Chapter 2 Quantum Mechanics

Quantum Information Science uses quantum properties to help store, process, and transmit information. In this chapter, we describe some basic background on quantum mechanics. We first use vector states to describe quantum systems. Then we demonstrate the formulation using density matrices.

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. Suppose a state $|x\rangle = c_1|u_1\rangle + c_2|u_2\rangle$ such that $A|u_i\rangle = a_i|u_i\rangle$ for $i \in \{1, 2\}$. 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

$$\hbar = 6.6260700410^{-34}m^2kg/s,$$

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

Remarks

1. The phase of the state does not matter, i.e., $|x\rangle$ and $e^{i\alpha}|x\rangle$ represents the same states.

2. In the finite dimensional case, if the state and the observable are represented by

$$|x\rangle = \sum_{j=1}^{n} c_j |u_j\rangle \in \mathbb{C}^n \quad \text{and} \quad A = \sum_{j=1}^{n} \lambda_j |u_j\rangle\langle u_j| = \sum_{j=1}^{n} \lambda_j P_j,$$

   then the projective measurement of the state is

$$\langle x|A|x\rangle = \sum_{j=1}^{n} \lambda_j |c_j|^2.$$

   Once the measurement is applied, the state becomes (collapses to)

$$\frac{P_i|x\rangle}{\sqrt{\langle x|P_i|x\rangle}} = \frac{P_i|x\rangle}{|c_i|}.$$

3. In the Schrödinger equation, if $H(t)$ does not depend on t, then

$$|x(t)\rangle = e^{-iHt/\hbar}|x(0)\rangle.$$

   Otherwise,

$$|x(t)\rangle = \exp\left(\frac{-i}{\hbar}\int_0^t H(s)ds\right)|x(0)\rangle.$$

Example If

$$H = \frac{-\hbar}{2} w \sigma_x \quad \text{and} \quad |\psi(0)\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{so that} \quad i\hbar \frac{\partial |\psi\rangle}{\partial t} = H|\psi\rangle,$$

then $|\psi(t)\rangle = \exp(i\frac{w}{2}\sigma_x t)|\psi(0)\rangle$. Hence,

$$|\psi(t)\rangle = ((\cos wt/2)I_2 + (i \sin wt/2)\sigma_x)|\psi(0)\rangle = \begin{pmatrix} \cos wt/2 \\ i \sin wt/2 \end{pmatrix}.$$

Two ways to compute

$$\exp(B) \quad \text{with} \quad B = (iwt/2)\sigma_x = (iwt/2)\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

Method 1. Use the fact that

$$B = (iwt/2)\sigma_x = (iwt/2)P_1 + (-iwt/2)P_2 \quad \text{with } P_1 = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}, P_2 = \frac{1}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}.$$

Thus,

$$\exp(B) = e^{iwt/2}P_1 + e^{-iwt/2}P_2 = \frac{1}{2}\begin{pmatrix} e^{iwt/2} + e^{-iwt/2} & e^{iwt/2} - e^{-iwt/2} \\ e^{iwt/2} - e^{-iwt/2} & e^{iwt/2} + e^{-iwt/2} \end{pmatrix} = \begin{pmatrix} \cos(wt/2) & i\sin(wt/2) \\ i\sin(wt/2) & \cos(wt/2) \end{pmatrix}.$$

Method 2. Use the fact that $\sigma_x^n = I_2$ if n is even, and $\sigma_x^n = \sigma_x$ if n is odd. Then

$$\exp(B) = \sum_n B^n/n! = \sum_{2j} B^{2j}/(2j)! + \sum_{2j-1} B^{2j-1}/(2j-1)! = \cos(wt/2)I_2 + i\sin(wt/2)\sigma_x.$$

The uncertainty principle

Let $\text{Exp}_x(A) = \langle x|A|x\rangle = \mu$ and

$$\text{Var}_x(A) = \text{Exp}_x((A - \mu I)^2) = \langle x|(A - \mu I)^2|x\rangle = \|(A - \mu I)|x\rangle\|^2.$$

In an deterministic model, the variance of measurements should go to zero as the apparatus is made very accurate.

