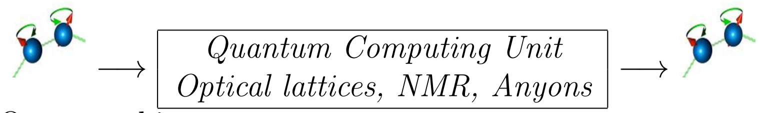
1. Quantum Information Science Research

Basic model



Quantum bit
(*Qubit*)

- Design a *quantum process* to use *quantum properties* to get useful information for a given problem.
- Choose a *suitable* quantum system to build the hardware.
- Prepare the initial (*entangled*) quantum states.
- Create a suitable environment for the quantum system to *evolve* according to quantum mechanical rules.
- Apply a suitable *measurement* to extract useful information.

Remarks

- In physics labs, one would prepare quantum states, manipulate them with quantum operations and measure the output states, where measuring quantum states is also a quantum operation.
- Mathematical theory is needed to help model and design the process.
- Computer Science theory is needed to develop the computation and communication algorithms.
- Knowledge in engineering, material science, chemistry, etc. are needed to build the system.
- We are interested in the mathematical theory.

2. Mathematical framework and notation

- Quantum states with n measurable states are represented as complex unit vectors $v \in \mathbb{C}^n$.
- One does not distinguish v and $e^{it}v$ for any $t \in \mathbb{R}$.
- The conjugate transpose of $v \in \mathbb{C}^n$ and $A \in M_{m,n}$ are denoted by $v^\dagger$ and $A^\dagger$, where $M_{m,n}$ is the set of $m \times n$ complex matrices.
- In physics literature, one uses the bracket notation for v and $v^\dagger$, namely, $|v\rangle$ and $\langle v|$.
- For example, a photon has two measurable states so that it is represented by vectors in $\mathbb{C}^2$.
- Upon measurement, one only sees $|e_1\rangle$ or $|e_2\rangle$. Sometimes, written as $|\uparrow\rangle$, $|\rightarrow\rangle$.
- A general quantum state has the form $a_1|e_1\rangle + a_2|e_2\rangle$ with probability of $|a_1|^2$ in $|e_1\rangle$ and $|a_2|^2$ in $|e_2\rangle$.
- We say that the quantum state is a *superposition* of its measurable states.
- Schrödinger cat interpretation of superposition...
- One may have a different measuring "frame" or "basis", say, $|f_1\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \end{bmatrix}, |f_2\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -1 \end{bmatrix}$, and the superposition has the form $b_1|f_1\rangle + b_2|f_2\rangle$.
- Quantum operations on a closed system with vector states in $\mathbb{C}^n$ are unitary matrices U, i.e., $U^\dagger U = I_n$.

Basic linear algebra [Nakahara and Ohmi, Chapter 1]

- Complex vectors.
- Inner product structure.
- Orthogonal and orthonormal vecotrs.
- Schur Triangularization Lemma.
- Special class of matrices: Hermitian, positive semidefinite, unitary, normal matrices.
- Spectral theorem of diagonalizable and normal matrices.

3. Quantum Mechanics

Here are the basic postulates of quantum mechanics in terms of vector states.

Copenhagen interpretation

A1 A vector state $|x\rangle$ is a unit vector in a Hilbert space $\mathcal{H}$ (usually $\mathbb{C}^n$). Linear combinations (superposition) of the physical states are allowed in the state space.

A2 Every physical quantity (observable) corresponds to a Hermitian operator (matrix) $A \in M_2$ such that A has orthonormal eigenvectors $|u_1\rangle$ and $|u_2\rangle$. Suppose a state $|x\rangle = c_1|u_1\rangle + c_2|u_2\rangle$. Then applying a measurement of $|x\rangle$ corresponding to A will cause the **wave function** (that describes the quantum state) to **collapse** to $|u_1\rangle$ or $|u_2\rangle$ with probability of $|c_1|^2$ and $|c_2|^2$, respectively. Here c_1, c_2 are called the probability amplitude of the state $|x\rangle$.

