Assignment 6: additional background

Density operator/matrix

1) Pure state $|\psi\rangle \in \mathcal{H}$

$$\rho = |\psi\rangle\langle\psi|$$

Example: $|\psi\rangle = c_0|0\rangle + c_1|1\rangle$:

$$\begin{aligned}
\rho &= (c_0|0\rangle + c_1|1\rangle)(c_0^*\langle 0| + c_1^*\langle 1|) \\
&= \left|c_0\right|^2 |0\rangle\langle 0| + c_0 c_1^*|0\rangle\langle 1| + c_0^* c_1|1\rangle\langle 0| + |c_1|^2 |1\rangle\langle 1| \\
&= \begin{pmatrix} \left|c_0\right|^2 & c_0 c_1^* \\ c_0^* c_1 & |c_1|^2 \end{pmatrix}
\end{aligned}$$

2) Mixed state

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

Example:

$p_1 = 0.4, \quad |\psi_1\rangle = (|0\rangle + i|1\rangle)/\sqrt{2}$

$p_2 = 0.6, \quad |\psi_2\rangle = |1\rangle$:

$$\begin{aligned}
\rho &= 0.4 \, |\psi_1\rangle\langle\psi_1| + 0.6 \, |\psi_2\rangle\langle\psi_2| \\
&= 0.4 \left[\frac{1}{2}(|0\rangle\langle 0| - i|0\rangle\langle 1| + i|1\rangle\langle 0| + |1\rangle\langle 1|)\right] + 0.6 \; [|1\rangle\langle 1|] \\
&= 0.2 \, |0\rangle\langle 0| - 0.2i \, |0\rangle\langle 1| + 0.2i \, |1\rangle\langle 0| + 0.8 \, |1\rangle\langle 1| \\
&= \begin{pmatrix} 0.2 & -0.2i \\ 0.2i & 0.8 \end{pmatrix} = \frac{1}{2}\left(\mathbb{I} + 0 \, \sigma_x + 0.4 \, \sigma_y - 0.6 \, \sigma_z\right)
\end{aligned}$$

Reduced density operator

Suppose we have physical system consisting of the subsystems A and B whose joint state is described by the density matrix ρ^{AB}. The reduced density operator for the subsystem A is

$$\rho_A = \mathrm{tr}_B\, \rho^{AB}$$

where tr_B is an operator map known as *partial trace* over system B. It is defined as

$$\rho_A = \mathrm{tr}_B\, |a_1 b_1\rangle\langle a_2 b_2| = \mathrm{tr}_B\, \left(|a_1\rangle\langle a_2| \otimes |b_1\rangle\langle b_2|\right) = |a_1\rangle\langle a_2| \quad \mathrm{tr}\, \left(|b_1\rangle\langle b_2|\right)$$

where $|a_1\rangle$ and $|a_2\rangle$ are any two vectors in A, and $|b_1\rangle$ and $|b_2\rangle$ are any two vectors in B. $\mathrm{tr}\, (|b_1\rangle\langle b_2|)$ is the usual trace, so, using the completeness relation, we get

$$\mathrm{tr}\, \left(|b_1\rangle\langle b_2|\right) = \sum_k \langle k|b_1\rangle\langle b_2|k\rangle = \sum_k \langle b_2|k\rangle\langle k|b_1\rangle = \langle b_2|\left(\sum_k |k\rangle\langle k|\right)|b_1\rangle = \langle b_2|b_1\rangle$$

Example

$$\rho = \frac{1}{2}\left(|00\rangle\langle 00| + |00\rangle\langle 11| + |11\rangle\langle 00| + |11\rangle\langle 11|\right)$$

The partial trace over the second qubit is

$$\begin{aligned}
\rho_1 &= \mathrm{tr}_2\left[\frac{1}{2}\left(|00\rangle\langle 00| + |00\rangle\langle 11| + |11\rangle\langle 00| + |11\rangle\langle 11|\right)\right] \\
&= \frac{1}{2}\left(|0\rangle\langle 0|\langle 0|0\rangle + |0\rangle\langle 1|\langle 1|0\rangle + |1\rangle\langle 0|\langle 0|1\rangle + |1\rangle\langle 1|\langle 1|1\rangle\right) \\
&= \frac{1}{2}\left(|0\rangle\langle 0| + |1\rangle\langle 1|\right)
\end{aligned}$$

