# Lecture 10
# The Density Operator

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# Table of Contents

# Pure and Mixed Ensembles in QM

- So far, our discussion of QM has dealt with describing particles in a definite quantum state. If we are given a collection, or ensemble of such particles, then we can describe all members of the ensemble with a common state vector.
- However there are instances where the ensemble is described by a collection of particles in different quantum states. For such ensembles, there is no one state vector that describes the ensemble, therefore we need to expand our formalism to deal with such ensembles.
- If you recall, we said that the atoms exiting the oven in the S-G experiment where unpolarized, that is if we sent the beam of particles into a S-G analyzer, we would measure a 50%/50% distribution of spin-up and spin-down particles regardless of the direction in which we oriented the S-G analyzer.
- If we place a S-G analyzer in front of the beam exiting the oven, say along the $z-$direction, then the state of the particles exiting the analyzer is either spin-up ($|+\rangle$) or spin-down ($|-\rangle$). We refer to ensembles in which all members of the ensemble have a definite polarization as pure ensembles.

# Pure and Mixed Ensembles in QM

- In a pure ensemble, all members of the ensemble have a common state vector

$$|\psi\rangle = \sum_n c_n |a_n\rangle$$

- Note, with the appropriate unitary transformation, we can always transform to a basis in which the state $|\psi\rangle$ may be expressed in terms of a single ket $|\psi\rangle = |b_n\rangle$ in some other complete basis $\{|b\rangle\}$.
- In contrast to pure ensembles, there is no single ket that describes the state of a particles coming out of the oven in the S-G experiment. Such unpolarized states are described as a statistical admixtures of pure ensembles.
- How do we operationally distinguish mixed ensembles from pure ones?
- Imagine we are given a beam of particles of an unknown polarization, and we are asked to identify whether they belong to mixed of pure ensembles. How would we figure this out?
- We have a S-G analyzer with which we can measure the state of the particles along any direction in space.
- Suppose we orient the analyzer in the $x-$direction and we find a $50\%/50\%$ distribution of spin-up and spin-down particles. This is certainly consistent with having an unpolarized distribution, however the particles can also be in either the $|\pm\rangle$ state, for example and produce the same distribution.

# Pure and Mixed Ensembles in QM

- To identify whether the particles belong to a pure or mixed ensemble, we need to rotate the S-G analyzer over all angles in space. If we find that the there is a direction in which we only get spin-up or spin-down, then the particles belong to a pure ensemble. However, if we find that we get a $50\%/50\%$ distribution regardless of the angle, then the particles belong to a mixed ensemble.
- To be clear, a completely unploarized ensemble is referred to as being fully mixed. In reality, we rarely deal with systems that are fully mixed or completely pure. In real-world experiments, we are usually dealing with ensembles that are a mixture of the two.
- Now that we motivated pure and mixed ensembles, let's provide some definitions:
- Pure Ensembles: All members of the ensemble are represented by a single quantum state vector.
- Mixed Ensembles: Members of the ensemble are represented by a statistical admixture of states.

# The Density Operator

- A systematic way of working with both types of ensembles is by introducing the density operator $\hat{\rho}$.
- For the state $|\psi\rangle = \sum_n c_n |n\rangle$, consider the probability of measuring the state $|m\rangle$.

$$
\begin{aligned}
P_m &= |\langle m|\psi\rangle|^2 \\
&= \langle m|\psi\rangle \langle m|\psi\rangle^* = \langle m| \underbrace{|\psi\rangle\langle\psi|}_{\hat{\rho}} |m\rangle
\end{aligned}
$$

- We define the density operator corresponding to a state $|\psi\rangle$ as $\hat{\rho} := |\psi\rangle\langle\psi|$.
- For a pure state, the density operator is equivalent to the projection operator.
- $\hat{\rho}$ is a Hermitian operator.

$$
\begin{aligned}
\hat{\rho}_{ij} &= \langle i|\hat{\rho}|j\rangle = \langle i|\psi\rangle \langle\psi|j\rangle \\
\hat{\rho}^*_{ji} &= (\langle j|\hat{\rho}|i\rangle)^* = (\langle j|\psi\rangle \langle\psi|i\rangle)^* \\
&= \langle j|\psi\rangle^* \langle\psi|i\rangle^* = \langle\psi|i\rangle \langle j|\psi\rangle = \langle i|\psi\rangle \langle\psi|j\rangle = \hat{\rho}_{ij} \\
\hat{\rho}_{ij} &= \hat{\rho}^*_{ji} \quad \Rightarrow \quad \boxed{\hat{\rho} = \hat{\rho}^\dagger}
\end{aligned}
$$

