Today's outline - March 28, 2023

- Mixed and pure states
- Properties of traces
- Density operators
- Properties of density operators

Reading Assignment: Reiffel: 10.2

Homework Assignment #06:
Due Thursday, April 06, 2023

Mixed and pure states (ensembles)

In order to better understand what can be measured in a quantum system it is useful to understand the difference between pure and mixed quantum states

An example of a pure state is the $|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ state

By measuring this state in the standard basis, there is a 50% chance of getting $|0\rangle$ and 50% chance of getting $|1\rangle$ but a single measurement will only measure one of these

In order to reveal the probabilities, it is necessary to prepare a pool of many such systems and measure them in the same way

A mixed state is a statistical distribution of the possible states

Many states are prepared in an equal distribution of $|0\rangle$ and $|1\rangle$ states and then are measured

When all these systems are measured, the results are the same as for the measurement of the pure states but the system is fundamentally different since pure states have phase information that can produce interference effects not found in mixed states

Quantum subsystems and mixed states

It is often the case that one has access only to a part of a larger quantum system

For example, Alice only has access to the first qubit of an EPR pair, $|\psi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$

If she measures in the standard basis, she has a 50% chance of getting $|0\rangle$ or $|1\rangle$ but her qubit cannot be described as being in the state $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ because if it is measured in the Hadamard basis, there is a 50% chance of getting $|+\rangle$ or $|-\rangle$

It is therefore important to be able to describe measurements on m-qubit subsystems of identically prepared n-qubit systems and what can be learned from such

This information is encapsulated in a structure called the mixed state of the m-qubit subsystem

Density operators are transformations which can be used to extract this information

Just because the subsystem can be described as a mixed state, does not mean that they are well-defined and not entangled in the larger system

Knowing the mixed states of all the subsystems only provides full knowledge of the system when it is unentangled in that specific subspace decomposition

Tools of the "trade"

In order to understand how density operators function, it is necessary to develop a few identities which relate to quantum subsystems

- The trace of an operator and its relation to inner products
- Operators which are restricted to subsystems and their independence on basis
- The partial trace of an operator

The trace of an operator

Given a space V with basis $\{|v_i\rangle\}$ and an operator $O : V \longrightarrow V$ with a matrix representation M whose trace is

$$\text{Tr}(M) = \sum_i \langle v_i|M|v_i\rangle$$

Given the identity $\text{Tr}(M_1 M_2) = \text{Tr}(M_2 M_1)$, for an invertible matrix C we can write

$$\text{Tr}(C^{-1}MC) = \text{Tr}(MCC^{-1}) = \text{Tr}(M)$$

Since $C^{-1}MC$ can represent a change of basis for M it follows that the trace of a matrix is invariant under basis change which can be written $\text{Tr}(O)$

Given a basis $\{|v_i\rangle\}$ for space V

$$\text{Tr}(|\psi_1\rangle\langle\psi_2|O) = \sum_i \langle v_i|\psi_2\rangle\langle\psi_1|O|v_i\rangle = \sum_i \langle\psi_1|O|v_i\rangle\langle v_i|\psi_2\rangle = \langle\psi_1|O\Big(\sum_i |v_i\rangle\langle v_i|\Big)|\psi_2\rangle$$

$$= \langle\psi_1|OI|\psi_2\rangle = \langle\psi_1|O|\psi_2\rangle$$

This is a useful method of computing an inner product

Restricting operators to subsystems

For any operator O_{AB} on $A \otimes B$, there is a family of operators on subsystem A that is defined by any pair of states $|b_1\rangle$ and $|b_2\rangle$ in B as $\langle b_1|O_{AB}|b_2\rangle : A \to A$ such that

$$|x\rangle \mapsto \sum_i \langle \alpha_i|\langle b_1|O_{AB}|x\rangle|b_2\rangle\, |\alpha_i\rangle$$

where $|\alpha_i\rangle$ are basis states of A

The goal is to show that the operator $\langle b_1|O_{AB}|b_2\rangle$ is independent of the basis of A by which it is defined

Suppose both $\{|\alpha_i\rangle\}$ and $\{|a'_j\rangle\}$ are basis for A with $|a'_j\rangle = \sum_i a_{ij}|\alpha_i\rangle$

