Density Matrices and Mixed States

Quantum Foundations · Module 5 — Decoherence

Node 5.1

Position in Knowledge Graph

System: Quantum Foundations **Structural Domain:** Decoherence **Node:** 5.1

The state postulate (Node 2.1) identified quantum states with rays in Hilbert space — pure states. This node generalizes the state concept to **mixed states**: statistical ensembles of pure states. The mathematical object is the **density matrix**, and it is the right state object whenever the system is open, noisy, partially traced out, or simply uncertain.

Density matrices are the most important object in this course after the Hilbert space itself. Modules 5–9 all live on density matrices.

Formal Definition

A **density operator** (or **density matrix**) on a Hilbert space $\mathcal{H}$ is an operator $\rho : \mathcal{H} \to \mathcal{H}$ satisfying:

1. **Hermiticity:** $\rho = \rho^\dagger$.
2. **Positivity:** $\langle\psi|\rho|\psi\rangle \geq 0$ for all $|\psi\rangle \in \mathcal{H}$.
3. **Unit trace:** $\mathrm{tr}(\rho) = 1$.

A density operator is **pure** if $\mathrm{tr}(\rho^2) = 1$, and **mixed** otherwise.

For a pure state $|\psi\rangle$, the corresponding density operator is the projector

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

For a statistical ensemble $\{(p_k, |\psi_k\rangle)\}$ with $p_k \geq 0$ and $\sum_k p_k = 1$, the density operator is the convex combination

$$\rho = \sum_k p_k \, |\psi_k\rangle\langle\psi_k|.$$

The set of density operators is closed and convex; the extreme points are the pure states.

Born Rule for Density Matrices

For an observable A and density matrix ρ, the expectation value is

$$\langle A\rangle_\rho = \mathrm{tr}(\rho A).$$

For a projective measurement $\{P_i\}$, the probability of outcome i is

$$p(i) = \mathrm{tr}(\rho P_i),$$

and the post-measurement state, conditional on outcome i, is

$$\rho' = \frac{P_i\,\rho\,P_i}{\mathrm{tr}(\rho P_i)}.$$

Both of these reduce to the pure-state Born rule (Node 2.3) when $\rho = |\psi\rangle\langle\psi|$.

Intuition

A density matrix is the most general quantum state. It encodes:

- **Quantum uncertainty** (intrinsic to a pure state — non-zero variance of incompatible observables).
- **Classical uncertainty** (about which pure state the system is actually in).

The two are conceptually distinct but the formalism does not separate them. This is the structural reason that density matrices have multiple ensemble decompositions: many different convex combinations $\{(p_k, |\psi_k\rangle)\}$ can give the same ρ.

The textbook example: the maximally mixed qubit state

$$\rho = \frac{I}{2} = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1| = \frac{1}{2}|+\rangle\langle +| + \frac{1}{2}|-\rangle\langle -|$$

— two completely different "ensembles," same density matrix, identical predictions for every measurement.

Structural Role

Density matrices are required wherever the pure-state formalism breaks down:

- **Subsystems of entangled states** (Node 5.2): tracing out part of an entangled pure state gives a mixed reduced state.
- **Open systems** (Module 8): system-environment coupling drives pure states to mixed states.
- **Noisy quantum hardware** (relevant to VQA): real circuits do not produce pure outputs.
- **Measurement statistics**: pre-readout, the system is described by a density matrix conditional on the previous measurement record.
- **Quantum information**: channels (Module 7) act on density matrices, not on rays.

The density matrix is also the right object for **quantum statistical mechanics**: the Gibbs state $\rho = e^{-\beta H}/Z$ is a density matrix (Node 9.1), and quantum thermodynamics builds entirely on this.

Mathematical Development

Bloch ball representation (qubit)

Every 2×2 density matrix can be written

$$\rho = \frac{1}{2}(I + \vec{r} \cdot \vec{\sigma})$$

where $\vec{r} \in \mathbb{R}^3$ with $\|\vec{r}\| \leq 1$, and $\vec{\sigma} = (X, Y, Z)$ is the vector of Pauli matrices.

- $\|\vec{r}\| = 1$: pure state, on the Bloch sphere.
- $\|\vec{r}\| < 1$: mixed state, in the interior of the Bloch ball.
- $\vec{r} = 0$: maximally mixed state $I/2$, at the center.

The pure-state postulate (Node 2.1) maps states to the *surface* of the ball; the density-matrix generalization fills in the interior.

Purity

The **purity** of ρ is

$$\gamma(\rho) = \mathrm{tr}(\rho^2) \in [1/d, 1],$$

where $d = \dim \mathcal{H}$. It equals 1 for pure states and $1/d$ for the maximally mixed state.

Worked Example

Mixture of $|0\rangle$ and $|1\rangle$ versus $|+\rangle$

Consider two preparations:

1. With probability 1/2, the qubit is in $|0\rangle$; with probability 1/2, it is in $|1\rangle$. Density matrix: $\rho_1 = I/2$.
2. The qubit is definitely in $|+\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$. Density matrix: $\rho_2 = |+\rangle\langle+|$.

These are *very* different states. Measuring X on ρ_1 gives outcome ± 1 with equal probability; measuring X on ρ_2 gives $+1$ with certainty.

The lesson: a mixed state and a pure superposition look similar in computational-basis measurements but diverge sharply when measured in other bases. The density matrix captures this correctly.

Cross-Links

- **Linear Algebra:** Hermitian, positive semidefinite operators with unit trace.
- **Statistics:** Density matrices generalize probability distributions; the diagonal of ρ in any basis is a classical distribution over that basis.
- **Quantum Information:** All channels and entropies are defined on density matrices.
- **VQA:** Cost functions $\langle H \rangle = \mathrm{tr}(\rho H)$ on noisy circuits use this trace formula.
- **Statistics $\to$ Bayesian inference:** The density matrix is to a quantum state what the posterior is to a Bayesian belief — a complete summary of "what we know."

Structural Compression

Invariant: A density operator is positive, Hermitian, and unit-trace; the set of density operators is convex with pure states as extreme points.

Mechanism: Convex hull of $\{|\psi\rangle\langle\psi| : |\psi\rangle \in \mathcal{H}, \||\psi\rangle\| = 1\}$.

Cross-System Echo: Probability simplices in classical statistics are also convex with pure (delta) measures as extreme points. The density operator is the non-commutative generalization. Both are the most general state objects in their respective theories.

Exercises

1. Show that for any density matrix ρ, $\mathrm{tr}(\rho^2) \leq 1$, with equality iff ρ is pure.
2. Verify that $\rho = \frac{1}{2}|+\rangle\langle+| + \frac{1}{2}|-\rangle\langle-| = I/2$.
3. Show that the Bloch ball parameterization $\rho = \frac{1}{2}(I + \vec{r} \cdot \vec{\sigma})$ is positive iff $\|\vec{r}\| \leq 1$.
4. Compute the purity of $\rho = p|0\rangle\langle 0| + (1-p)|+\rangle\langle+|$ as a function of p. For what p is it most mixed?
5. Construct two distinct ensembles $\{(p_k, |\psi_k\rangle)\}$ and $\{(q_l, |\phi_l\rangle)\}$ that produce the same density matrix ρ, and verify they make identical predictions for every observable.

Quantum Foundations · Module 5 — Decoherence · Node 5.1
Concepts: density-matrix, expectation-value, probability-space
Prerequisites: 2.1, 2.3, 1.5
Enables: 5.2, 5.3, 7.1

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