- Recall from linear algebra that the trace of a matrix is the sum of its diagonal elements, and the trace is independent of the choice of basis we choose to represent the matrix.

$$\mathrm{Tr}\{A\} := \sum_i A_{ii}$$

- Statement 1: The trace of the density operator for a pure ensemble is equal to 1 for any complete basis representation.
- Proof: Let $|\psi\rangle$ have normalization $\langle\psi|\psi\rangle = 1$, and $\hat{\rho} = |\psi\rangle\langle\psi|$

$$\mathrm{Tr}\{\hat{\rho}\} = \sum_i \hat{\rho}_{ii} = \sum_i \langle i|\psi\rangle \langle\psi|i\rangle = \sum_i \langle\psi|i\rangle \langle i|\psi\rangle$$

$$\sum_i |i\rangle\langle i| = \mathbb{1} \quad \text{Completeness}$$

$$\therefore \quad \mathrm{Tr}\{\hat{\rho}\} = \langle\psi|\mathbb{1}|\psi\rangle = \langle\psi|\psi\rangle = 1$$

- We will see shortly that $\mathrm{Tr}\{\hat{\rho}\} = 1$ for pure and mixed ensembles.
- Statement 2: $\hat{\rho}^2 = \hat{\rho}$ for pure ensemble.
- Proof:

$$\hat{\rho}^2 = (|\psi\rangle\langle\psi|)(|\psi\rangle\langle\psi|) = |\psi\rangle \underbrace{\langle\psi|\psi\rangle}_{1} \langle\psi| = |\psi\rangle\langle\psi| = \hat{\rho}$$

$$\therefore \quad \mathrm{Tr}\left\{\hat{\rho}^2\right\} = 1 \quad \text{for pure ensembles.}$$

- Statement 3: Given a state $|\psi\rangle$, the probability of measuring the state $|\phi\rangle$ is

$$\text{Prob.} = |\langle\phi|\psi\rangle|^2 = \mathrm{Tr}\left\{\hat{P}_\phi\,\hat{\rho}\right\}$$

where $\hat{P}_\phi = |\phi\rangle\langle\phi|$ is the projection operator for the state $|\phi\rangle$.

- Proof:

$$\mathrm{Tr}\left\{\hat{P}_\phi\,\hat{\rho}\right\} = \sum_i \langle i|\phi\rangle\,\langle\phi|\psi\rangle\,\langle\psi|i\rangle$$
$$= \langle\phi|\psi\rangle \sum_i \langle\psi|i\rangle\,\langle i|\phi\rangle$$
$$= \langle\phi|\psi\rangle\,\langle\psi|\phi\rangle = |\langle\phi|\psi\rangle|^2$$

- Statement 4: The expectation value of operator $\hat{A}$ for the state $|\psi\rangle$ is

$$\langle\psi|\hat{A}|\psi\rangle = \mathrm{Tr}\left\{\hat{A}\,\hat{\rho}\right\}$$

- Proof:

$$\langle\psi|\hat{A}|\psi\rangle = \sum_i \langle\psi|i\rangle\;\langle i|\hat{A}|\psi\rangle \quad \text{using } \sum_i |i\rangle\langle i| = \mathbb{1}$$
$$= \sum_i \langle i|\hat{A}|\psi\rangle\,\langle\psi|i\rangle$$
$$= \sum_i \langle i|\hat{A}\,\hat{\rho}|i\rangle = \mathrm{Tr}\left\{\hat{A}\,\hat{\rho}\right\}$$

# Example 1

- Example 1: Use the density matrix formalism to calculate $\langle S_z \rangle$ and $\langle S_y \rangle$ for the states $|\pm\rangle$.

$$\hat{\rho}_+ = |+\rangle\langle +| = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

$$\langle +|S_z|+\rangle = \mathrm{Tr}\{S_z\, \hat{\rho}_+\} = \mathrm{Tr}\left\{ \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \right\} = \mathrm{Tr}\left\{ \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \right\}$$

$$\langle +|S_z|+\rangle = \frac{\hbar}{2}$$

$$\hat{\rho}_- = |-\rangle\langle -| = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\langle -|S_z|-\rangle = \mathrm{Tr}\{S_z\, \hat{\rho}_-\} = \mathrm{Tr}\left\{ \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \right\} = \mathrm{Tr}\left\{ \frac{\hbar}{2} \begin{pmatrix} 0 & 0 \\ 0 & -1 \end{pmatrix} \right\}$$