Apply $\langle b_1|O_{AB}|b_2\rangle$ to a state $|a\rangle$ and convert it to a trace as shown previously

$$\langle b_1|O_{AB}|b_2\rangle|a\rangle = \sum_j \langle a'_j|\langle b_1|O_{AB}|b_2\rangle|a\rangle|a'_j\rangle$$

Restricting operators to subsystems

$$\begin{aligned}
\langle b_1|O_{AB}|b_2\rangle|a\rangle &= \sum_j \langle a'_j|\langle b_1|O_{AB}|b_2\rangle|a\rangle|a'_j\rangle \\
&= \sum_j \left(\sum_i \overline{a_{ij}}\langle\alpha_i| \right) \langle b_1|O_{AB}|a\rangle|b_2\rangle \left(\sum_k a_{kj}|\alpha_k\rangle \right) \\
&= \sum_i \sum_k \sum_j \overline{a_{ij}} a_{kj} \langle\alpha_i|\langle b_1|O_{AB}|a\rangle|b_2\rangle|\alpha_k\rangle
\end{aligned}$$

Recall that the two bases $|\alpha_i\rangle$ and $|a'_j\rangle$ are related by $|a'_j\rangle = \sum_i a_{ij}|\alpha_i\rangle$

Thus we know that $\sum_j \overline{a_{ij}} a_{kj} \equiv \delta_{ik}$ and we have

$$\langle b_1|O_{AB}|b_2\rangle|a\rangle = \sum_i \langle\alpha_i|\langle b_1|O_{AB}|a\rangle|b_2\rangle|\alpha_i\rangle$$

Such restricted operators are used in defining the partial trace, the restriction of operator O_{AB} to subsystem A, and the operator sum decomposition

The partial trace

For any operator O_{AB} on $A \otimes B$, the partial trace of O_{AB} with respect to subsystem B and basis $\{|\beta_i\rangle\}$ is an operator $\mathrm{Tr}_B(O_{AB})$ on subsystem A

$$\mathrm{Tr}_B(O_{AB}) = \sum_j \langle\beta_j|O_{AB}|\beta_j\rangle$$

As a trace, this operator is basis-independent and has entries in terms of bases $\{|\alpha_i\rangle\}$ and $\{|\beta_j\rangle\}$

$$\mathrm{Tr}_B(O_{AB})_{ik} = \sum_{j=0}^{M-1} \langle\alpha_i|\langle\beta_j|O_{AB}|\alpha_k\rangle|\beta_j\rangle$$

The matrix representation for the $\mathrm{Tr}_B(O_{AB})$ operator is given by

$$\mathrm{Tr}_B(O_{AB}) = \sum_{i=0}^{N-1}\sum_{k=0}^{N-1}\left(\sum_{j=0}^{M-1}\langle\alpha_i|\langle\beta_j|O_{AB}|\alpha_k\rangle|\beta_j\rangle\right)|\alpha_i\rangle\langle\alpha_k|$$

If $O_{AB} = |x\rangle\langle x|$ such that $x_{ij}\overline{x_{kl}}$ are the entries of the O_{AB} matrix in the $\{|\alpha_i\rangle|\beta_j\rangle\}$ basis

$$O_{AB} = \sum_{i=0}^{N-1}\sum_{j=0}^{M-1} x_{ij}|\alpha_i\rangle|\beta_j\rangle \sum_{k=0}^{N-1}\sum_{l=0}^{M-1}\overline{x_{kl}}\langle\alpha_k|\langle\beta_l| = \sum_{i=0}^{N-1}\sum_{j=0}^{M-1}\sum_{k=0}^{N-1}\sum_{l=0}^{M-1} x_{ij}\overline{x_{kl}}|\alpha_i\rangle|\beta_j\rangle\langle\alpha_k|\langle\beta_l|$$

The partial trace

$$O_{AB} = \sum_{i=0}^{N-1} \sum_{j=0}^{M-1} \sum_{k=0}^{N-1} \sum_{l=0}^{M-1} x_{ij}\overline{x_{kl}} |\alpha_i\rangle|\beta_j\rangle\langle\alpha_k|\langle\beta_l|$$

