ar\rangle\langle ar| = \int_a^{a+\Delta a}\mathrm{d}a\ \hat{P}(a)$ (continuous).

MEASUREMENT POSTULATE IN THE CASE OF DEGENERACY

For non-degenerate and state has normalized cases:

a. measurement outcome: $\hat{A}|\psi_n\rangle = A + n|\psi_n\rangle$

b. probability: $p(n) = |C_n|^2$ (discrete) $p(a \sim \Delta a) = |C(a)|^2 \Delta a$ (continuous)

c. collapse: after measurement, at that time, the state become a certain state (outcome state).

Conditions: the state may be not normalized and is degenerate.

Revised b. probability:

$$p(A_n) = norm(\sum_{i=1}^{g_n} |C_n^i|^2) = norm(\sum_{i=1}^{g_n} \langle\psi|u_n^i\rangle\langle u_n^i|\psi\rangle)$$
$$= \frac{\langle\psi|\hat{P}_n|\psi\rangle}{\langle\psi|\psi\rangle}. \quad (24)$$

Revised c. collapse:

$$|\psi\rangle \to \frac{|\psi_n\rangle}{\sqrt{\langle\psi_n|\psi_n\rangle}} = \frac{\hat{P}_n|\psi\rangle}{\sqrt{\langle|\hat{P}_n|\psi\rangle}}. \quad (25)$$

Here, $\hat{A}_n\hat{P}_n|\psi\rangle = \sum_{i=1}^{g_n} \hat{A}_n|u_n^i\rangle\langle u_n^i|\psi\rangle = A_n\hat{P}_n|\psi\rangle$, therefore, $\hat{P}_n|\psi\rangle$ is a set of eigenfunctions of $\hat{A}_n$.

For conrinuous cases $\sum \to \int$, $\hat{P}_n \to \hat{P}_{\Delta a}$.

Exception: easy to proof, $\langle\hat{A}\rangle = \frac{\langle\psi|\hat{A}|\psi\rangle}{\langle\psi|\psi\rangle}$.

Variance: $\hat{\sigma}_A = \langle\hat{A}^2\rangle - \langle\hat{A}\rangle^2$.

PAULI MATRIX

Pauli matrix:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (26)$$

Every matrix can be describe by using a Hermitian and a skew-Hermitian (anti-Hermitian) matrix.

$$\hat{A} = \frac{1}{2}(\hat{A} + \hat{A}^\dagger) + \frac{1}{2}(\hat{A} - \hat{A}^\dagger). \quad (27)$$

Here, the first term is Hermitian, the second term is anti-Hermitian.

SPECIAL UNITARY MATRIX (SU(2))

a. unitary $\hat{M}^\dagger = \hat{M}$

b. special det $\hat{M} = 1$

$\Rightarrow \hat{M} = x_0\hat{\sigma}_0 + i\vec{x}\hat{\vec{\sigma}}$, $(x_0, \vec{x} \in \mathbb{R})$, which means diagonal elements of this matrix are imagine, off-diagonal elements of this matrix are real.

DENSITY OPERATOR

Origin:

For any state $|\psi\rangle$, about a parameter λ, the exception of an observable is:

$$\overline{\hat{A}} = \int \mathrm{d}\lambda\ f(\lambda)\langle\psi(\lambda)|\hat{A}|\psi(\lambda)\rangle, \quad (28)$$

where $f(\lambda)$ denotes probability. $\int \mathrm{d}\lambda\ f(\lambda) = 1$. We assume:

$$\hat{\rho} = \int \mathrm{d}\lambda\ f(\lambda)|\psi(\lambda)\rangle\langle\psi(\lambda)|,\ \textit{continuous}$$
$$\hat{\rho} = \sum_i f_i|\psi_i\rangle\langle\psi_i|,\ \textit{discrete}$$
$$\overline{\hat{A}} = \mathrm{Tr}(\hat{\rho}\hat{A}). \quad (29)$$

easy to proof, based on the properties of trace.

Properties:

a. Hermitian: $\hat{\rho}^\dagger = \hat{\rho}$

b. closed system: $\mathrm{Tr}(\hat{\rho}) = 1$

c. $\mathrm{Tr}(\hat{\rho^2})$<1, iff pure state, =1 ($\hat{\rho} = |\psi\rangle\langle\psi|$)

d. $\hat{\rho} = \sum_{i,j} \rho_{ij}|i\rangle\langle j|$, $\rho_{ij} = \rho_{ji}^*$

Pure & mixed state:

a. pure state: $\hat{\rho} = |\psi\rangle\langle\psi|$

b. mixed state: $\hat{\rho} = \sum_i f_i|\psi\rangle\langle\psi|$