$$\langle -|S_z|-\rangle = -\frac{\hbar}{2}$$

# Example 1

$$\langle +|S_y|+\rangle = \mathrm{Tr}\{S_y\,\hat{\rho}_+\} = \mathrm{Tr}\left\{\frac{\hbar}{2}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & 0\end{pmatrix}\right\} = \mathrm{Tr}\left\{\frac{\hbar}{2}\begin{pmatrix}0 & 0\\ i & 0\end{pmatrix}\right\}$$

$$\langle +|S_y|+\rangle = 0$$

$$\langle -|S_y|-\rangle = \mathrm{Tr}\{S_y\,\hat{\rho}_-\} = \mathrm{Tr}\left\{\frac{\hbar}{2}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}\begin{pmatrix}0 & 0\\ 0 & 1\end{pmatrix}\right\} = \mathrm{Tr}\left\{\frac{\hbar}{2}\begin{pmatrix}0 & -i\\ 0 & 0\end{pmatrix}\right\}$$

$$\langle -|S_y|-\rangle = 0$$

- Note: When calculating $\mathrm{Tr}\left\{\hat{A}\,\hat{\rho}\right\}$, both $\hat{A}$ and $\hat{\rho}$ must be represented in the same basis.
- Home exercise: Calculate $\langle +y|S_y|+y\rangle$ using the density operator $\hat{\rho} = |+y\rangle\langle +y|$ in the $S_z$ basis.

# The Density Operator for Mixed Ensembles

- While density operators can be used to calculate expectation values for pure ensembles, they are especially useful for calculating mixed ensembles.
- For a mixed ensemble

$$\hat{\rho} = \sum_k P_k \left|\psi_k\right\rangle\!\left\langle\psi_k\right|$$

where $P_k$ is the probability that a member of the ensemble is in the state $|\psi_k\rangle$.

$$\sum_k P_k = 1$$

$$\hat{\rho}_{ij} = \sum_k P_k \langle i|\psi_k\rangle \langle\psi_k|j\rangle$$

$$\mathrm{Tr}\{\hat{\rho}\} = \sum_i \hat{\rho}_{ii} = \sum_i \sum_k P_k \langle i|\psi_k\rangle \langle\psi_k|i\rangle$$

$$= \sum_k P_k \sum_i \langle \psi_k | i \rangle \langle i | \psi_k \rangle$$

$$= \sum_k P_k \underbrace{\langle \psi_k | \psi_k \rangle}_{1} = \sum_k P_k = 1$$

- Statement 5: For mixed ensembles $\mathrm{Tr}\{\hat{\rho}^2\} < 1$
- Proof:

$$\mathrm{Tr}\{\hat{\rho}^2\} = \sum_i \sum_k \sum_l P_k P_l \langle i | \psi_k \rangle \langle \psi_k | \psi_l \rangle \langle \psi_l | i \rangle$$

$$= \sum_k \sum_l P_k P_l \langle \psi_k | \psi_l \rangle \underbrace{\sum_i \langle \psi_l | i \rangle \langle i | \psi_k \rangle}_{\langle \psi_k | \psi_l \rangle^*}$$

$$= \sum_k \sum_l P_k P_l |\langle \psi_k | \psi_l \rangle|^2$$

# The Density Operator for Mixed Ensembles

- From the Cauchy-Schwarz inequality, we know

$$\underbrace{\langle\psi_k|\psi_k\rangle}_{1}\underbrace{\langle\psi_l|\psi_l\rangle}_{1} \geq |\langle\psi_k|\psi_l\rangle|^2$$

$$|\langle\psi_k|\psi_l\rangle|^2 \leq 1$$

$$\therefore \quad \sum_k \sum_l P_k P_l |\langle\psi_k|\psi_l\rangle|^2 \leq 1$$

$$\mathrm{Tr}\left\{\hat{\rho}^2\right\} \leq 1$$

- This is an important distinguishing feature of mixed ensembles. Given a density matrix, we can determine if it corresponds to pure ensemble by calculating $\mathrm{Tr}\left\{\hat{\rho}^2\right\}$.

Pure Ensembles: $\mathrm{Tr}\left\{\hat{\rho}^2\right\} = 1$

Mixed Ensembles: $\mathrm{Tr}\left\{\hat{\rho}^2\right\} < 1$

# Example 2

- Example 2: Consider the density operator $\hat{\rho} = \frac{1}{2}\,|+\rangle\langle+| + \frac{1}{2}\,|-\rangle\langle-|$.
- Show that this density operator corresponds to a mixed ensemble.

$$\hat{\rho} = \tfrac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \tfrac{1}{2}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = \tfrac{1}{2}\mathbb{1}$$

$$\hat{\rho}^2 = \tfrac{1}{4}\mathbb{1}$$

$$\mathrm{Tr}\left\{\hat{\rho}^2\right\} = \tfrac{1}{4} + \tfrac{1}{4} = \tfrac{1}{2} < 1$$

- Show that the density operator corresponds to a *maximally* mixed ensemble.
- We think of a maximally mixed ensemble as one in which there is no preferred polarization. Therefore, if we orient the S-G analyzer along any direction in space, we will always get a $50\%/50\%$ distribution.

