PART A : IDEAL QUANTUM COMPUTING

I - Basics of Quantum Computing

1 - Postulates of quantum mechanics for isolated systems

Quantum mechanics (QM) is a mathematical framework for the development of physical theories.
The 5 following postulates formulate mathematically how we describe 1) states of a system, 2) observables, 3) measurements, 4) dynamics 5) Composition of several systems.

① States of a (closed) system

- Associated with any physical isolated system is a complex vector space, which is the state space of the system, known as Hilbert space $\mathcal{H}$.

  (note: we will only consider finite-dimensional $\mathcal{H}$)

- The vectors in $\mathcal{H}$ are denoted by kets $|\psi\rangle$.
  (Dirac notation)

- The physical states of the system are represented by rays in $\mathcal{H}$

  A ray $R(\psi) = \{ e^{i\alpha} |\psi\rangle, \alpha \in \mathbb{R} \}$ is a ket up to a global phase.

$\Rightarrow$ $|\psi\rangle$ & $e^{i\alpha}|\psi\rangle$ represent the same physical state.

⇒ Properties of the Hilbert space $\mathcal{H}$:

- linear combination of 2 states is another state :

$$c_1 |\psi_1\rangle + c_2 |\psi_2\rangle = |\psi_3\rangle \quad \forall c_1, c_2 \in \mathbb{C}$$

⚠ the relative phase is meaningful

$$\left(c_1 |\psi_1\rangle + c_2 |\psi_2\rangle \neq c_1 |\psi_1\rangle + e^{i\alpha} c_2 |\psi_2\rangle \right)$$

⇒ superposition : the system described by $|\psi_3\rangle$ is in both state $|\psi_1\rangle$ & $|\psi_2\rangle$ with certain proba amplitude.

- ket $|\psi\rangle \longleftrightarrow$ bra $\langle\psi| = |\psi\rangle^\dagger$

- inner product $\langle\psi_1|\psi_2\rangle \in \mathbb{C}$

→ positivity : $\langle\psi|\psi\rangle > 0 \quad (\in \mathbb{R})$ for $|\psi\rangle \neq 0$

→ linearity : $\langle\psi| \left(c_1|\psi_1\rangle + c_2|\psi_2\rangle \right)$

$$= c_1 \langle\psi|\psi_1\rangle + c_2 \langle\psi|\psi_2\rangle$$

→ Hermiticity : $\langle\varphi|\psi\rangle = \langle\psi|\varphi\rangle^*$

- norm : $\|\psi\| = \sqrt{\langle\psi|\psi\rangle} > 0$ → typically will choose $\|\psi\| = 1$
  (for $|\psi\rangle \neq 0$)

② <u>Observables</u> = properties of a system that (in principle) can be measured

In QM, observables $\mathcal{A}$ are represented by linear Hermitian operators $\hat{A} = \hat{A}^{\dagger}$ acting on the kets
= self-adjoint

$$\mathcal{A}: \quad |\psi\rangle \longmapsto \hat{A}|\psi\rangle$$

$$\mathcal{A}: \quad c_1|\psi_1\rangle + c_2|\psi_2\rangle \longmapsto c_1\hat{A}|\psi_1\rangle + c_2\hat{A}|\psi_2\rangle$$

$$\hat{A} = \hat{A}^{\dagger} \Rightarrow \quad \langle\varphi|\hat{A}|\psi\rangle = \langle\varphi|\hat{A}^{\dagger}|\psi\rangle = \langle\psi|\hat{A}|\varphi\rangle^{*}$$

$\hat{A} = \hat{A}^{\dagger} \Rightarrow$ the eigenstates of $\hat{A}$ form a complete orthonormal basis in $\mathcal{H}$.

