Foundations of Quantum Programming (Lecture 1)

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Outline

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Let $\{|\psi_n\rangle\}$ be a sequence of vectors in $\mathcal{H}$ and $|\psi\rangle \in \mathcal{H}$.

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2. If for any $\epsilon > 0$, there exists a positive integer N such that $||\psi_n - \psi|| < \epsilon$ for all $n \geq N$, then $|\psi\rangle$ is a limit of $\{|\psi_n\rangle\}$, $|\psi\rangle = \lim_{n\to\infty} |\psi_n\rangle$.

Hilbert spaces

A Hilbert space is a complete inner product space; that is, an inner product space in which each Cauchy sequence of vectors has a limit.

Bases

A finite or countably infinite family $\{|\psi_i\rangle\}$ of unit vectors is an orthonormal basis of $\mathcal{H}$ if

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- If $\dim \mathcal{H} = n$, *fix* an orthonormal basis $\{|\psi_1\rangle, ..., |\psi_n\rangle\}$, then a vector $|\psi\rangle = \sum_{i=1}^{n} \lambda_i |\psi_i\rangle \in \mathcal{H}$ is represented by the vector in $\mathbb{C}^n$:

$$\begin{pmatrix} \lambda_1 \\ \ldots \\ \lambda_n \end{pmatrix}$$

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- Complex coefficients λ_i are called *probability amplitudes*.

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$$|+\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad |-\rangle = \frac{|0\rangle - |1\rangle}{\sqrt{2}} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

Linear Operators

Let $\mathcal{H}$ and $\mathcal{K}$ be Hilbert spaces. A mapping

$$A : \mathcal{H} \to \mathcal{K}$$

is a linear operator if it satisfies the conditions:

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2. $A(\lambda|\psi\rangle) = \lambda A|\psi\rangle$.

Positive operators

An operator $A \in \mathcal{L}(\mathcal{H})$ is positive if for all states $|\psi\rangle \in \mathcal{H}$:

$$\langle\psi|A|\psi\rangle \geq 0.$$

Matrix Representation of Operators

- When $\dim \mathcal{H} = n$, *fix* orthonormal basis $\{|\psi_1\rangle, ..., |\psi_n\rangle\}$, A can be represented by the $n \times n$ complex matrix:

$$A = \left(a_{ij}\right)_{n\times n} = \begin{pmatrix} a_{11} & ... & a_{1n} \\ & ... & \\ a_{n1} & ... & a_{nn} \end{pmatrix}$$

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Unitary Transformations

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- If $\dim \mathcal{H} = n$, then a unitary operator is represented by an $n \times n$ unitary matrix U: $U^\dagger U = I_n$.

Postulate of quantum mechanics 2

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- Suppose that the states of a closed quantum system (i.e. a system without interactions with its environment) at times t_0 and t are $|\psi_0\rangle$ and $|\psi\rangle$, respectively.
- Then they are related to each other by a unitary operator U which depends only on the times t_0 and t,

$$|\psi\rangle = U|\psi_0\rangle.$$

Example: Hadamard transformation

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

$$H|0\rangle = H \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = |+\rangle,$$
$$H|1\rangle = H \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} = |-\rangle.$$

Postulate of quantum mechanics 3

- A quantum measurement on a system with state Hilbert space $\mathcal{H}$ is described by a collection $\{M_m\} \subseteq \mathcal{L}(\mathcal{H})$ of operators satisfying the normalisation condition:

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- If the state of a quantum system is $|\psi\rangle$ immediately before the measurement, then for each m,
  - the probability that result m occurs in the measurement is

$$p(m) = ||M_m|\psi\rangle||^2 = \langle\psi|M_m^\dagger M_m|\psi\rangle \qquad \text{(Born rule)}$$

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- The index m stands for the measurement outcomes that may occur in the experiment.
- If the state of a quantum system is $|\psi\rangle$ immediately before the measurement, then for each m,
  - the probability that result m occurs in the measurement is

$$p(m) = ||M_m|\psi\rangle||^2 = \langle\psi|M_m^\dagger M_m|\psi\rangle \qquad \text{(Born rule)}$$

  - the state of the system after the measurement with outcome m is

$$|\psi_m\rangle = \frac{M_m|\psi\rangle}{\sqrt{p(m)}}.$$

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  - the probability of outcome 1 is $p(1) = |\beta|^2$, the state after the measurement is $|1\rangle$.

Hermitian Operators, Observables

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- The set of eigenvalues of A is called the (point) spectrum of A and denoted $\mathit{spec}(A)$.

Eigenspaces

- For each eigenvalue $\lambda \in spec(A)$, the set

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$$M = \sum_{\lambda \in spec(M)} \lambda P_\lambda$$

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- The expectation — average value — of M in state $|\psi\rangle$:

$$\langle M\rangle_\psi = \sum_{\lambda\in spec(M)} p(\lambda)\cdot\lambda = \langle\psi|M|\psi\rangle.$$

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$$|\psi_{1j_1}, ..., \psi_{nj_n}\rangle = |\psi_{1j_1} \otimes ... \otimes \psi_{nj_n}\rangle = |\psi_{1j_1}\rangle \otimes ... \otimes |\psi_{nj_n}\rangle.$$

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- Then the tensor product of $\mathcal{H}_i$ $(i = 1, ..., n)$ is the Hilbert space with $\mathcal{B}$ as an orthonormal basis:

$$\bigotimes_i \mathcal{H}_i = span\mathcal{B}.$$

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- S is a quantum system composed by subsystems $S_1, ..., S_n$ with state Hilbert space $\mathcal{H}_1, ..., \mathcal{H}_n$.
- If for each $1 \leq i \leq n$, S_i is in state $|\psi_i\rangle \in \mathcal{H}_i$, then S is in the *product state* $|\psi_1, ..., \psi_n\rangle$.

