4.2 Density operator

For any square matrix A, the trace of A is the sum of its diagonal elements,

$$\mathrm{tr}(A) = \sum_i A_{i,i}.$$

The trace operator has the following properties.

- Linearity: $\mathrm{tr}(A+B) = \mathrm{tr}(A) + \mathrm{tr}(B)$.
- Cyclic property: $\mathrm{tr}(AB) = \mathrm{tr}(BA)$.
- For any unitary U, $\mathrm{tr}(UAU^\dagger) = \mathrm{tr}(A)$.
- $\langle\psi|\phi\rangle = \mathrm{tr}(|\phi\rangle\langle\psi|)$. Proof: $\langle\psi|\phi\rangle = \sum_i \langle\psi|i\rangle\langle i|\phi\rangle = \sum_i \langle i|\phi\rangle\langle\psi|i\rangle = \mathrm{tr}(|\phi\rangle\langle\psi|)$.

Consider a quantum system that is in state $|\psi_i\rangle$ with probability p_i. The density operator is defined as

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|.$$

The density operator is indispensable for describing ensembles of states and also for dealing with subsystems of a given system.

The density evolves under unitary transformation as

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i| \xrightarrow{U} \sum_i p_i U|\psi_i\rangle\langle\psi_i|U^\dagger = U\rho U^\dagger$$

An observable A acting on a density ρ has expectation

$$\begin{aligned} \langle A\rangle &= \sum_i p_i \langle\psi_i|A|\psi_i\rangle \\ &= \sum_i p_i \ \mathrm{tr}(A|\psi_i\rangle\langle\psi_i|) \\ &= \mathrm{tr}(A\rho). \end{aligned}$$

A GM $\{M_m\}$ acting on a pure state $|\psi_i\rangle$ produces outcome

$$|\psi_i^m\rangle = \frac{M_m|\psi_i\rangle}{\sqrt{\langle\psi_i|M_m^\dagger M_m|\psi_i\rangle}}$$

with probability

$$p(m|i) = \langle\psi_i|M_m^\dagger M_m|\psi_i\rangle = \mathrm{tr}(M_m^\dagger M_m|\psi_i\rangle\langle\psi_i|).$$

So, the same measurement acting on

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$$

produces the outcome m with probability

$$p(m) = \sum_i p_i p(m|i) = \mathrm{tr}(M_m^\dagger M_m \rho).$$

Given that outcome m is observed, the state after measurement equals

$$|\psi_i^m\rangle = \frac{M_m|\psi_i\rangle}{\sqrt{\mathrm{tr}(M_m^\dagger M_m |\psi_i\rangle\langle\psi_i|)}}$$

with probability

$$p(i|m) = \frac{p_i p(m|i)}{p(m)} = \frac{p_i\ \mathrm{tr}(M_m^\dagger M_m |\psi_i\rangle\langle\psi_i|)}{\mathrm{tr}(M_m^\dagger M_m \rho)}$$

So, the density after measuring m is

$$\begin{aligned}
\rho_m &= \sum_i p(i|m)|\psi_i^m\rangle\langle\psi_i^m| \\
&= \sum_i p(i|m)\frac{M_m|\psi_i\rangle\langle\psi_i^m|M_m^\dagger}{\mathrm{tr}(M_m^\dagger M_m|\psi_i\rangle\langle\psi_i|)} \\
&= \sum_i p_i \frac{M_m|\psi_i\rangle\langle\psi_i^m|M_m^\dagger}{\mathrm{tr}(M_m^\dagger M_m\rho)} \\
&= \frac{M_m\rho M_m^\dagger}{\mathrm{tr}(M_m^\dagger M_m\rho)}
\end{aligned}$$

If the outcome is unknown, the density is

$$\begin{aligned}
\rho &= \sum_m p(m)\rho_m \\
&= \sum_m \mathrm{tr}(M_m^\dagger M_m\rho)\frac{M_m\rho M_m^\dagger}{\mathrm{tr}(M_m^\dagger M_m\rho)} \\
&= \sum_m M_m\rho M_m^\dagger
\end{aligned}$$

Finally, we note a few important points.