- Can express $\hat{A} = \sum_n a_n \hat{P}_n$

where $\boxed{\hat{P}_n = \text{orthogonal projector onto the space of eigenvect. with eigenvalue } a_n.}$

- if no degeneracies (one eigenvec. $|n\rangle$ per eigenvalue a_n: $\hat{A}|n\rangle = a_n|n\rangle$)

$\hat{P}_n = |n\rangle\langle n|$ projects onto one eigenstate

• otherwise $\hat{P}_n = \sum_i |n,i\rangle\langle n,i|$ → extra label to distinguish eigenvec.

where $\hat{A}|n,i\rangle = a_n |n,i\rangle$

project onto subspace assoc. to a_n.

properties: $\begin{cases} \hat{P}_n^{\dagger} = \hat{P}_n & \text{(easy to see)} \\ \hat{P}_n^{2} = \hat{P}_n & \text{(projector)} \end{cases}$

$$\sum_n \hat{P}_n = \hat{\mathbb{1}} \quad \text{(closure / completness relation)}$$

⇒ • Any ket $|\psi\rangle \in \mathcal{H}$ can be expressed as:

$$|\psi\rangle = \left(\sum_n \hat{P}_n\right)|\psi\rangle$$

$$= \sum_n \underbrace{\langle n|\psi\rangle}_{\equiv c_n \in \mathbb{C}} |n\rangle . \quad \text{(if no deg)}$$

(if degen ⇒ $|\psi\rangle = \sum_{n,i} |n,i\rangle \underbrace{\langle n,i|\psi\rangle}_{c_n^{(i)}}$)

③ **Measurement** = Process in which information about the state of a physical system is acquired by an observer.

in QM: When a measurement of an observable $\hat{A}$ is performed, the state of the system becomes an eigenstate of $\hat{A}$ and the observer learns the corresponding eigenvalue a_n.

if system is in arbitrary state $|\psi\rangle$ before the measurement, the probability that a given a_n is measured is

$$p(a_n) = \|\hat{P}_n |\psi\rangle\|^2 = \langle\psi|\hat{P}_n|\psi\rangle$$

=> measurements are orthogonal projections

and the quantum state after measurement is: $\frac{\hat{P}_n |\psi\rangle}{\|\hat{P}_n |\psi\rangle\|}$

→ "Born Rule"

(if no degeneracies: $|\psi\rangle = \sum_n c_n |n\rangle$, $\hat{P}_n = |n\rangle\langle n|$

=> $p(a_n) = |c_n|^2$ and state after meas. is

$\frac{c_n}{|c_n|} |n\rangle$ = phase x $|n\rangle$

Notes :

- Measurements are probabilistic
(there is no definite outcome, instead have a proba distribution of the possible outcomes $\sum_n p(a_n) = 1$)

- if we measure again (immediately after) we will get the same outcome with proba = 1. (project twice)

- if many identical systems are prepared in $|\psi\rangle$ and measured, we obtain the expectation value of $\hat{A}$ = average outcome (from large # of measurements):

$$\sum_n a_n \, p(a_n) = \langle \psi | \hat{A} | \psi \rangle \equiv \langle A \rangle$$

↳ weighted average of the eigenvalues a_n.

④ Dynamics → how a state evolves over time.

In QM : the time evolution of a closed system is governed by the time-dependent Schrödinger equation :

$$\frac{d}{dt}|\psi(t)\rangle = -i\underbrace{\hat{H}(t)}_{\text{Hamiltonian of the system.}}|\psi(t)\rangle$$

$$\hat{H}(t) = \hat{H}^{\dagger}(t)$$

(can be time-dependent - ex: in the lab when applying ext field etc...)

(Note : we use $\hbar = 1$)

⇒ For infinitesimal time step dt :

$$\underbrace{d|\psi(t)\rangle}_{} = -i\hat{H}(t)\,dt\,|\psi(t)\rangle$$

$$|\psi(t+dt)\rangle - \psi(t) = -i\hat{H}(t)\,dt\,|\psi(t)\rangle$$

$$\Rightarrow |\psi(t+dt)\rangle = (\mathbb{1} - i\hat{H}(t)\,dt)\,|\psi(t)\rangle$$

$$\simeq e^{-i\hat{H}(t)\,dt}\,|\psi(t)\rangle$$

(to linear order in dt)