Operator sum representation

is a representation of quantum operations in terms of the operators on the principal system only:

Let $|e_k\rangle$ be the orthonormal basis for the finite dimensional Hilbert space of the environment, and let $\rho = |e_0\rangle\langle e_0|$ be the initial (pure) state of the environment. Then we can express a quantum operation as

$$\mathcal{E}(\rho) = \mathrm{tr}_{\,env}\left[U\,(\rho \otimes \rho_{env})\,U^\dagger\right] = \sum_k \langle e_k|U(\rho \otimes |e_0\rangle\langle e_0|)U^\dagger|e_k\rangle = \sum_k \; E_k\,\rho\,E_k^\dagger$$

where $E_k = \langle e_k|U|e_o\rangle$ is an operator on the Hilbert space of the principal system called an *operation element* of the quantum operation. They satisfy

$$\sum_k E_k^\dagger\,E_k = \mathbb{I}.$$

Example:

Assume the system is one qubit in the state ρ, and the environment is one qubit in the initial state $|0\rangle$, and the unitary operation is $CNOT$ with the system as the control:

$$
\begin{aligned}
\mathcal{E}(\rho) &= \mathrm{tr}_{env}\left[U_{CNOT}\,(\rho \otimes |0\rangle\langle 0|)\,U^{\dagger}_{CNOT}\right] \\
&= \mathrm{tr}_{env}\left[(P_0 \otimes I + P_1 \otimes X)\,(\rho \otimes |0\rangle\langle 0|)\,(P_0 \otimes I + P_1 \otimes X)\right] \\
&= \mathrm{tr}_{env}\left[(P_0 \otimes I)\,(\rho \otimes |0\rangle\langle 0|)\,(P_0 \otimes I) + (P_0 \otimes I)\,(\rho \otimes |0\rangle\langle 0|)\,(P_1 \otimes X)\right. \\
&\qquad \left. + (P_1 \otimes X)\,(\rho \otimes |0\rangle\langle 0|)\,(P_0 \otimes I) + (P_1 \otimes X)\,(\rho \otimes |0\rangle\langle 0|)\,(P_1 \otimes X)\right] \\
&= \mathrm{tr}_{env}\left[P_0\rho P_0 \otimes |0\rangle\langle 0| + P_0\rho P_1 \otimes |0\rangle\langle 0|X + P_1\rho P_0 \otimes X|0\rangle\langle 0| + P_1\rho P_1 \otimes X|0\rangle\langle 0|X\right] \\
&= \mathrm{tr}_{env}\left[P_0\rho P_0 \otimes |0\rangle\langle 0| + P_0\rho P_1 \otimes |0\rangle\langle 1| + P_1\rho P_0 \otimes |1\rangle\langle 0| + P_1\rho P_1 \otimes |1\rangle\langle 1|\right] \\
&= P_0\rho P_0\ \langle 0|0\rangle + P_0\rho P_1\ \langle 1|0\rangle + P_1\rho P_0\ \langle 0|1\rangle + P_1\rho P_1\ \langle 1|1\rangle \\
&= P_0\,\rho\,P_0 + P_1\,\rho\,P_1
\end{aligned}
$$

Assignment 7: background

Problem 5:

The energy eigenstates of harmonic oscillator $|n\rangle$:

$$\hat{H}|n\rangle = \hbar\omega\left(n + \frac{1}{2}\right)|n\rangle$$

A density operator for the state of harmonic oscillator in the representation given by the energy eigenstates

$$\rho = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\rho_{mn}|m\rangle\langle n|.$$

The action of the Hamiltonian $\hat{H} = \hat{H}^\dagger$ onto the density matrix

$$
\begin{aligned}
\hat{H}\rho &= \sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\rho_{mn}\hat{H}|m\rangle\langle n| = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\hbar\omega\left(m+\frac{1}{2}\right)\rho_{mn}|m\rangle\langle n| \\
\rho\hat{H} &= \sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\rho_{mn}|m\rangle\langle n|\hat{H} = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\hbar\omega\left(n+\frac{1}{2}\right)\rho_{mn}|m\rangle\langle n|.
\end{aligned}
$$

The density operator elements in this representation become just multiplied by the Hamiltonian eigenvalues given by the corresponding eigenstate.