Theorem For any observable A and B and for any state $|x\rangle$, we have

$$\text{Var}_x(A)\text{Var}_x(B) \geq \frac{1}{4}\langle x|[A, B]|x\rangle,$$

where $[A, B] = AB - BA$ is the commutator of A and B.

Bipartite systems

A system may have two components described by two Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$. Then the bipartite system is represented by $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$. A general state in $\mathcal{H}$ has the form

$$|x\rangle = \sum_{i,j} c_{ij} |e_{1,i}\rangle \otimes |e_{2,j}\rangle \quad \text{with} \quad \sum_{i,j} |c_{ij}|^2 = 1,$$

where $\{|e_{r,1}\rangle, |e_{r,2}\rangle, \ldots\}$ is an orthonormal basis for $\mathcal{H}_r$ with $r \in \{1,2\}$.

A state of the form $|x\rangle = |x_1\rangle \otimes |x_2\rangle$ is a separable state or a tensor product state. Otherwise, it is an entangled state.

Theorem Every state $|x\rangle$ in $\mathcal{H}_1 \otimes \mathcal{H}_2$ admits a Schmidt decomposition

$$|x\rangle = \sum_{j=1}^{r} \sqrt{s_j} |u_j\rangle \otimes |v_j\rangle,$$

where $s_j > 0$ are the Schmidt coefficients satisfying $\sum_{j=1}^{r} s_j = 1$, r is the Schmidt number of $|x\rangle$, $\{|u_1\rangle, \ldots, |u_r\rangle\}$ is an orthonormal set of $\mathcal{H}_1$ and $\{|v_1\rangle, \ldots, |v_r\rangle\}$ is an orthonormal set of $\mathcal{H}_2$.

Remark Extending the results to $\mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_k$ for $k \geq 3$ is an open problem.

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 there is only one possible state, i.e., $p_1 = 1$, then the system is in pure state. The mean value of the measurement of the system corresponding to the observable described by the Hermitian matrix A is

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

where

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

is a density operator (matrix).

Description of a quantum system 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 $\langle A \rangle = \operatorname{tr}(\rho A)$.

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.

Theorem 2.1 The following conditions are equivalent for a given state (density matrix) ρ.

(a) ρ is pure. (b) $\rho^2 = \rho$. (c) $\operatorname{tr}(\rho^2) = 1$.

Remarks

- A mixed state ρ is a Hermitian matrix with nonnegative eigenvalues (Exercise 2.3) summing up to one. Equivalently, $\langle v|\rho|v\rangle \geq 0$ for all vectors $|v\rangle$ and $\operatorname{tr}\rho = 1$.

  Note ρ is a nonnegative combination of Hermitian matrices so that it is Hermitian, and has real eigenvalues. If ρ has a negative eigenvalue λ_1, then ...

- A density matrix ρ is a pure state $\rho = |\psi\rangle\langle\psi|$, i.e., ρ has eigenvalues $1, 0, \dots, 0$. This is the same as saying that $\operatorname{tr}\rho = 1$ (Exercise 2.4).

  Suppose ρ has eigenvalues $\lambda_1, \dots, \lambda_n$. Then $\operatorname{tr}\rho^2 = \sum_{j=1}^n \lambda_j^2$.

Definition 2.1 Suppose $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$. A state ρ is **uncorrelated** if $\rho = \rho_1 \otimes \rho_2$; it is **separable** if it is a convex combination of uncorrelated states, i.e.,

$$\rho = \sum_{j=1}^{r} p_j \rho_{1,j} \otimes \rho_{2,j}.$$

Otherwise, it is **inseparable**.

Partial transpose

Let $\rho = \sum_{j=1}^{r} c_j \rho_{1,j} \otimes \rho_{2,j} \in \mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$. The **partial transpose** of ρ with respect to $\mathcal{H}_2$ is

$$\rho^{\mathrm{pt}} = \sum_{j=1}^{r} \rho_{1,j} \otimes \rho_{2,j}^{t}.$$

In matrix form, if $\rho = (\rho_{ij}) \in M_m(M_n)$, then $\rho^{\mathrm{pt}} = (\rho_{ij}^{t})$.

