CS 599 P1: Introduction to Quantum Computation — Boston University, Fall 2025
Instructor: Alexander Poremba

LECTURE # 18: DENSITY MATRIX FORMALISM

In this lecture, we introduce the density matrix formalism—a generalization of the pure state formalism we relied on in the first half of the class. While the pure state formalism describes *closed* quantum systems (i.e. isolated quantum systems in which evolution is *unitary*), the density matrix formalism is significantly more general as it also captures *open* quantum systems, i.e. systems which may interact with an outside environment (and where evolution may be even be irreversible, e.g., in the form of a quantum channel). Importantly, the density matrix formalism can also capture the purely classical notion of *statistical* uncertainty arising from probability distributions.

1 Classical probability distributions

Before we introduce the notion of a density matrix, it will be instructive to first formally define what we mean by a classical probability distribution.

Classical probability distribution

A probability distribution on N outcomes is a *probability vector* $\mathbf{p} = (p_0, p_1, \dots, p_{N-1})$ such that

- outcome $j \in \{0, 1, \dots, N-1\}$ occurs with probability $p_j \geq 0$ and
- the total probability sums to 1, i.e. $\sum_{j=0}^{N-1} p_j = 1$.

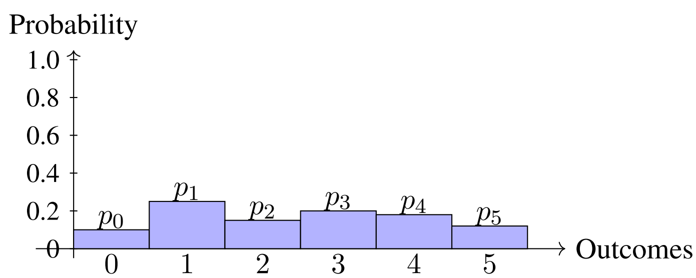


Figure 1: A histogram representing a probability vector $\mathbf{p} = (p_0, \dots, p_5)$.

2 Density matrices (or mixed states)

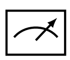
A density matrix (or quantum *mixed* state) captures a statistical mixture/ensemble of multiple different (and not necessarily orthogonal) d-dimensional quantum states $\{|\psi_j\rangle\}_{j=0}^{N-1}$. For example, we may find

$$\text{the quantum system in the state ...} \qquad \begin{cases} |\psi_0\rangle & \text{with probability } p_0 \\ |\psi_1\rangle & \text{with probability } p_1 \\ \vdots & \\ |\psi_{N-1}\rangle & \text{with probability } p_{N-1}. \end{cases}$$

What would we observe if we measured the system above in some basis $\{|b_i\rangle\}_{i=1}^{d}$? By the law of total probability, we would observe

$$\text{the outcome } |b_i\rangle \text{ with probability ...} \qquad \begin{cases} p_0 \cdot |\langle b_i|\psi_0\rangle|^2, & \text{if } |\psi_0\rangle \\ p_1 \cdot |\langle b_i|\psi_1\rangle|^2, & \text{if } |\psi_1\rangle \\ \vdots & \\ p_{N-1} \cdot |\langle b_i|\psi_{N-1}\rangle|^2, & \text{if } |\psi_{N-1}\rangle. \end{cases}$$

In other words, we have a convex combination (or *mixture*) of the form



$$\begin{aligned} \Pr\left[\boxed{} = |b_i\rangle \right] &= \sum_{j=0}^{N-1} p_j \cdot |\langle b_i|\psi_j\rangle|^2 && \text{(law of total probability)} \\ &= \sum_{j=0}^{N-1} p_j \cdot \langle b_i|\psi_j\rangle \langle \psi_j|b_i\rangle && \text{(skew symmetry)} \\ &= \langle b_i| \left(\underbrace{\sum_{j=0}^{N-1} p_j |\psi_j\rangle\langle\psi_j|}_{=\rho} \right) |b_i\rangle && \text{(by linearity)} \\ &= \mathrm{Tr}\left[\langle b_i|\,\rho\,|b_i\rangle\right] && \text{(trace applied to a scalar)} \\ &= \mathrm{Tr}\left[|b_i\rangle\langle b_i|\rho\right]. && \text{(cyclicity of the trace)} \end{aligned}$$

In other words, the operator ρ alone captures all of the aspects of the statistical mixture we discussed earlier.

