

# Density Operators in Quantum Physics

Podcast Learn & Fun \*

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The concept of the density operator is pivotal in describing quantum systems, especially when dealing with mixed states, statistical ensembles, and systems that cannot be fully described by pure state vectors alone.

In quantum physics, the state of a system can be described in two major ways: pure states and mixed states. *Pure states* correspond to quantum systems that are in a definite state, typically represented by a state vector,  $|\psi\rangle$ , in a Hilbert space. *Mixed states* are used to describe situations where we have a statistical ensemble of pure states, or the system is in a probabilistic combination of different states.

The density operator formalism provides a unified and convenient way to handle both pure and mixed states, making it especially useful in situations involving partial information, measurements, or systems interacting with environments.

## 1 Definition of a Density Operator

A *density operator* is a mathematical object that generalizes the state vector formalism to mixed states.

For a quantum system, the density operator  $\hat{\rho}$  is defined as a sum over pure states, weighted by their respective probabilities. The general definition is:

$$\hat{\rho} = \sum_i p_i |\psi_i\rangle \langle \psi_i|$$

where  $|\psi_i\rangle$  are the pure states (state vectors) that the system might be in and  $p_i$  are the probabilities that the system is in the state  $|\psi_i\rangle$ . The sum is over all possible pure states.

For pure states, the density operator has a simpler form. If the system is in a single pure state  $|\psi\rangle$ , the density operator is:

$$\hat{\rho} = |\psi\rangle \langle \psi|$$

Thus, for a pure state, the density operator is a rank-1 projection operator.

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## 2 Pure States

Let our system be described by a state vector  $|\psi\rangle$ , which can be written as:

$$|\psi\rangle = \sum_i c_i |u_i\rangle$$

where  $\{|u_i\rangle\}$  is an orthonormal basis for the Hilbert space, meaning that:

$$\langle u_i | u_j \rangle = \delta_{ij}$$

where  $\delta_{ij}$  is the *Kronecker delta* which equals 1 when  $i = j$  and 0 otherwise. The coefficients  $c_i$  are complex numbers, and they describe the expansion of the state  $|\psi\rangle$  in the basis  $\{|u_i\rangle\}$ .

The *density operator* for a pure quantum state  $|\psi\rangle$  is defined as:

$$\hat{\rho} = |\psi\rangle\langle\psi|$$

This is a projection operator onto the state  $|\psi\rangle$ . Now, we will calculate the matrix elements of the density operator in the  $\{|u_i\rangle\}$  basis:

$$\rho_{ij} = \langle u_i | \hat{\rho} | u_j \rangle = \langle u_i | \psi \rangle \langle \psi | u_j \rangle = c_i c_j^*$$

Thus, the components of the density operator in this basis are the complex conjugates of the coefficients  $c_i$  and  $c_j$ :

$$\hat{\rho} \rightarrow \begin{pmatrix} c_1 c_1^* & c_1 c_2^* & \cdots \\ c_2 c_1^* & c_2 c_2^* & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}$$

This matrix is *Hermitian* because  $c_i c_j^* = c_j c_i^*$ , as required for a valid quantum operator.

### Hermiticity

The density operator is *Hermitian*, meaning that:

$$\hat{\rho}^\dagger = \hat{\rho}$$

For the density operator  $\hat{\rho} = |\psi\rangle\langle\psi|$ , the adjoint is:

$$\hat{\rho}^\dagger = (|\psi\rangle\langle\psi|)^\dagger = |\psi\rangle\langle\psi| = \hat{\rho}$$

This confirms that  $\hat{\rho}$  is Hermitian.

### Idempotency

The density operator is *idempotent*, meaning that:

$$\hat{\rho}^2 = \hat{\rho}$$

To see this, we compute:

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

Since  $\langle\psi|\psi\rangle = 1$  for a pure state, idempotency holds.

### Positivity

The density operator is positive semi-definite. For any state vector  $|\phi\rangle$ :

$$\langle\phi|\hat{\rho}|\phi\rangle = \langle\phi|\psi\rangle\langle\psi|\phi\rangle = |\langle\psi|\phi\rangle|^2 \geq 0$$

This means that all its eigenvalues are non-negative. This condition ensures that the probabilities derived from the density operator are non-negative.

### No Global Phase Ambiguity

The density operator is *invariant under global phase changes*. If we multiply the state vector by a global phase factor  $|\psi'\rangle = e^{i\theta}|\psi\rangle$ , we will get:

$$\hat{\rho}' = |\psi'\rangle\langle\psi'| = e^{i\theta}|\psi\rangle\langle\psi|e^{-i\theta} = \hat{\rho}$$

This shows that multiplying the state by a global phase factor does not change the density operator.

### Normalization of the State and Density Operator

The normalization condition for a pure state is:

$$\langle\psi|\psi\rangle = 1$$

In terms of the coefficients  $c_i$ , this can be written as:

$$\langle\psi|\psi\rangle = \sum_i c_i^* c_i = \sum_i |c_i|^2 = 1$$

Similarly, the trace of the density operator must also be 1, since:

$$\text{Tr}(\hat{\rho}) = \sum_i \rho_{ii} = \sum_i |c_i|^2 = 1$$

Thus, the trace of the density operator for a pure state is always 1.

