# The Density Operator

Suppose a quantum system is in state $|\psi_i\rangle$ with probability $p_i$, we call $\{p_i, |\psi_i\rangle\}$ an **ensemble of quantum states**. The **density operator** (or **density matrix**) for the system is defined as

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

The evolution of the density matrix (of a closed system) described by unitary operator $\mathbf{U}$ is

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

After measurement described by $\mathbf{M}_m$, outcome $m$ occurs with probability

$$\begin{aligned} p(m) &= \sum_i p_i p(m|i) \\ &= \sum_i p_i \langle\psi_i|\mathbf{M}_m^\dagger \mathbf{M}_m|\psi_i\rangle \\ &= \sum_i p_i \mathrm{tr}\left(\mathbf{M}_m^\dagger \mathbf{M}_m |\psi_i\rangle\langle\psi_i|\right) \\ &= \mathrm{tr}\left(\mathbf{M}_m^\dagger \mathbf{M}_m \rho\right). \end{aligned}$$

while the new state (density operator) in this case is

$$
\begin{aligned}
\rho' &= \sum_i p(i|m) \frac{\mathbf{M}_m |\psi_i\rangle\langle\psi_i| \mathbf{M}_m^\dagger}{\mathrm{tr}\left(\mathbf{M}_m^\dagger \mathbf{M}_m |\psi_i\rangle\langle\psi_i|\right)} \\
&= \sum_i \frac{p(m|i) p_i}{p(m)} \frac{\mathbf{M}_m |\psi_i\rangle\langle\psi_i| \mathbf{M}_m^\dagger}{\mathrm{tr}\left(\mathbf{M}_m^\dagger \mathbf{M}_m |\psi_i\rangle\langle\psi_i|\right)} \\
&= \sum_i p_i \frac{\mathbf{M}_m |\psi_i\rangle\langle\psi_i| \mathbf{M}_m^\dagger}{\mathrm{tr}\left(\mathbf{M}_m^\dagger \mathbf{M}_m \rho\right)} \\
&= \frac{\mathbf{M}_m \rho \mathbf{M}_m^\dagger}{\mathrm{tr}\left(\mathbf{M}_m^\dagger \mathbf{M}_m \rho\right)}
\end{aligned}
$$

# Pure and Mixed States

States described by a state vector $|\psi\rangle$ are called **pure states**. Pure state density matrices have the form $\rho = |\psi\rangle\langle\psi|$, density matrices not expressable in this form is in a **mixed state**. For example, the density matrix $\rho = |0\rangle\langle 0| + |1\rangle\langle 1|$ for a qubit is in a mixed state.

The density operator represents a pure state if and only if $\mathrm{tr}\left(\rho^2\right) = 1$.

A density operator can also be formed from an ensemble of density operators $\{p_i, \rho_i\}$, each of which arises from some ensemble $\{p_{ij}, |\psi_{ij}\rangle\}$, so that each $|\psi_{ij}\rangle$ has probability $p_i p_{ij}$,

$$\rho = \sum_{ij} p_i p_{ij} |\psi_{ij}\rangle\langle\psi_{ij}| = \sum_i p_i \rho_i.$$

We can say that the density matrix $\rho$ is a mixture of density matrices $\rho_i$, each of which is a mixture of quantum states $|\psi_{ij}\rangle$.

# General Properties of the Density Operator

An operator $\rho$ is a density operator for some ensemble $\{p_i, |\psi_i\rangle\}$ if and only if

1. $\rho$ is self-adjoint.

2. $\text{tr}\,(\rho) = 1$.

3. $\rho$ is positive.

# The Postulates Restated With Density Operators

**Postulate 1** The state of a physical system is described by a density operator (a positive operator with unit trace) on its state space (a Hilbert space). A system with probability $p_i$ of being in the state $\rho_i$ has density operator $\rho = \sum_i p_i \rho_i$.