Background: the trace. In the calculation above, we relied on the so-calld *trace*. Roughly speaking, the trace is simply the linear operator which takes the sum over all of the diagonal entries of a given matrix.

Trace of a matrix

The *trace* of a matrix $A \in \mathbb{C}^{d\times d}$ is defined as the operation

$$\mathrm{Tr}[A] = \sum_{i=1}^{d} A_{ii} = \sum_{i=1}^{d} \langle i| A |i\rangle .$$

where $\{|i\rangle\}_{i=1}^{d}$ is the standard basis of $\mathbb{C}^d$. In other words, the trace corresponds to a sum over all of the diagonal entries of the matrix. Mathematically speaking, the trace has the following properties:

1. **Linearity (over $\mathbb{C}$):** For all $A, B \in \mathbb{C}^{d\times d}$ and $\alpha, \beta \in \mathbb{C}$,

$$\mathrm{Tr}[\alpha A + \beta B] = \alpha\ \mathrm{Tr}[A] + \beta\ \mathrm{Tr}[B].$$

2. **Cyclicity:** For all $A, B \in \mathbb{C}^{d\times d}$,

$$\mathrm{Tr}[AB] = \mathrm{Tr}[BA].$$

   More generally, for any finite product of square matrices whose products are well defined,

$$\mathrm{Tr}[A_1 A_2 \cdots A_n] = \mathrm{Tr}[A_2 \cdots A_n A_1].$$

3. **Invariance under change of basis:** For any $A \in \mathbb{C}^{d\times d}$ and any unitary U (i.e. $U^\dagger U = UU^\dagger = I$),

$$\mathrm{Tr}[UAU^\dagger] = \mathrm{Tr}[A] = \mathrm{Tr}[U^\dagger AU].$$

   In particular, for *any* orthonormal basis $\{|b_i\rangle\}_{i=1}^{d}$ of $\mathbb{C}^d$ with $|b_i\rangle = U|i\rangle$, we have

$$\mathrm{Tr}[A] = \mathrm{Tr}[U^\dagger AU] = \sum_{i=1}^{d} \langle i| U^\dagger AU |i\rangle = \sum_{i=1}^{d} \langle b_i| A |b_i\rangle .$$

This motivates the following definition of a density matrix.

Density matrix

A density matrix corresponding to the statistical ensemble $(\mathbf{p}, \{|\psi_j\rangle\}_{i=0}^{N-1})$ of d-dimensional quantum states with associated *probability vector* $\mathbf{p} = (p_0, p_1, \ldots, p_{N-1})$ is the matrix $\rho \in \mathbb{C}^{d\times d}$ given by

$$\rho = \sum_{j=0}^{N-1} p_j |\psi_j\rangle\langle\psi_j|.$$

where for $j \in \{0, 1, \ldots, N-1\}$ the state $|\psi_j\rangle$ occurs with probability $p_j \geq 0$ and $\sum_{j=0}^{N-1} p_j = 1$. Formally, any density matrix $\rho \in \mathbb{C}^{d\times d}$ satisfies the following properties:

- ρ is a hermitian with $\rho^\dagger = \rho$;
- ρ has unit trace, i.e., $\mathrm{Tr}[\rho] = 1$;
- ρ is positive semi-definite, i.e. $\rho \geq 0$, and thus all eigenvalues are non-negative.

A density matrix of rank 1, e.g. $\rho = |\psi\rangle\langle\psi|$, is called a *pure* state; otherwise, we call it a *mixed* state. We use $\mathcal{D}(\mathcal{H})$ to denote density operators over $\mathcal{H}$, and we use $\mathcal{L}(\mathcal{H})$ to denote all linear operators.

Despite the fact that ρ is now a *matrix* (and thus an operator) rather than a complex quantum state, we will nevertheless call ρ a quantum state in the new density matrix formalism. To get a better sense of what density matrices look like, let us consider a few examples.

Examples.