A3 The time dependence of a state is governed by the Schrödinger equation

$$i\hbar\frac{\partial|x\rangle}{\partial t} = H|x\rangle,$$

where $\hbar$ is the Planck constant with

$$\hbar = 6.62607004 \times 10^{-34} m^2 kg/s,$$

and H is a Hermitian operator (matrix) corresponding to the energy of the system known as the Hamiltonian.

Multipartite systems

- Suppose $|v_1\rangle \in \mathbb{C}^m, |v_2\rangle \in \mathbb{C}^n$ are quantum state. Then the $|v_1\rangle \otimes |v_2\rangle = |v_1 v_2\rangle$ is a **composite state** (**uncorrelated state**) in the bipartite system.

- For example, $|v_1\rangle = \begin{bmatrix} a_1 \\ a_2 \end{bmatrix}, |v_2\rangle = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix}$, then

  $$|v_1\rangle \otimes |v_2\rangle = |v_1\rangle|v_2\rangle = |v_1 v_2\rangle = \begin{bmatrix} a_1|v_2\rangle \\ a_2|v_2\rangle \end{bmatrix} = \begin{bmatrix} a_1 b_1 \\ a_1 b_2 \\ a_2 b_1 \\ a_2 b_2 \end{bmatrix}.$$

- A state $|v\rangle \in \mathbb{C}^m \otimes \mathbb{C}^n$ is **entangled** if it is not a composite state.

- The orthonormal basis $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$ for $\mathbb{C}^4 = \mathbb{C}^2 \otimes \mathbb{C}^2$ consists of decomposable states.

- The orthonormal basis

  $$\Big\{\tfrac{1}{\sqrt{2}}(|00\rangle + |11\rangle),\ \tfrac{1}{\sqrt{2}}(|00\rangle - |11\rangle),$$
  $$\tfrac{1}{\sqrt{2}}(|01\rangle + |10\rangle),\ \tfrac{1}{\sqrt{2}}(|01\rangle - |10\rangle)\Big\}$$

  consists of entangled states known as Bell states.

- Suppose an observable corresponds to the Hermitian matrix with eigenvectors $|00\rangle, |01\rangle, |10\rangle, |11\rangle$, say, $H = \text{diag}\,(3/2, 1/2, -1/2, -3/2)$.

  Then the measurement of $\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$ will yield $|00\rangle$ or $|11\rangle$ each with 50%.

  In particular, the first Schrödinger cat is alive (dead) if and only if the second one is alive (dead).

- We can construct **multipartite system** from k systems to get $\mathbb{C}^{n_1} \otimes \cdots \otimes \mathbb{C}^{n_k} = \mathbb{C}^{n_1 \cdots n_k}$.

- For example, $\mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^2$ is a 3 qubit system.

Quantum operations on multipartite systems

We focus on qubit systems.

- Local (unitary) operations. If $U_1, U_2 \in M_2$ are unitary, then $U_1 \otimes U_2$ is unitary
$$(U_1 \otimes U_2)|v_1 v_2\rangle = |U_1 v_1\rangle|U_2 v_2\rangle.$$

- General $U \in M_4$ is a product of local unitary gates $U_1 \otimes U_2$ and controlled unitary gates of the form $I_2 \oplus V$ and $V \oplus I_2$.

- Proof. Let U be unitary.

  Find $P_1 = U_1 \otimes V_1$ so that $P_1 U$ has zero $(4,1)$ entry.

  Find $P_2 = U_2 \oplus I_2$ so that $P_2 P_1 U$ has zero $(4,1)$ and $(2,1)$ entry.

  Find $P_3 = U_3 \otimes I_2$ so that the first column of $P_3 P_2 P_1 U$ is $(1,0,0,0)^t$. Then $P_2 P_1 = [1] \oplus B$.

  Find $P_4 = I_2 \oplus V_4$ such that $P_4 P_3 P_2 P_1 U$ has zero $(3,2)$ entry.

  Find $P_5 = U_5 \otimes I_2$ such that $P_5 \cdots P_1 U = I_2 \oplus V_6$.

  If $P_6 = I_2 \oplus V_6^\dagger$, then $U = P_1^\dagger \cdots P_6^\dagger$.

- We can represent the operations on a circuit diagrams, and implement the operations using a quantum computers.

  See [Nakahara and Ohmi, Chapter 4].