$$= \underbrace{\hat{U}(dt)}_{\hookrightarrow \text{unitary}}\,|\psi(t)\rangle$$

In fact for finite time step $(t'-t)$ we have:

$$\boxed{\begin{aligned} |\psi(t')\rangle &= \hat{U}(t', t)\, |\psi(t)\rangle \\ \text{with } \hat{U}(t', t) &= \text{unitary operator} \end{aligned}}$$

$$\hat{U}(t', t) = \begin{cases} e^{-i(t'-t)\hat{H}} & \text{if } \hat{H} \text{ is time independent} \\ T\left(e^{-i\int_t^{t'} H(t'')\, dt''}\right) & \text{otherwise.} \end{cases}$$

↳ time-ordering operator

$\Rightarrow$ Time evolution proceeds via unitary operators.

<u>Note</u>: . As time goes on the state of the system moves through the Hilbert space

. unitarity is necessary to preserve normalization of the state and probability distributions.

(If we measure observable $\hat{A}$ (eigenbasis $\{|n\rangle\}$) on initial state $|\psi^{(0)}\rangle = \sum_n c_n |n\rangle$, the possible outcomes represent a proba distribution:

$$\sum_n p(a_n) = 1$$
$$\parallel$$
$$\langle\psi|\hat{P}_n|\psi\rangle$$
$$\parallel$$
$$|c_n|^2$$

This must remain true after evolution

$$\Rightarrow \quad |\psi(t)\rangle = \sum_n c_n(t)\, |n\rangle$$

with $\sum_n |c_n(t)|^2 = 1$

(preserving the norm means preserving proba dist°))

- For this reason, any non-measuring action is represented by a unitary operator.

- U unitary $\Rightarrow$ it is invertible ($U^{-1} = U^{\dagger}$)

$\Rightarrow$ non-measuring operations that we will deal with in quantum computing will be reversible ($\neq$ with classical computing)

⑤ Composite systems

If we want to describe a system made of several smaller subsystems – For ex:

$$\begin{cases} \text{Subsystem } A \longrightarrow \text{Hilbert space } \mathcal{H}_A, \text{ orthon. basis } \{|i\rangle_A\} \quad (\to \dim d_A) \\ \text{Subsystem } B \longrightarrow \text{Hilbert space } \mathcal{H}_B, \text{ orthon. basis } \{|\mu\rangle_B\} \quad (\to \dim d_B) \end{cases}$$

$\Rightarrow$ Hilbert space of the composite system AB is $\mathcal{H}_A \otimes \mathcal{H}_B$ with dimension $d_A d_B$

and $\{\underbrace{|i\rangle_A \otimes |\mu\rangle_B}_{\equiv |i,\mu\rangle_{AB}}\}$ is a basis for $\mathcal{H}_A \otimes \mathcal{H}_B$.

- inner product $\quad {}_{AB}\langle i,\mu | j,\nu\rangle_{AB} = \delta_{ij}\, \delta_{\mu\nu}$
- action of operators $\quad \hat{\mathcal{M}}_A \otimes \hat{N}_B\, |i,\mu\rangle_{AB}$
$$= \hat{\mathcal{M}}_A |i\rangle_A \otimes \hat{N}_B |\mu\rangle_B .$$
- State of the global system can be written

$$|\psi\rangle_{AB} = \sum_{i=0}^{d_A-1} \sum_{\mu=0}^{d_B-1} C_{i\mu}\, |i\rangle_A \otimes |\mu\rangle_B$$

This is called a <u>bi-partite</u> state

These 5 axioms provide a complete mathematical formulation of QM.

We note: Unitary evolution is deterministic
while
Measurement is probabilistic

$\rightarrow$ "measurement problem".