**Postulate 2** The evolution of a physical system is unitary:

$$\rho' = \mathbf{U}\rho\mathbf{U}^\dagger.$$

**Postulate 3** Quantum measurements are described by operators $\{\mathbf{M}_m\}$. If the state of the measured system is $\rho$ then result $m$ occurs with probability

$$p(m) = \mathrm{tr}\left(\mathbf{M}_m^\dagger \mathbf{M}_m \rho\right),$$

and the new state is

$$\frac{\mathbf{M}_m^\dagger \rho \mathbf{M}_m}{\text{tr}\left(\mathbf{M}_m^\dagger \mathbf{M}_m \rho\right)}.$$

**Postulate 4** The state of the composite system of systems 1 through $n$ is the density operator

$$\rho_1 \otimes \rho_2 \otimes \ldots \otimes \rho_n = \bigotimes_{i=1}^{n} \rho_i$$

acting on

$$\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \ldots \otimes \mathcal{H}_n = \bigotimes_{i=1}^{n} \mathcal{H}_i.$$

# Density Operators in the Bloch "Ball"

For the Bloch sphere state

$$\hat{n} = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$$

(spinup in the $(\theta, \varphi)$ direction), the density matrix is

$$\begin{aligned}
\rho(\hat{n}) &= |\hat{n}\rangle\langle\hat{n}| \\
&= \begin{pmatrix} \cos\frac{\theta}{2} \\ e^{i\varphi}\sin\frac{\theta}{2} \end{pmatrix} \begin{pmatrix} \cos\frac{\theta}{2} & e^{-i\varphi}\sin\frac{\theta}{2} \end{pmatrix} \\
&= \begin{pmatrix} \cos^2\frac{\theta}{2} & e^{-i\varphi}\sin\frac{\theta}{2}\cos\frac{\theta}{2} \\ e^{i\varphi}\sin\frac{\theta}{2}\cos\frac{\theta}{2} & \sin^2\frac{\theta}{2} \end{pmatrix} \\
&= \frac{1}{2}\mathbf{1} + \frac{1}{2}\begin{pmatrix} \cos\theta & e^{-i\varphi}\sin\theta \\ e^{i\varphi}\sin\theta & -\cos\theta \end{pmatrix} \\
&= \frac{1}{2}\mathbf{1} + \frac{1}{2}\Bigg(\sin\theta\cos\varphi\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\
&\qquad + \sin\theta\sin\varphi\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + \cos\theta\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\Bigg) \\
&= \frac{1}{2}(\mathbf{1} + n_1\sigma_1 + n_2\sigma_2 + n_3\sigma_3) \\
&= \frac{1}{2}(\mathbf{1} + \hat{n}\cdot\vec{\sigma})
\end{aligned}$$

The density matrix for the pure state $|\psi(\theta,\varphi)\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\varphi}\sin\frac{\theta}{2}|1\rangle$ is

$$\rho(\vec{n}) = \frac{1}{2}(\mathbf{1} + \vec{n}\cdot\vec{\sigma}).$$

Since density operators are positive,

$$\det\rho = \frac{1}{4}(1 - \vec{n}^2) \geq 0,$$

So $\vec{n}^2 \leq 0$ are all valid states. For density matrices, the Bloch sphere becomes a "ball".

The density operator is pure if and only if its Bloch "ball" representation is a unit vector.

# Ambiguity of the Ensemble Representation

For two ensembles of pure states $\{p_i, |\psi_i\rangle\}$ and $\{q_j, |\varphi_j\rangle\}$ if

$$\sqrt{p_i}|\psi_i\rangle = \sum_j u_{ij}\sqrt{q_j}|\varphi_j\rangle$$

for some unitary matrix $u_{ij}$, then

$$\rho = \sum_i p_i|\psi_i\rangle\langle\psi_i| = \sum_j q_j|\varphi_j\rangle\langle\varphi_j|.$$

A vector inside the Bloch "ball" can be written as the sum of unit vectors in infinite ways. A density operator can also be formed by the convex sum of other density operators:

$$\rho = \lambda_1\rho_1 + \lambda_2\rho_2,$$

where $0 \leq \lambda_1, \lambda_2 \leq 1$ and $\lambda_1 + \lambda_2 = 1$; $\rho$ is a density operator if both $\rho_1$ and $\rho_2$ are.