- Any positive operator ρ with $\mathrm{tr}(\rho) = 1$ is a valid density operator.
- If $\mathrm{tr}(\rho^2) = 1$, ρ is a pure state; if $\mathrm{tr}(\rho^2) < 1$, ρ is a mixed state.
- Ambiguity of ensemble interpretation. Consider the density

$$\rho = \frac{3}{4}|0\rangle\langle 0| + \frac{1}{4}|1\rangle\langle 1|.$$

Can we interpret ρ as consisting of an ensemble of 75% $|0\rangle$ and 25% $|1\rangle$ states? Notice that we also have

$$\rho = \frac{1}{2}|a\rangle\langle a| + \frac{1}{2}|b\rangle\langle b|$$

where

$$|a\rangle = \sqrt{\frac{3}{4}}|0\rangle + \sqrt{\frac{1}{4}}|1\rangle,$$
$$|b\rangle = \sqrt{\frac{3}{4}}|0\rangle - \sqrt{\frac{1}{4}}|1\rangle.$$

This example shows that ρ cannot be interpreted unambigously as an ensemble.

4.2.1 Reduced density operator

Consider a joint system AB with subsystems A and B. Let

$$|a_m b_n\rangle = |a_m\rangle \otimes |b_n\rangle$$

be a basis for AB where $\{|a_m\rangle\}$, $\{|b_n\rangle\}$ are bases for A and B, respectively.

Consider an observable $R = R^A \otimes I^B$ acting on AB.

$$R|a_m b_n\rangle = R^A|a_m\rangle \otimes b_n$$

Thus, R acts nontrivially only on A. Consider now the expectation of this observable on a density ρ^{AB}.

$$\begin{aligned}
\langle R\rangle &= \mathrm{tr}(\rho^{AB}R) \\
&= \sum_{m,n,m',n'} \langle a_m b_n|\rho^{AB}|a_{m'} b_{n'}\rangle\langle a_{m'} b_{n'}|R|a_m b_n\rangle \\
&= \sum_{m,n,m',n'} \langle a_m b_n|\rho^{AB}|a_{m'} b_{n'}\rangle\langle a_{m'}|R^A|a_m\rangle\langle b_{n'}|b_n\rangle \\
&= \sum_{m,m'}\sum_{n}\langle a_m b_n|\rho^{AB}|a_{m'} b_n\rangle\langle a_{m'}|R^A|a_m\rangle \\
&= \mathrm{tr}(\rho^A R^A)
\end{aligned}$$

where ρ^A is the matrix with elements

$$\langle a_m|\rho^A|a_{m'}\rangle = \sum_n \langle a_m b_n|\rho^{AB}|a_{m'} b_n\rangle.$$

This is also denoted as

$$\rho^A = \sum_n \langle b_n|\rho^{AB}|b_n\rangle.$$

Note that this notation may be misleading and must be carefully interpreted since the dimensions of the bra and ket vectors do not match that of the density matrix.

Partial trace

Consider a joint system in state

$$\rho^{AB} = \begin{bmatrix} R_{11} & R_{12} & R_{13} \\ R_{21} & R_{22} & R_{23} \\ R_{31} & R_{32} & R_{33} \end{bmatrix}$$

where $\{R_{ij}\}$ are square matrices with the same dimension n. Suppose that the columns and rows of ρ^{AB} are ordered in the standard lexicographic order. Then, subsystem A is 3-dimensional, B is n-dimensional; and

$$\rho^{A} = \mathrm{tr}_B(\rho^{AB}) = \begin{bmatrix} \mathrm{tr}(R_{11}) & \mathrm{tr}(R_{12}) & \mathrm{tr}(R_{13}) \\ \mathrm{tr}(R_{21}) & \mathrm{tr}(R_{22}) & \mathrm{tr}(R_{23}) \\ \mathrm{tr}(R_{31}) & \mathrm{tr}(R_{32}) & \mathrm{tr}(R_{33}) \end{bmatrix}$$

and

$$\rho^{B} = \mathrm{tr}_A(\rho^{AB}) = R_{11} + R_{22} + R_{33}.$$

4.2.2 Quantum teleportation

At this point we will discuss a paradoxical example to illustrate the above ideas. Consider a 3-qubit system in state

$$\begin{aligned} |\psi\rangle &= (\alpha|0\rangle + \beta|1\rangle) \otimes \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) \\ &= \frac{\alpha}{\sqrt{2}}(|000\rangle + |011\rangle) + \frac{\beta}{\sqrt{2}}(|100\rangle + |111\rangle) \end{aligned}$$

Alice possesses the first and second qubits, Bob the third. The goal is to convert the state of Bob's qubit into $\alpha|0\rangle + \beta|1\rangle$. The coefficients α and β are unknown. Alice and Bob are separated and have only a classical bit channel between them. How can the task be accomplished?