For this case, the partial trace of O_{AB} is given by

$$\mathrm{Tr}_B(O_{AB}) = \mathrm{Tr}_B(|x\rangle\langle x|) = \langle\beta_l| \sum_{i=0}^{N-1} \sum_{j=0}^{M-1} \sum_{k=0}^{N-1} \sum_{l=0}^{M-1} x_{ij}\overline{x_{kl}} |\alpha_i\rangle|\beta_j\rangle\langle\alpha_k|\cancelto{1}{\langle\beta_l|\beta_l\rangle}$$

$$= \sum_{i=0}^{N-1} \sum_{j=0}^{M-1} \sum_{k=0}^{N-1} \sum_{l=0}^{M-1} x_{ij}\overline{x_{kl}} |\alpha_i\rangle\cancelto{\delta_{lj}}{\langle\beta_l|\beta_j\rangle}\langle\alpha_k| = \sum_{i=0}^{N-1} \sum_{j=0}^{M-1} \sum_{k=0}^{N-1} x_{ij}\overline{x_{kj}} |\alpha_i\rangle\langle\alpha_k|$$

If the operator is the tensor product of two operators on the separate subsystems $O_{AB} = O_A \otimes O_B$ then the partial trace is particularly simple since $\langle\alpha_i|\langle\beta_j|O_A \otimes O_B|\alpha_k\rangle|\beta_j\rangle$ can be decomposed

$$\mathrm{Tr}_B(O_{AB}) = \sum_{i=0}^{N-1} \sum_{k=0}^{N-1} \langle\alpha_i|O_A|\alpha_k\rangle \cdot \left(\sum_{j=0}^{M-1} \langle\beta_j|O_B|\beta_j\rangle \right) |\alpha_i\rangle\langle\alpha_k| = O_A \mathrm{Tr}(O_B)$$

Density operators

Suppose A is an m-qubit subsystem for a larger n-qubit system, $X = A \otimes B$

Let $M = 2^m$, $L = 2^{n-m}$ with bases $\{|\alpha_0\rangle, \dots, |\alpha_{M-1}\rangle\}$ and $\{|\beta_0\rangle, \dots, |\beta_{L-1}\rangle\}$ for subsystems A and B

The basis $\{|\alpha_i\rangle \otimes |\beta_i\rangle\}$ spans the entire system X with states given by $|x\rangle$

$$|x\rangle = \sum_{i=0}^{M-1} \sum_{j=0}^{L-1} x_{ij} |\alpha_i\rangle |\beta_j\rangle$$

Let O be an observable which measures on A with projection operators $\{P_i\}$, $0 \le i < M-1$

When applied to the entire space, X, these measurements take the form $O \otimes I$ with projectors $P_I \otimes I$ and the probability that measurement of $|x\rangle$ by $O \otimes I$ is given by

$$\langle x|P \otimes I|x\rangle = \left(\sum_{i=0}^{M-1} \sum_{j=0}^{L-1} \overline{x_{ij}} \langle \alpha_i| \otimes \langle \beta_j| \right) (P \otimes I) \left(\sum_{k=0}^{M-1} \sum_{l=0}^{L-1} x_{kl} |\alpha_k\rangle \otimes |\beta_l\rangle \right)$$

$$= \sum_{i=0}^{M-1} \sum_{j=0}^{L-1} \sum_{k=0}^{M-1} \sum_{l=0}^{L-1} \overline{x_{ij}} x_{kl} \langle \alpha_i|P|\alpha_k\rangle \cancelto{\delta_{jl}}{\langle \beta_j|\beta_l\rangle} = \sum_{i=0}^{M-1} \sum_{j=0}^{L-1} \sum_{k=0}^{M-1} \overline{x_{ij}} x_{kj} \langle \alpha_i|P|\alpha_k\rangle$$

Density operators

We can write the identity operator for subspace A in terms of the the $\{|\alpha_u\rangle\}$ basis

$$I = \sum_{u=0}^{M-1} |\alpha_u\rangle\langle\alpha_u|$$

Substituting into the expression just derived for $\langle x|P \otimes I|x\rangle$

$$\langle x|P \otimes I|x\rangle = \sum_{i=0}^{M-1}\sum_{j=0}^{L-1}\sum_{k=0}^{M-1} \overline{x_{ij}} x_{kj} \langle\alpha_i|\, P\, |\alpha_k\rangle = \sum_{i=0}^{M-1}\sum_{j=0}^{L-1}\sum_{k=0}^{M-1} \overline{x_{ij}} x_{kj} \langle\alpha_i| P \left(\sum_{u=0}^{M-1} |\alpha_u\rangle\langle\alpha_u|\right) |\alpha_k\rangle$$