- We only need to check the actions of the quantum operations on measurable states, say, $|000\rangle, |001\rangle, \ldots, |111\rangle$.

- The standard gates and basic gates might vary from different quantum computer.

- We are working on a research project requiring a decomposition of a unitary $U \in M_8$ into simple unitary gates.

Mixed states and density matrices

A system is in a mixed state if there is a probability p_i that the system is in state $|x_i\rangle$ for $i = 1, \ldots, N$.

If $N = 1$, then the system is in pure state.

Consider an observable corresponds to the Hermitian matrix A.

- The mean value of the quantum system with quantum state $|x\rangle$ is given by $\langle A\rangle = \langle x|A|x\rangle$.
- The mean value of the quantum system with a mixed state $\sum_{j=1}^{N} p_j|x_j\rangle$ is given by

$$\langle A\rangle = \sum_{j=1}^{N} p_j\langle x_j|A|x_j\rangle = \mathrm{tr}\,(A\rho) = \mathrm{tr}\,(\rho A),$$

  where

$$\rho = \sum_{j=1}^{N} p_j|x_j\rangle\langle x_j|$$

  is a density operator (matrix).

Description of quantum systems in mixed states.

A1' A physical state is specified by a density matrix $\rho : \mathcal{H} \to \mathcal{H}$, which is positive semidefinite with trace equal to one.

A2' The mean value of an observable associate with the Hermitian matrix A is $\langle A\rangle = \mathrm{tr}\,(\rho A)$.

A3' The temporal evolution of the density matrix is given by the Liouville-von Neumann equation

$$i\hbar\frac{d}{dt}\rho = [H, \rho] = H\rho - \rho H,$$

where H is the system Hamiltonian.

Multipartitle systems

- Let $\rho_1 \in M_{n_1}, \rho_2 \in M_{n_2}$ be mixed states. Then

  $$\rho_1 \otimes \rho_2 \in M_{n_1} \otimes M_{n_2} \equiv M_{n_1 n_2}$$

  is a composite (uncorrelated) state in the bipartite system.

- General states ρ in $M_{n_1} \otimes M_{n_2}$ are density matrices in $M_{n_1 n_2}$.

- Let ρ be a density matrix in the bipartite system $M_{n_1} \otimes M_{n_2}$. It is **separable** if it is a probabilistic (convex) combination of composite state, i.e.,

  $$\rho = \sum_{j=1}^{N} p_j \sigma_j \otimes \tau_j$$

  with quantum states $\sigma_j \in M_{n_1}, \tau_j \in M_{n_2}$.

- Otherwise, it is **entangled**.

- Note that ρ is always a **linear combination** of composite states.

- Checking whether a state is separable is an NP-hard problem.

- A common test is to use the **partial transposes** defined by

  $$(\rho_1 \otimes \rho_2)^{pt_1} = \rho_1^t \otimes \rho_2, \;\; (\rho_1 \otimes \rho_2)^{pt_2} = \rho_1 \otimes \rho_2^t.$$

- If ρ is separable, then the partial transposes are also quantum states, i.e., positive semi-definite.

- If ρ is a state such that ρ^{pt_1} is positive semidefinite, we say that ρ is a ppt (positive partial trace) state.

- One can extend the concepts to multipartite systems.

Partial traces

- If ρ is quantum state in the bipartite system $M_{n_1} \otimes M_{n_2}$, the partial traces of ρ are defined by

$$\mathrm{tr}_1(\rho_1 \otimes \rho_2) = \mathrm{tr}(\rho_1)\rho_2 = \rho_2 \in M_{n_2},$$

$$\mathrm{tr}_2(\rho_1 \otimes \rho_2) = \rho_1 \mathrm{tr}(\rho_2) = \rho_1 \in M_{n_1}.$$

- One may regard ρ_1 lies in the principal system, and ρ_2 is the environment.
- There are many problems concerning partial traces.

  * Given quantum states $\rho_1 \in M_m, \rho_2 \in M_n$, determine

$$\mathcal{S}(\rho_1, \rho_2) = \{\rho \in D_{n_1 n_2} : \mathrm{tr}_1(\rho) = \rho_2, \mathrm{tr}_2(\rho) = \rho_1\}.$$

  * Find a quantum state in $\mathcal{S}(\rho_1, \rho_2)$ with lowest rank.