It is easy to check that

$$\begin{aligned} |\psi\rangle &= \frac{\alpha}{\sqrt{2}}(|000\rangle + |011\rangle) + \frac{\beta}{\sqrt{2}}(|100\rangle + |111\rangle) \\ &= \frac{1}{2}\,|\phi_1\rangle\ (\alpha|0\rangle + \beta|1\rangle) + \\ &\quad\ \frac{1}{2}\,|\phi_2\ \rangle\ (\alpha|0\rangle - \beta|1\rangle) + \\ &\quad\ \frac{1}{2}\,|\phi_3\rangle\ (\alpha|1\rangle + \beta|0\rangle) + \\ &\quad\ \frac{1}{2}\,|\phi_4\rangle\ (\alpha|1\rangle - \beta|0\rangle), \end{aligned}$$

where

$$\begin{aligned}
|\phi_1\rangle &= \frac{|00\rangle + |11\rangle}{\sqrt{2}} \\
|\phi_2\rangle &= \frac{|00\rangle - |11\rangle}{\sqrt{2}} \\
|\phi_3\rangle &= \frac{|01\rangle + |10\rangle}{\sqrt{2}} \\
|\phi_4\rangle &= \frac{|01\rangle - |10\rangle}{\sqrt{2}}
\end{aligned}$$

are an orthonormal set known as the Bell states. Alice performs a projective measurement with $P_i = |\phi_i\rangle\langle\phi_i|$.

Alice measures	Alice sends	Bob's state	Bob's action
$\lvert\phi_1\rangle$	00	$\alpha\lvert 0\rangle + \beta\lvert 1\rangle$	I
$\lvert\phi_2\rangle$	01	$\alpha\lvert 0\rangle - \beta\lvert 1\rangle$	Z
$\lvert\phi_3\rangle$	10	$\alpha\lvert 1\rangle + \beta\lvert 0\rangle$	X
$\lvert\phi_4\rangle$	11	$\alpha\lvert 1\rangle - \beta\lvert 0\rangle$	iY

Bob's qubit has final state $\alpha|0\rangle + \beta|1\rangle$ in each case, as desired.

The unknown quantum state has been teleported to Bob by sending two classical bits, utilizing the prior entanglement.

Density viewpoint of teleportation

Before Alice's measurement the densities are

$$\begin{aligned}
\rho^{AB} &= |\psi\rangle\langle\psi| \\
&= \frac{1}{2}\begin{bmatrix}
|\alpha|^2 & 0 & 0 & |\alpha|^2 & \alpha\beta^* & 0 & 0 & \alpha\beta^* \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
|\alpha|^2 & 0 & 0 & |\alpha|^2 & \alpha\beta^* & 0 & 0 & \alpha\beta^* \\
\alpha^*\beta & 0 & 0 & \alpha^*\beta & |\beta|^2 & 0 & 0 & |\beta|^2 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\alpha^*\beta & 0 & 0 & \alpha^*\beta & |\beta|^2 & 0 & 0 & |\beta|^2
\end{bmatrix}
\end{aligned}$$

$$
\rho^A = \frac{1}{2} \begin{bmatrix} |\alpha|^2 & 0 & \alpha\beta^* & 0 \\ 0 & |\alpha|^2 & 0 & \alpha\beta^* \\ \alpha^*\beta & 0 & |\beta|^2 & 0 \\ 0 & \alpha^*\beta & 0 & |\beta|^2 \end{bmatrix}
$$

$$
\begin{aligned}
\rho^B &= \frac{1}{2} \begin{bmatrix} |\alpha|^2 + |\beta|^2 & 0 \\ 0 & |\alpha|^2 + |\beta|^2 \end{bmatrix} \\
&= \begin{bmatrix} 1/2 & 0 \\ 0 & 1/2 \end{bmatrix}
\end{aligned}
$$

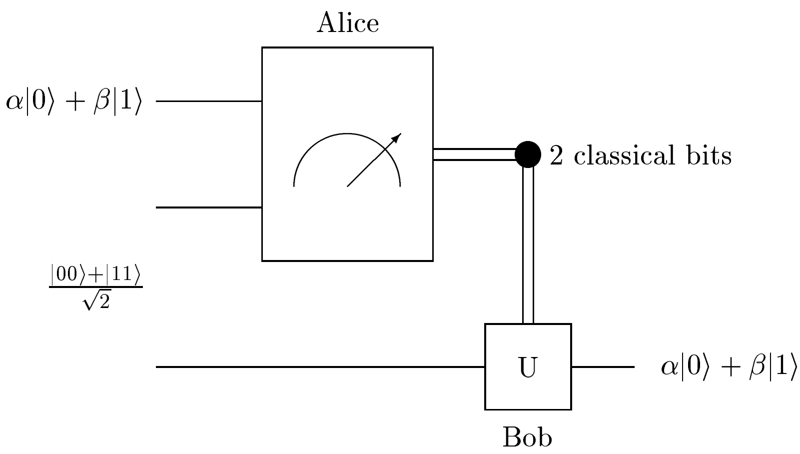
Since Bob's density has no dependence on α and β, he cannot create a copy of $\alpha|0\rangle + \beta|1\rangle$ by himself.