Appendix : Vector, Matrices and Tensor products

a) Column representation of vector :

If $\mathcal{H}$ is N-dimensional Hilbert space and $\{|n\rangle\} = |0\rangle, |1\rangle, \ldots |N-1\rangle$ is an orthonormal basis of $\mathcal{H}$ – An arbitrary state $|\psi\rangle \in \mathcal{H}$ can be written as a superposition of these basis states :

$$|\psi\rangle = \sum_n c_n |n\rangle$$

where $c_n = \langle n|\psi\rangle$

Often we write $|\psi\rangle$ as a column-vector of its amplitudes :

$$|\psi\rangle = \begin{pmatrix} c_0 \\ c_1 \\ \vdots \\ c_{N-1} \end{pmatrix} \in \mathbb{C}^N$$

The bra is a line vector :

$$\langle\psi| = (c_0^* \quad c_1^* \quad \ldots\ldots \quad c_{N-1}^*)$$

b) Matrix representation of an operator

Consider linear operator $\hat{O}$

$$\hat{O} = \sum_{nm} |n\rangle \underbrace{\langle n|\hat{O}|m\rangle}_{} \langle m| \qquad \text{(using closure relations)}$$

matrix elements forming the matrix O of $\hat{O}$ in the basis $\{|n\rangle\}$.

$$O = \begin{pmatrix} \langle 0|\hat{O}|0\rangle & \langle 0|\hat{O}|1\rangle & \cdots \\ \langle 1|\hat{O}|0\rangle & \langle 1|\hat{O}|1\rangle & \cdots \\ \vdots & & \ddots \\ & & & \langle N-1|\hat{O}|N-1\rangle \end{pmatrix}$$

Then the action of $\hat{O}$ on the ket $|\psi\rangle$ can be represented by action of O on column vector :

$$\hat{O}|\psi\rangle = \begin{pmatrix} & & \\ & O & \\ & & \end{pmatrix} \begin{pmatrix} c_0 \\ \vdots \\ c_{N-1} \end{pmatrix} = \begin{pmatrix} \sum_{j=0}^{N-1} \langle 0|\hat{O}|j\rangle c_j \\ \vdots \\ \sum_j \langle N-1|\hat{O}|j\rangle c_j \end{pmatrix}$$

c) Tensor products

$$A = \begin{pmatrix} A_{00} & A_{01} & \cdots & A_{0N-1} \\ A_{10} & A_{11} & \cdots & A_{1N-1} \\ \vdots & & \ddots & \\ \vdots & & & A_{N-1\,N-1} \end{pmatrix}$$

$$B = \begin{pmatrix} B_{00} & \cdots & B_{0\,N-1} \\ \vdots & \ddots & \\ \vdots & & B_{N-1\,N-1} \end{pmatrix}$$

$$A \otimes B = \begin{pmatrix} A_{00}B & A_{01}B & \cdots & A_{0N-1}\,B \\ A_{10}\,B & A_{11}B & & \\ \vdots & & \ddots & \\ & & & A_{N-1;N-1}\,B \end{pmatrix}$$

Example:

$$\begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & -1/\sqrt{2} \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1/\sqrt{2} & 0 & 1/\sqrt{2} \\ -1/\sqrt{2} & 0 & -1/\sqrt{2} & 0 \\ 0 & 1/\sqrt{2} & 0 & -1/\sqrt{2} \\ -1/\sqrt{2} & 0 & 1/\sqrt{2} & 0 \end{pmatrix}$$

Tensor prod of 2 vectors :

$$|\psi_1\rangle = \begin{pmatrix} c_0 \\ \vdots \\ c_{N-1} \end{pmatrix} \qquad |\psi_2\rangle = \begin{pmatrix} b_0 \\ \vdots \\ b_{N-1} \end{pmatrix}$$

$$|\psi_1\rangle \otimes |\psi_2\rangle = \begin{pmatrix} c_0 \begin{pmatrix} b_0 \\ \vdots \\ b_{N-1} \end{pmatrix} \\ \vdots \\ c_{N-1} \begin{pmatrix} b_0 \\ \vdots \\ b_{N-1} \end{pmatrix} \end{pmatrix} = \begin{pmatrix} c_0 b_0 \\ \vdots \\ c_0 b_{N-1} \\ \vdots \\ c_{N-1} b_0 \\ \vdots \\ c_{N-1} b_{N-1} \end{pmatrix}$$