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- A state of the composite system is *entangled* if it is not a product of states of its component systems.

Example

- The state space of the system of n qubits:

$$\mathcal{H}_2^{\otimes n} = \mathbb{C}^{2^n} = \left\{ \sum_{x \in \{0,1\}^n} \alpha_x |x\rangle : \alpha_x \in \mathbb{C} \textit{ for all } x \in \{0,1\}^n \right\}.$$

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- A two-qubit system can be in a product state like $|00\rangle, |1\rangle|+\rangle$.
- It can also be in an entangled state like the Bell states or the EPR (Einstein-Podolsky-Rosen) pairs:

$$|\beta_{00}\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle), \quad |\beta_{01}\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle),$$
$$|\beta_{10}\rangle = \frac{1}{\sqrt{2}}(|00\rangle - |11\rangle), \quad |\beta_{11}\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle).$$

Controlled-NOT

- The controlled-NOT or CNOT operator C in $\mathcal{H}_2^{\otimes 2} = \mathbb{C}^4$:

$$C|00\rangle = |00\rangle, \quad C|01\rangle = |01\rangle, \quad C|10\rangle = |11\rangle, \quad C|11\rangle = |10\rangle$$

$$C = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}.$$

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- Transform product states into entangled states:

$$\mathsf{C}|+\rangle|0\rangle = \beta_{00}, \quad \mathsf{C}|+\rangle|1\rangle = \beta_{01}, \quad \mathsf{C}|-\rangle|0\rangle = \beta_{10}, \quad \mathsf{C}|-\rangle|1\rangle = \beta_{11}.$$

Ensembles

- The state of a quantum system is not completely known: it is in one of a number of pure states $|\psi_i\rangle$, with respective probabilities p_i, where $|\psi_i\rangle \in \mathcal{H}$, $p_i \geq 0$ for each i, $\sum_i p_i = 1$.

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- A pure state $|\psi\rangle$ may be seen as a special mixed state $\{(|\psi\rangle, 1)\}$, its density operator is $\rho = |\psi\rangle\langle\psi|$.

Density Operators

- The trace $tr(A)$ of operator $A \in \mathcal{L}(\mathcal{H})$:

$$tr(A) = \sum_i \langle \psi_i | A | \psi_i \rangle$$

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- A density operator ρ is a positive operator with $tr(\rho) = 1$.
- The operator ρ defined by any ensemble $\{(|\psi_i\rangle, p_i)\}$ is a density operator. Conversely, any density operator ρ is defined by an (but not necessarily unique) ensemble $\{(|\psi_i\rangle, p_i)\}$.

Postulates of Quantum Mechanics in the Language of Density Operators

- A closed quantum system from time t_0 to t is described by unitary operator U depending on t_0 and t:

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- If the state of a quantum system was ρ before measurement $\{M_m\}$ is performed, then the probability that result m occurs:

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the system after the measurement:

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- For open quantum systems that interact with the outside, we need a more general notion of quantum operation.
- A linear operator in vector space $\mathcal{L}(\mathcal{H})$ is called a *super-operator* in $\mathcal{H}$.
- Let $\mathcal{H}$ and $\mathcal{K}$ be Hilbert spaces. For any super-operator $\mathcal{E}$ in $\mathcal{H}$ and super-operator $\mathcal{F}$ in $\mathcal{K}$, their tensor product $\mathcal{E} \otimes \mathcal{F}$ is the super-operator in $\mathcal{H} \otimes \mathcal{K}$: for each $C \in \mathcal{L}(\mathcal{H} \otimes \mathcal{K})$,

$$(\mathcal{E} \otimes \mathcal{F})(C) = \sum_k \alpha_k (\mathcal{E}(A_k) \otimes \mathcal{F}(B_k))$$

where $C = \sum_k \alpha_k (A_k \otimes B_k)$, $A_k \in \mathcal{L}(\mathcal{H})$, $B_k \in \mathcal{L}(\mathcal{K})$ for all k.

Quantum Operations

- Let the states of a system at times t_0 and t are ρ and ρ', respectively. Then they must be related to each other by a super-operator $\mathcal{E}$ depending only on the times t_0 and t:

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  1. $tr[\mathcal{E}(\rho)] \leq tr(\rho) = 1$ for each density operator ρ in $\mathcal{H}$;
  2. (Complete positivity) For any extra Hilbert space $\mathcal{H}_R$, $(\mathcal{I}_R \otimes \mathcal{E})(A)$ is positive provided A is a positive operator in $\mathcal{H}_R \otimes \mathcal{H}$, where $\mathcal{I}_R$ is the identity operator in $\mathcal{L}(\mathcal{H}_R)$.

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$$\mathcal{E}(\rho) = tr_E \left[PU(|e_0\rangle\langle e_0| \otimes \rho)U^{\dagger}P \right]$$
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3. (*Kraus operator-sum representation*) There exists a finite or countably infinite set of operators $\{E_i\}$ in $\mathcal{H}$ such that $\sum_i E_i^\dagger E_i \sqsubseteq I$ and
$$\mathcal{E}(\rho) = \sum_i E_i \rho E_i^\dagger$$
for all density operators ρ in $\mathcal{H}$. We write: $\mathcal{E} = \sum_i E_i \circ E_i^\dagger$.