- (*Uniform bit*) Suppose we have random bit $b \in \{0, 1\}$ such that $\Pr[b = 0] = \Pr[b = 1] = \frac{1}{2}$. We can express this in quantum notation as

  $$\text{a qubit in the state ...} \quad \begin{cases} |0\rangle\,, & \text{with probability } \frac{1}{2} \\ |1\rangle\,, & \text{with probability } \frac{1}{2}. \end{cases}$$

  Hence, this ensemble corresponds to the maximally mixed state given by the density matrix

  $$\rho = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1| = \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|) = \frac{I}{2}.$$

  Note that the maximally mixed state corresponds to a *diagonal* matrix of the form

  $$\frac{I}{2} = \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{bmatrix}.$$

- (*Uniform superposition*) Suppose we have a quantum system which is in the state $|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ (with probability 1). This corresponds to the density matrix

  $$\begin{aligned} \rho = |+\rangle\langle +| &= \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)\frac{1}{\sqrt{2}}(\langle 0| + \langle 1|) \\ &= \frac{1}{2}(|0\rangle\langle 0| + |0\rangle\langle 1| + |1\rangle\langle 0| + |1\rangle\langle 1|) \;=\; \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix}. \end{aligned}$$

Notice the difference compared to the maximally mixed state $\frac{I}{2}$. Unlike the maximally mixed state from before, ρ above has *off-diagonal* elements which capture the *quantumness* of the state. As we previously noticed in one of the earlier lectures, $|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ is not the same as a random bit.

- (*General qubit*) Suppose $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$ is an arbitrary qubit. Then, $|\psi\rangle$ corresponds to the rank-1 pure state density operator

$$\begin{aligned}\rho = |\psi\rangle\langle\psi| &= (\alpha|0\rangle + \beta|1\rangle)(\bar{\alpha}\langle 0| + \bar{\beta}\langle 1|) \\ &= |\alpha|^2 \cdot |0\rangle\langle 0| + \alpha\bar{\beta} \cdot |0\rangle\langle 1| + \bar{\alpha}\beta \cdot |1\rangle\langle 0| + |\beta|^2 \cdot |1\rangle\langle 1| \;=\; \begin{bmatrix} |\alpha|^2 & \alpha\bar{\beta} \\ \bar{\alpha}\beta & |\beta|^2 \end{bmatrix}.\end{aligned}$$

  Notice the appearance of off-diagonal elements!

- (*Classical distribution*) Suppose we have a classical probability distribution on N outcomes given by $\mathbf{p} = (p_0, p_1, \ldots, p_{N-1})$ such that outcome $j \in \{0, 1, \ldots, N-1\}$ occurs with probability $p_j \geq 0$ and $\sum_{j=0}^{N-1} p_j = 1$. We can represent this ensemble as a density matrix on $\log N$ qubits:

$$\rho = \sum_{j=0}^{N-1} p_j |j\rangle\langle j| = \begin{pmatrix} p_0 & & & \\ & p_1 & & \\ & & \ddots & \\ & & & p_{N-1} \end{pmatrix}.$$

  Therefore, a classical distribution is a special case of a *diagonal* density matrix.

3 Density matrices on multiple systems

The density matrix formalism also naturally extends to multiple quantum systems (or, multiple Hilbert spaces). For example, suppose we consider the single-qubit Bell pair

$$|\Phi^+\rangle_{AB} \;=\; \frac{1}{\sqrt{2}}(|0\rangle_A |0\rangle_B + |1\rangle_A |1\rangle_B).$$

The corresponding two-qubit density matrix is given by

$$\rho_{AB} = |\phi^+\rangle\langle\phi^+|_{AB} = \frac{1}{2}(|00\rangle\langle 00| + |00\rangle\langle 11| + |11\rangle\langle 00| + |11\rangle\langle 11|).$$

Note that the density matrix ρ_{AB} describes the global (or joint) quantum state on both systems. We will now see the full power of the density matrix formalism: we can calculate *reduced states* which describe the *local* state, say from either Alice's or Bob's perspective. Crucially, either of the two parties only has access to a single sub-system of the global state; this induces *statistical uncertainty* with respect to the additional system which is outside their view.

