Foundations of Quantum Programming

Lecture 2: Basics of Quantum Mechanics

Mingsheng Ying

University of Technology Sydney, Australia

Outline

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- vector addition $+ : \mathcal{H} \times \mathcal{H} \to \mathcal{H}$

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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 an orthonormal basis contains infinitely many vectors, then $\dim \mathcal{H} = \infty$.
- 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 $\mathbb{C}^n$:

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

Closed-subspace

Let $\mathcal{H}$ be a Hilbert space.

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4. Let X, Y be two subspaces of $\mathcal{H}$. Then

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- Complex coefficients λ_i are called *probability amplitudes*.

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

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- The space of square summable sequences:

$$\mathcal{H}_\infty = \left\{ \sum_{n=-\infty}^{\infty} \alpha_n |n\rangle : \alpha_n \in \mathbb{C} \text{ for all } n \in \mathbb{Z} \text{ and } \sum_{n=-\infty}^{\infty} |\alpha_n|^2 < \infty \right\}.$$

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- $\{|n\rangle : n \in \mathbb{Z}\}$ is an orthonormal basis, $\mathcal{H}_\infty$ is infinite-dimensional.

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is a linear operator if it satisfies the conditions:

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- Identity operator maps each vector in $\mathcal{H}$ to itself, denoted $I_{\mathcal{H}}$.

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Examples

- Identity operator maps each vector in $\mathcal{H}$ to itself, denoted $I_{\mathcal{H}}$.
- Zero operator maps every vector in $\mathcal{H}$ to the zero vector, denoted $0_{\mathcal{H}}$.

Linear Operators

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

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

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- Zero operator maps every vector in $\mathcal{H}$ to the zero vector, denoted $0_{\mathcal{H}}$.
- For vectors $|\varphi\rangle, |\psi\rangle \in \mathcal{H}$, their outer product is the operator $|\varphi\rangle\langle\psi|$ in $\mathcal{H}$:
$$(|\varphi\rangle\langle\psi|)|\chi\rangle = \langle\psi|\chi\rangle|\varphi\rangle.$$

Projection

- Let X be a closed subspace of $\mathcal{H}$ and $|\psi\rangle \in \mathcal{H}$. Then there exist uniquely $|\psi_0\rangle \in X$ and $|\psi_1\rangle \in X^\perp$ such that

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- Vector $|\psi_0\rangle$ is called the projection of $|\psi\rangle$ onto X, $|\psi_0\rangle = P_X|\psi\rangle$.
- For closed subspace X of $\mathcal{H}$, the operator

$$P_X : \mathcal{H} \to X, \quad |\psi\rangle \mapsto P_X|\psi\rangle$$

is the *projector* onto X.

Bounded operators

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- $\mathcal{L}(\mathcal{H})$ stands for the set of bounded operators in $\mathcal{H}$.

Operations of operators

$$(A+B)|\psi\rangle = A|\psi\rangle + B|\psi\rangle,$$
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Positive operators

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

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

Löwner order

$A \sqsubseteq B$ if and only if $B - A = B + (-1)A$ is positive.

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Distance between operators

$$d(A, B) = \sup_{|\psi\rangle} ||A|\psi\rangle - B|\psi\rangle||$$

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:

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

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$$A|\psi\rangle = A \begin{pmatrix} \alpha_1 \\ ... \\ \alpha_n \end{pmatrix} = \begin{pmatrix} \beta_1 \\ ... \\ \beta_n \end{pmatrix}$$

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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

- 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.

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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

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

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

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- $T_L = T_{-1}$ and $T_R = T_1$. They moves a particle on the line one position to the left and to the right, respectively.

Outline

Hilbert Spaces

Linear Operators

Quantum Measurements

Tensor Products

Density Operators

Quantum Operations

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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  - 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 $spec(A)$.

Eigenspaces

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

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Spectral Decomposition

- All eigenvalues of an observable (i.e. a Hermitian operator) M are real numbers.
- $$M = \sum_{\lambda \in spec(M)} \lambda P_\lambda$$

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the state of the system after the measurement is
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- The expectation — average value — of M in state $|\psi\rangle$:
$$\langle M\rangle_\psi = \sum_{\lambda\in spec(M)} p(\lambda)\cdot\lambda = \langle\psi|M|\psi\rangle.$$

Outline

Tensor Product of Hilbert Spaces

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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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- 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:

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

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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:

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

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- 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:

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

Implementing a General Measurement by a Projective Measurement

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- Then for each m, we have:

$$p_{\overline{M}}(m) = p_M(m)$$

$$|\overline{\psi}_m\rangle = |m\rangle|\psi_m\rangle$$

Outline

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 $A \in \mathcal{L}(\mathcal{H})$:

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- 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:

$$p(m) = tr\left(M_m^\dagger M_m \rho\right)$$

  the system after the measurement:

$$\rho_m = \frac{M_m \rho M_m^\dagger}{p(m)}.$$

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$$tr_T : \mathcal{L}(\mathcal{H}_S \otimes \mathcal{H}_T) \to \mathcal{L}(\mathcal{H}_S)$$

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- Let ρ be a density operator in $\mathcal{H}_S \otimes \mathcal{H}_T$. Its reduced density operator for system S:

$$\rho_S = tr_T(\rho).$$

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- Unitary transformations are suited to describe the dynamics of closed quantum systems.
- 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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  1. For each m, if for any system state ρ before measurement, define

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  2. For any system state ρ before measurement, the post-measurement state is

  $$\mathcal{E}(\rho) = \sum_m \mathcal{E}_m(\rho) = \sum_m M_m\rho M_m^\dagger$$

  whenever the measurement outcomes are ignored. Then $\mathcal{E}$ is a quantum operation.

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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: $\mathcal{E} = \sum_i E_i \circ E_i^\dagger$.