  * Find a quantum state in $\mathcal{S}(\rho_1, \rho_2)$ with the lowest von Neumann entropy

$$S(\rho) = -\mathrm{tr}\,\rho \log \rho.$$

  * Find all possible eigenvalues of $\rho \in \mathcal{S}(\rho_1, \rho_2)$.

- One can extend the concepts to multipartite systems.

Research questions about quantum states

Quantum State tomography

Determine $\rho = (\rho_{ij})$.

- For a Hermitian matrix $A = (a_{ij})$, we can determine $\mathrm{tr}\,(a_{ij})X$ for $X \in \mathcal{B}$, where

$$\mathcal{B} = \{E_{rr} : 1 \le r \le n\} \cup \{E_{rs} + E_{sr} : 1 \le r < s \le n\}$$
$$\cup \{i(E_{rs} - E_{sr}) : 1 \le r < s \le n\}.$$

  Then $A = (a_{ij})$ is completely determined.

- If we know that $\mathrm{tr}\, A = 1$, we may skip the checking of $\mathrm{tr}\, AE_{nn}$.

- If $\rho = (\rho_{ij}) = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} (\bar{x}_1, \dots, \bar{x}_n)$ is a pure state, we only need to get information for $\rho_{12}, \dots, \rho_{1n}$. If $x_1 > 0$, then we can solve x_1 in the equation

$$x_1^2 + \sum_{j=2}^{n} |\rho_{1j}/x_1|^2 = 1.$$

  Thus, one only need to check $\mathrm{tr}\,\rho X$ for

  $X = E_{1j} + E_{j1}$, $X = i(E_{1j} - E_{j1})$, $j = 2, \dots, n$.

- Can we write a computer program to do that?

- Can we set up physical experiments to to that?

- Consider the Pauli matrices: $\sigma_0 = I_2$,

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

  For an n-qubit states in M_{2^n}, the test set can be

$$\{T_1 \otimes \cdots \otimes T_n : T_j \in \{\sigma_0, \sigma_x, \sigma_y, \sigma_z\}\}.$$

- Suppose $\mathcal{S} \subseteq M_n$ is a special set of quantum states. Can we find a small test set $\mathcal{S}$ of observable to determine whether $\rho \in \mathcal{S}$ or not?

- For example, determine all ρ with specific norm, eigenvalues, specific the Renyi entropy

  $H_\alpha = \frac{1}{1-\alpha} \log \mathrm{tr}\, \rho^\alpha$ for $\alpha \in (0,1) \cup (1, \infty)$.

  For $\alpha = 2$, we get $\quad H_2(\rho) = -\mathrm{tr}\, \log \rho^2$.

  When $\alpha \to 1$, we get the

  von Neumann entropy $\quad H(\rho) = -\mathrm{tr}\,(\rho \log \rho)$.

Multipartite states

Determine multipartite states with special properties.

- Let $\rho_1 \in M_{n_1}, \rho_2 \in M_{n_2}$. Determine the set

  $$\mathcal{S}(\rho_1, \rho_2) = \{\rho \in M_{n_1} \otimes M_{n_2} : \operatorname{tr}_1 \rho = \rho_2, \operatorname{tr}_1 \rho = \rho_2\}.$$

- One may consider the special case when $\rho_2 = I_{n_2}/n_2$.

- Determine all possible norms, eigenvalues, Renyi entropy of $\rho \in \mathcal{S}(\rho_1, \rho_2)$.

  Use projection methods to find the elements.

- Extend the problems to multipatite systems.

- For example, determine the set of states

  $$\rho \in M_{n_1} \otimes M_{n_2} \otimes M_{n_3}$$

  with specific $\operatorname{tr}_1(\rho) = \rho_{23} \in M_{n_2} \otimes M_{n_3}$,

  and $\operatorname{tr}_3(\rho) = \rho_{12} \in M_{n_1} \otimes M_{n_2}$.

- If the set is non-empty, determine all possible norms, eigenvalues, Renyi entropy of $\rho \in \mathcal{S}(\rho_1, \rho_2)$.