Reduced density matrices and the partial trace

Suppose $\rho_{AB} \in \mathcal{D}(\mathcal{H}_A \otimes \mathcal{H}_B)$ is a density matrix on two systems A and B, where $d_A = \dim(\mathcal{H}_A)$ and $d_B = \dim(\mathcal{H}_B)$. Let $\{|b_i\rangle\}_{i=1}^{d_B}$ be any orthonormal basis of $\mathcal{H}_B$. Then, the *reduced state* on system A when *discarding* system B is given by the density matrix

$$\rho_A = \mathrm{Tr}_B\left[\rho_{AB}\right]$$

where $\mathrm{Tr}_B : \mathcal{L}(\mathcal{H}_A \otimes \mathcal{H}_B) \to \mathcal{L}(\mathcal{H}_A)$ is the so-called *partial trace* map given by

$$\mathrm{Tr}_B\left[\rho_{AB}\right] = \sum_{i=1}^{d_B} (I_A \otimes \langle b_i|_B)\, \rho_{AB}\, (I_A \otimes |b_i\rangle_B).$$

The partial trace has the following properties:

1. **Linearity (over $\mathbb{C}$):** For all linear operators $\rho_{AB}, \sigma_{AB} \in \mathcal{L}(\mathcal{H}_A \otimes \mathcal{H}_B)$ and $\alpha, \beta \in \mathbb{C}$,

$$\mathrm{Tr}_B[\alpha\rho_{AB} + \beta\sigma_{AB}] = \alpha\ \mathrm{Tr}_B[\rho_{AB}] + \beta\ \mathrm{Tr}_B[\sigma_{AB}].$$

2. **Tensor products:** If $\rho_{AB} \in \mathcal{L}(\mathcal{H}_A \otimes \mathcal{H}_B)$ is a product state $\rho_{AB} = \rho_A^{(1)} \otimes \rho_B^{(2)}$, then

$$\mathrm{Tr}_B[\rho_{AB}] = \rho_A^{(1)} \cdot \mathrm{Tr}[\rho_B^{(2)}].$$

To get some familiarity with the partial trace, let us consider the following example.

Reduced state of the Bell pair. Consider the density operator for the Bell state

$$|\phi^+\rangle\langle\phi^+|_{AB} = \frac{1}{2}(|00\rangle\langle 00| + |00\rangle\langle 11| + |11\rangle\langle 00| + |11\rangle\langle 11|).$$

To compute the reduced state $\rho_A = \mathrm{Tr}_B[|\phi^+\rangle\langle\phi^+|_{AB}]$, we can simply use the properties of the partial trace.

$$\begin{aligned}
\rho_A &= \mathrm{Tr}_B[|\phi^+\rangle\langle\phi^+|_{AB}] \\
&= \frac{1}{2}\mathrm{Tr}_B\big[|00\rangle\langle 00| + |00\rangle\langle 11| + |11\rangle\langle 00| + |11\rangle\langle 11|\big] \\
&= \frac{1}{2}\left(\mathrm{Tr}_B\big[|00\rangle\langle 00|\big] + \mathrm{Tr}_B\big[\,|00\rangle\langle 11|\,\big] + \mathrm{Tr}_B\big[\,|11\rangle\langle 00|\,\big] + \mathrm{Tr}_B\big[|11\rangle\langle 11|\big]\right) \\
&= \frac{1}{2}\big(\mathrm{Tr}_B\big[|0\rangle\langle 0|_A \otimes |0\rangle\langle 0|_B\big] + \mathrm{Tr}_B\big[\,|0\rangle\langle 1|_A \otimes |0\rangle\langle 1|_B\,\big] \\
&\qquad + \mathrm{Tr}_B\big[\,|1\rangle\langle 0|_A \otimes |1\rangle\langle 0|_B\,\big] + \mathrm{Tr}_B\big[|1\rangle\langle 1|_A \otimes |1\rangle\langle 1|_B\big]\big) \\
&= \frac{1}{2}\big(|0\rangle\langle 0|_A \cdot \mathrm{Tr}\big[|0\rangle\langle 0|_B\big] + |0\rangle\langle 1|_A \cdot \underbrace{\mathrm{Tr}\big[\,|0\rangle\langle 1|_B\,\big]}_{=0} + |1\rangle\langle 0|_A \cdot \underbrace{\mathrm{Tr}\big[\,|1\rangle\langle 0|_B\,\big]}_{=0} + |1\rangle\langle 1|_A \cdot \mathrm{Tr}\big[|1\rangle\langle 1|_B\big]\big) \\
&= \frac{1}{2}|0\rangle\langle 0|_A + \frac{1}{2}|1\rangle\langle 1|_A \;=\; \frac{I_A}{2}.
\end{aligned}$$

Thus the reduced state on system A is the *maximally mixed state*. Even though the joint state ρ_{AB} is pure, subsystem A alone is fully mixed due to its entanglement with B.