# Example 2

- To see if the ensemble described by $\hat{\rho}$ is fully mixed, we calculate the expectation value of the angular momentum operator in the $\hat{\mathbf{n}}-$direction.

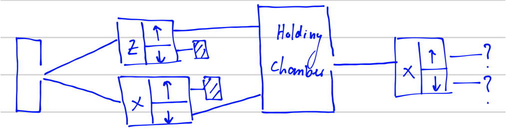
$$S_n = \frac{\hbar}{2}\begin{pmatrix} \cos\theta & \sin\theta e^{-i\phi} \\ \sin\theta e^{i\phi} & -\cos\theta \end{pmatrix}$$

$$\langle S_n \rangle = \mathrm{Tr}\{S_n\,\hat{\rho}\} = \mathrm{Tr}\left\{\frac{\hbar}{2}\begin{pmatrix} \cos\theta & \sin\theta e^{-i\phi} \\ \sin\theta e^{i\phi} & -\cos\theta \end{pmatrix}\frac{1}{2}\mathbb{1}\right\} = 0$$

- We see that $\langle S_n \rangle = 0$ for any direction, therefore the spin state is completely unpolarized, or maximally mixed.

# Example 3

- Consider the density operator $\hat{\rho} = \frac{1}{2}|+\rangle\langle+| + \frac{1}{2}|-x\rangle\langle-x|$.
- Conceptually, we can think of composing an ensemble of spins that corresponds to $\hat{\rho}$ by constructing a holding chamber that collects the output of two S-G analyzers, as shown in the figure below.




- The holding chamber creates an equal mix of particles in the $|+\rangle$ and $|-\rangle_x$ states, i.e., if you reach into the holding chamber and grab a particle, you are equally likely to get a spin in the $|+\rangle$ or $|-\rangle_x$ state.
- Show that this density operator corresponds to a mixed ensemble.

$$\hat{\rho} = \frac{1}{2}\begin{pmatrix}1\\0\end{pmatrix}\begin{pmatrix}1 & 0\end{pmatrix} + \frac{1}{4}\begin{pmatrix}1\\-1\end{pmatrix}\begin{pmatrix}1 & -1\end{pmatrix} = \frac{1}{2}\begin{pmatrix}1 & 0\\0 & 0\end{pmatrix} + \frac{1}{4}\begin{pmatrix}1 & -1\\-1 & 1\end{pmatrix}$$

# Example 3

$$\hat{\rho} = \begin{pmatrix} \frac{3}{4} & -\frac{1}{4} \\ -\frac{1}{4} & \frac{1}{4} \end{pmatrix}$$

- $\mathrm{Tr}\{\hat{\rho}\} = 1$
- Show $\mathrm{Tr}\left\{\hat{\rho}^2\right\} < 1$

$$\hat{\rho}^2 = \frac{1}{16}\begin{pmatrix} 3 & -1 \\ -1 & 1 \end{pmatrix}\begin{pmatrix} 3 & -1 \\ -1 & 1 \end{pmatrix} = \frac{1}{8}\begin{pmatrix} 5 & -2 \\ -2 & 1 \end{pmatrix}$$

$$\mathrm{Tr}\left\{\hat{\rho}^2\right\} = \tfrac{3}{4} < 1$$

- Calculate $\langle S_x \rangle$

$$\langle S_x \rangle = \mathrm{Tr}\{S_x\, \hat{\rho}\} = \mathrm{Tr}\left\{\frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\frac{1}{4}\begin{pmatrix} 3 & -1 \\ -1 & 1 \end{pmatrix}\right\} = -\frac{\hbar}{4}$$

# Example 3

- The expectation value $\langle S_x \rangle$ for the state $\hat{\rho}$ can be thought of as

$$\langle S_x \rangle = \underbrace{\text{Prob.}(|+\rangle)}_{\frac{1}{2}} \underbrace{\langle + | S_x | + \rangle}_{0} + \underbrace{\text{Prob.}(|-\rangle_x)}_{\frac{1}{2}} \underbrace{\langle -x | S_x | -x \rangle}_{-\frac{\hbar}{2}}$$

$$\therefore \quad \langle S_x \rangle = -\frac{\hbar}{4}$$

- Home exercise: If a measurement of $S_x$ is performed, what is the probability of obtaining $\frac{\hbar}{2}$ and $-\frac{\hbar}{2}$?