Projection methods and gradient methods

- It is difficult to construct mutlipartite states with prescribed reduced states with overlapped subsystems. For example, construct $\rho \in M_{n_1} \otimes M_{n_2} \otimes M_{n_3}$ with prescribed ρ_{12} and ρ_{23}.

- One may construct a tripartite state ρ with prescribed $\rho \in M_{n_1} \otimes M_{n_2} \otimes M_{n_2}$ using alternating projection methods between the two convex sets:

$$S_1 = \{\rho \in D_{n_1 n_2 n_3} : \mathrm{tr}\,_3(\rho) = \rho_{12}\},$$

$$S_2 = \{\rho \in D_{n_1 n_2 n_3} : \mathrm{tr}\,_1(\rho) = \rho_{23}\}.$$

- We know that set

$$\mathcal{S}(\rho_1, \rho_2) = \{\rho \in D_{n_1 n_2} : \mathrm{tr}\,_1(\rho) = \rho_2, \mathrm{tr}\,_2(\rho) = \rho_1\}$$

  is non-empty. One may determine $\rho \in \mathcal{S}(\rho_1, \rho_2)$ with the maximum / minimum entropy $H(\rho)$, say, using gradient method, i.e., find the steepest descent direction $\nabla H(\rho)$ and change ρ to

$$\rho + t\nabla H(\rho)$$

  for some suitable step size $t > 0$.

Quantum Operations/channels

- Quantum operations $\mathcal{E} : M_n \to M_n$ of a close system with density matrices in M_n is a unitary similarity transform

$$\mathcal{E}(A) = UAU^\dagger, \qquad A \in M_n,$$

where $U \in M_n$ is unitary.

- Here $U = U_t$ may be a function of t: time.

- A mixed unitary channel $\mathcal{E}$ has the form

$$\mathcal{E}(A) = \sum_{j=1}^{r} p_j U_j A U_j^\dagger, \qquad A \in M_n,$$

where $U_1, \ldots, U_r \in M_n$ are unitary, and $p_1, \ldots, p_r$ are positive numbers summing up to 1.

- For an open system which may interact with the environment, $\mathcal{E} : M_n \otimes M_n$ has the form

$$\mathcal{E}(A) = \mathrm{tr}_2(U(A \otimes B)U^\dagger) = \sum_{j=1}^{r} F_j A F_j^\dagger, \quad A \in M_n,$$

where $F_1, \ldots, F_r \in M_n$ satisfy $\sum_{j=1}^{r} F_j^\dagger F_j = I_n$.

- More generally, a quantum operations $\mathcal{E} : M_n \to M_m$ has the operator sum representation

$$\mathcal{E}(A) = \mathrm{tr}_2(U(A \otimes B)U^\dagger) = \sum_{j=1}^{r} F_j A F_j^\dagger, \quad A \in M_n,$$

where $F_1, \ldots, F_r \in M_{m,n}$ satisfy $\sum_{j=1}^{r} F_j^\dagger F_j = I_n$.

- By a result of Choi, $\Phi : M_n \to M_m$ is a quantum channel if the Choi matrix of Φ

$$C(\Phi) = [\Phi(E_{ij})] = [P_{ij}] \in M_n(M_m)$$

is positive semidefinite, $\mathrm{tr}\, P_{jj} = 1$ for all $j = 1, \ldots, n$, and $\mathrm{tr}\, P_{ij} = 0$ for all $1 \le i < j \le n$.

- System tomography can be done by determining the states

$$\mathcal{E}(E_{kk}),\ \mathcal{E}(E_{ii} + E_{jj} + E_{ij} + E_{ji})/2,$$
$$\text{and}\ \ \mathcal{E}(E_{ii} + E_{jj} + iE_{ij} - iE_{ji})/2$$

for $k = 1, \ldots, n$, $1 \le i < j \le n$.

Additional open problems

- Determine the existence and construct quantum operations $\Phi : M_n \to M_m$ sending quantum states $\rho_1, \ldots, \rho_k \in D_n$ to $\tau_1, \ldots, \tau_k \in D_m$.
- If such quantum operation exists, construct one with minimum/maximum channel entropy.
- Determine whether a given channel has special properties, say, a mixed unitary channel.
- Construct quantum error correction codes and schemes for a quantum channel.
- Determine the quantum complexity, capacity, etc. of a quantum channel.