Commutator of the Hamiltonian and the density operator

$$
\begin{aligned}
[\hat{H},\rho] &= \hat{H}\rho - \rho\hat{H} = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\rho_{mn}\left(\hat{H}|m\rangle\langle n| - |m\rangle\langle n|\hat{H}\right) \\
&= \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} \hbar\,\omega\,(m-n)\,\rho_{mn}\,|m\rangle\langle n| \\
&= \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} \hbar\,\omega_{mn}\,\rho_{mn}\,|m\rangle\langle n|
\end{aligned}
$$

where $\omega_{mn} = \omega(m-n)$.

For any function of the commutator we will get

$$
f\left([\hat{H},\rho]\right) = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} f\left(\hbar\,\omega_{mn}\right)\,\rho_{mn}\,|m\rangle\langle n|.
$$

The **Schrödinger equation** for a density operator:

We start with the Schrödinger equation for a ket $|\psi\rangle$ and its adjoint $\langle\psi|$

$$\frac{\mathrm{d}}{\mathrm{d}t}|\psi\rangle = -\frac{i}{\hbar}\, H\, |\psi\rangle \qquad\qquad \frac{\mathrm{d}}{\mathrm{d}t}\langle\psi| = \frac{i}{\hbar}\, \langle\psi|\, H$$

and combine these as follows

$$\begin{aligned}
\frac{\mathrm{d}\rho}{\mathrm{d}t} &= \frac{\mathrm{d}}{\mathrm{d}t}|\psi\rangle\langle\psi| = \left(\frac{\mathrm{d}}{\mathrm{d}t}|\psi\rangle\right)\langle\psi| + |\psi\rangle\left(\frac{\mathrm{d}}{\mathrm{d}t}\langle\psi|\right) \\
&= -\frac{i}{\hbar}\,(H|\psi\rangle\langle\psi| - |\psi\rangle\langle\psi|H) \\
&= -\frac{i}{\hbar}\,(H\rho - \rho H) \\
&= -\frac{i}{\hbar}\,[H,\rho]
\end{aligned}$$

This holds also when the state is mixed, i.e. $\rho = \sum_i p_i\, \rho_i$, as $\frac{\mathrm{d}\rho}{\mathrm{d}t} = \sum_i p_i\, \frac{\mathrm{d}\rho_i}{\mathrm{d}t}$.

Unitary evolution of a density operator

$$\rho(t) = e^{-\frac{i}{\hbar}[H,\,.\,]t}\rho(0) = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} e^{-i\omega(m-n)t}\,\rho_{mn}(0)\,|m\rangle\langle n| = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} e^{-i\omega_{mn}t}\,\rho_{mn}(0)\,|m\rangle\langle n|$$

where the matrix elements transform as $\rho_{mn}(0) \rightarrow \rho_{mn}(t) = e^{-i\omega_{mn}t}\,\rho_{mn}(0)$.

This is completely equivalent to the expression

$$\begin{aligned}\rho(t) &= U\rho(0)U^{\dagger} = e^{-iHt/\hbar}\rho(0)e^{iHt/\hbar} = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\rho_{mn}(0)\,e^{-i\omega\left(m+\frac{1}{2}\right)t}\,|m\rangle\langle n|\,e^{i\omega\left(n+\frac{1}{2}\right)t}\\ &= \sum_{m=0}^{\infty}\sum_{n=0}^{\infty}e^{-i\omega(m-n)t}\rho_{mn}(0)\,|m\rangle\langle n| = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\,e^{-i\omega_{mn}}\,\rho_{mn}(0)\,|m\rangle\langle n|.\end{aligned}$$