$$= \sum_{u=0}^{M-1}\sum_{i=0}^{M-1}\sum_{j=0}^{L-1}\sum_{k=0}^{M-1} \overline{x_{ij}} x_{kj} \langle\alpha_u|\alpha_k\rangle\langle\alpha_i|P|\alpha_u\rangle$$

$$= \sum_{u=0}^{M-1} \langle\alpha_u| \left(\sum_{i=0}^{M-1}\sum_{j=0}^{L-1}\sum_{k=0}^{M-1} \overline{x_{ij}} x_{kj} |\alpha_k\rangle\langle\alpha_i|P\right) |\alpha_u\rangle = \mathrm{Tr}(\rho_x^A P)$$

Where ρ_x^A is the density operator for $|x\rangle$ on subsystem A

$$\rho_x^A = \sum_{i=0}^{M-1}\sum_{j=0}^{L-1}\sum_{k=0}^{M-1} \overline{x_{ij}} x_{kj} |\alpha_k\rangle\langle\alpha_i| = \mathrm{Tr}_B(|x\rangle\langle x|)$$

All information from subsystem A alone can be obtained with the density operator

Properties of density operators

Suppose the subsystem is the whole system, that is $A = X$, then the system is in a pure state $|x\rangle = \sum_i x_i|\chi_i\rangle$ with basis $\{|\chi_i\rangle\}$

$$\rho_x^A = \rho_x^X = \sum_{i=0}^{N-1}\sum_{k=0}^{N-1} \overline{x_i} x_k |\chi_k\rangle\langle\chi_i| = |x\rangle\langle x|$$

Clearly, the density operator of a pure state such as $|x\rangle$ is not basis-dependent

Given a basis $\{|\chi_i\rangle\}$, the matrix elements of the density operator are

$$(\rho_x^X)_{ij} = \overline{x_j} x_i$$

and the diagonal elements, $\overline{x_i} x_i$ are related to the projection operator $P_i = |\chi_i\rangle\langle\chi_i|$

$$\langle x|P_i|x\rangle = \langle x|\chi_i\rangle\langle\chi_i|x\rangle = \overline{x_j} x_i$$

In the more general case where $X = A \otimes B$ with bases $\{|\alpha_i\rangle\}$ and $\{|\beta_i\rangle\}$

$$|x\rangle = \sum_{i=0}^{M-1}\sum_{j=0}^{L-1} x_{ij}|\alpha_i\rangle|\beta_j\rangle$$

$$(\rho_x^X)_{ij} = \overline{x_{ij}} x_{kl}$$

The density operator is thus

$$\rho_x^X = \sum_{i,k=0}^{M-1}\sum_{j,l=0}^{L-1} \overline{x_{ij}} x_{kl} |\alpha_k\rangle|\beta_l\rangle\langle\alpha_i|\langle\beta_j|$$

Properties of density operators

To obtain the density matrix ρ_x^A use the partial trace over B of ρ_x^X

$$\rho_x^A = \mathrm{Tr}_B(\rho_x^X) = \mathrm{Tr}_B\left(\sum_{i=0}^{M-1}\sum_{j=0}^{L-1}\sum_{k=0}^{M-1}\sum_{l=0}^{L-1}\overline{x_{ij}}x_{kl}|\alpha_k\rangle|\beta_l\rangle\langle\alpha_i|\langle\beta_j|\right)$$

$$= \sum_{u=0}^{M-1}\sum_{v=0}^{M-1}\left[\sum_{w=0}^{L-1}\langle\alpha_u|\langle\beta_w|\left(\sum_{i=0}^{M-1}\sum_{j=0}^{L-1}\sum_{k=0}^{M-1}\sum_{l=0}^{L-1}\overline{x_{ij}}x_{kl}|\alpha_k\rangle|\beta_l\rangle\langle\alpha_i|\langle\beta_j|\right)|\alpha_v\rangle|\beta_w\rangle\right]|\alpha_u\rangle\langle\alpha_v|$$

$$= \sum_{u=0}^{M-1}\sum_{v=0}^{M-1}\sum_{w=0}^{L-1}\overline{x_{vw}}x_{uw}|\alpha_u\rangle\langle\alpha_v|$$

Because the partial trace is basis-independent, so is the density operator

However, it is not possible to recover the state of the entire system from the set of all subsystem density operators