After Alice's measurement, but before Bob learns the measurement result, Bob's density is

$$
\begin{aligned}
\rho^B &= \frac{1}{4}(\alpha|0\rangle + \beta|1\rangle)(\alpha^*\langle 0| + \beta^*\langle 1|) + \\
&\quad \frac{1}{4}(\alpha|0\rangle - \beta|1\rangle)(\alpha^*\langle 0| - \beta^*\langle 1|) + \\
&\quad \frac{1}{4}(\alpha|1\rangle + \beta|0\rangle)(\alpha^*\langle 1| + \beta^*\langle 0|) + \\
&\quad \frac{1}{4}(\alpha|1\rangle - \beta|0\rangle)(\alpha^*\langle 1| - \beta^*\langle 0|) \\
&= \begin{bmatrix} 1/2 & 0 \\ 0 & 1/2 \end{bmatrix}
\end{aligned}
$$

Bob still can't do anything to effect teleportation. Only after Bob learns the measurement result that Bob's density collapses to one of four possible pure states.

Teleportation operation can be represented as a circuit acting on three qubits as follows.



4.2.3 Principle of deferred measurement

In teleportation, we first apply a projective measurement on a quantum subsystem, then apply classical controls on another subsystem based on the measurement outcome. The general form of this is illustrated in the following figure. The joint state is initially

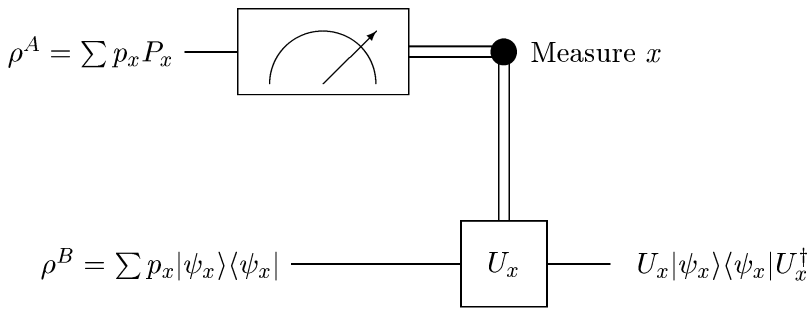
$$\rho^{AB} = \sum_x p_x P_x \otimes |\psi_x\rangle\langle\psi_x|$$

where $\{P_x\}$ are the projectors for the measurement that follows. Subsystem A is in a state

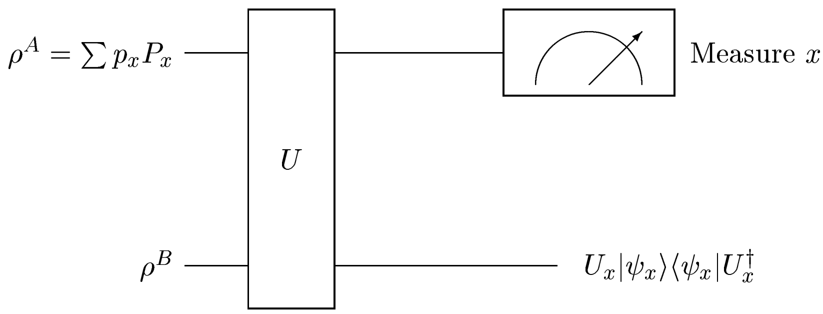
$$\rho^A = \sum_x p_x P_x$$

and subsystem B is in state

$$\rho^B = \sum_x p_x |\psi_x\rangle\langle\psi_x|.$$



The alternative circuit is given below.



The joint state before the measurement is

$$U\rho^{AB}U^\dagger \triangleq \sum_x p_x P_x \otimes U_x|\psi_x\rangle\langle\psi_x|U_x^\dagger.$$

Output $U_x|\psi_x\rangle\langle\psi_x|U_x^\dagger$ is obtained with probability p_x in both cases.