Remark If ρ is separable, then so is ρ^{pt}. If ρ^{pt} has negative eigenvalues, which can be detected by $N(A) = (\sum_j |\lambda_i(A)| - 1)/2$, then it is not physical and ρ is not separable. Converse holds for $\mathbb{C}^r \otimes \mathbb{C}^s$ for $r + s \leq 5$.

See Example 2.5 and 2.6.

Partial Trace and Purification

Let $A \in \mathcal{H}_1 \otimes \mathcal{H}_2$. The partial trace of A over $\mathcal{H}_2$ is an operator acting on $\mathcal{H}_1$ defined by

$$A_1 = \operatorname{tr}_2 A = \sum_u (I_m \otimes \langle u|)A(I_m \otimes |u\rangle),$$

where m, n are the dimension of $\mathcal{H}_1$ and $\mathcal{H}_2$.

In matrix form, if $\rho = (\rho_{ij}) \in M_m(M_n)$, then $\operatorname{tr}_2(\rho) = (\operatorname{tr} \rho_{ij}) \in M_n$. One can define $\operatorname{tr}_1(\rho_{ij}) = \rho_{11} + \cdots + \rho_{mm}$, which corresponds to

$$A_2 = \operatorname{tr}_1 A = \sum_u (\langle u| \otimes I_n)A(|u\rangle \otimes I_n).$$

Theorem (Purification) Let $\rho_1 = \sum_{j=1}^n p_j |x_j\rangle\langle x_j|$. Suppose $|\psi\rangle = \sum_{j=1}^n \sqrt{p}_j |x_j\rangle \otimes |y_j\rangle$. Then $\operatorname{tr}_2(|\psi\rangle\langle\psi|) = \rho_1$.

Fidelity

Definition 2.2 The fidelity of two density matrices ρ_1 and ρ_2 is defined as

$$F(\rho_1, \rho_2) = \mathrm{tr}\,((\rho_1^{1/2}\rho_2\rho_1^{1/2})^{1/2}) \geq 0.$$

Remarks

1. If $A = \sum_j \lambda_j P_j$ with $\lambda_j \geq 0$, then $A^{1/2} = \sum_j \sqrt{\lambda_j} P_j$.

2. If A, B are $m \times n$ and $n \times m$, then AB and BA have the same nonzero eigenvalues.

   Proof. Note that

   $$\begin{pmatrix} AB & 0 \\ B & 0_n \end{pmatrix} \begin{pmatrix} I_m & A \\ 0 & I_n \end{pmatrix} = \begin{pmatrix} AB & ABA \\ B & BA \end{pmatrix} = \begin{pmatrix} I_m & A \\ 0 & I_n \end{pmatrix} \begin{pmatrix} 0_m & 0 \\ B & BA \end{pmatrix}.$$

   So, $\begin{pmatrix} AB & 0 \\ B & 0 \end{pmatrix}$ and $\begin{pmatrix} 0_m & 0 \\ B & BA \end{pmatrix}$ are similar. The result follows.

3. We have $F(\rho_1, \rho_2) = F(\rho_2, \rho_1)$ as $\rho_1^{1/2}\rho_2\rho_1^{1/2}$ and $\rho_2^{1/2}\rho_1\rho_2^{1/2}$ have the same eigenvalues.

4. For any unitary U, $F(U\rho_1 U^\dagger, U\rho_2 U^\dagger) = F(\rho_1, \rho_2)$. (Exercise 2.10).

5. Suppose ρ_1, ρ_2 have eigenvalues $a_1 \geq \cdots \geq a_n$ and $b_1 \geq \cdots \geq b_n$. Then

   $$F(\rho_1, \rho_2) = \max\{|\mathrm{tr}\,(\rho_1^{1/2}\rho_2^{1/2}U)| : U \text{ unitary}\} \leq \sum_{j=1}^{n} \sqrt{a_j b_j} \leq 1.$$

6. For any two density matrices ρ_1 and ρ_2, we have

   $$0 \leq F(\rho_1, \rho_2) \leq 1.$$

   The first equality holds if and only if $\rho_1\rho_2 = 0$; the second equality holds if and only if $\rho_1 = \rho_2$.