### Expectation Values

The expectation value of an observable  $\hat{A}$  in the state  $|\psi\rangle$  is given by:

$$\langle\hat{A}\rangle = \langle\psi|\hat{A}|\psi\rangle$$

Using the density operator, this can be written as:

$$\langle\hat{A}\rangle = \text{Tr}(\hat{\rho}\hat{A})$$

**Proof:** We expand  $\langle\hat{A}\rangle$  in terms of the basis states  $\{|u_i\rangle\}$ :

$$\langle\hat{A}\rangle = \sum_{i,j} c_i^* c_j \langle u_i|\hat{A}|u_j\rangle$$

Using the matrix formulation of quantum operators  $A_{ij} = \langle u_i | \hat{A} | u_j \rangle$ :

$$\langle \hat{A} \rangle = \sum_{i,j} c_i^* c_j A_{ij} = \text{Tr}(\hat{\rho} \hat{A})$$

The last step comes from the definition of matrix multiplication. This demonstrates that the expectation value can be written as the trace of the product of the density operator and the observable.

### Probability of Measurement Outcomes

The probability of obtaining a measurement outcome corresponding to an eigenvalue  $\lambda_n$  of an observable  $\hat{A}$  is given by:

$$P(\lambda_n) = \langle \psi | \hat{P}_n | \psi \rangle$$

where  $\hat{P}_n = |u_n\rangle\langle u_n|$  is the projection operator onto the eigenspace corresponding to  $|u_n\rangle$ . In terms of the density operator, this probability is:

$$P(\lambda_n) = \text{Tr}(\hat{\rho} \hat{P}_n)$$

**Proof:** The projection operator  $\hat{P}_n$  is given by:

$$\hat{P}_n = \sum_{i=1}^{g_n} |u_n^i\rangle\langle u_n^i|$$

where  $g_n$  is the degeneracy of the eigenvalue  $\lambda_n$ , and  $|u_n^i\rangle$  are the corresponding eigenstates of  $\hat{A}$ . Thus, the probability of measuring  $\lambda_n$  is:

$$P(\lambda_n) = \text{Tr}(\hat{\rho} \hat{P}_n)$$

### Time Evolution of the Density Operator

We consider the time evolution of a quantum system. The state vector evolves according to the Schrödinger equation:

$$\frac{d}{dt} |\psi(t)\rangle = \frac{1}{i\hbar} \hat{H}(t) |\psi(t)\rangle$$

The corresponding evolution of the density operator is:

$$\frac{d}{dt} \hat{\rho}(t) = \frac{d}{dt} (|\psi(t)\rangle\langle\psi(t)|)$$

Using the product rule, this becomes:

$$\frac{d}{dt} \hat{\rho}(t) = \frac{1}{i\hbar} \hat{H}(t) |\psi(t)\rangle\langle\psi(t)| - \frac{1}{i\hbar} |\psi(t)\rangle\langle\psi(t)| \hat{H}(t)$$

This simplifies to the commutator form:

$$\frac{d}{dt} \hat{\rho}(t) = \frac{1}{i\hbar} [\hat{H}(t), \hat{\rho}(t)]$$

Thus, the density operator evolves according to the commutator of the Hamiltonian with the density operator. This is known as the *Liouville-von Neumann equation*.

In the Schrödinger picture, the time evolution of a pure state  $|\psi(t)\rangle$  is governed by the time-dependent Schrödinger equation:

$$|\psi(t)\rangle = e^{-i\hat{H}t/\hbar}|\psi(0)\rangle$$

For a density operator, the time evolution is given by:

$$\rho(t) = e^{-\frac{i}{\hbar}\hat{H}t}\rho(0)e^{\frac{i}{\hbar}\hat{H}t}$$

### 3 Mixed States

For a mixed state, the system is in a statistical ensemble of pure states  $|\psi_k\rangle$ , each occurring with a probability  $p_k$ . The total density operator for the mixed state is:

$$\hat{\rho} = \sum_k p_k \hat{\rho}_k = \sum_k p_k |\psi_k\rangle\langle\psi_k|$$

The probability of measuring the eigenvalue  $\lambda_n$  of the observable  $\hat{A}$  in a mixed state is:

$$P(\lambda_n) = \sum_k p_k P_k(\lambda_n) = \sum_k p_k \text{Tr}(\hat{\rho}_k \hat{P}_n)$$

Since the trace is a linear operator, we can rewrite this expression by moving the sum into the trace:

$$P(\lambda_n) = \text{Tr} \left( \left( \sum_k p_k \hat{\rho}_k \right) \hat{P}_n \right) = \text{Tr}(\hat{\rho} \hat{P}_n)$$

Thus, the probability of measuring the eigenvalue  $\lambda_n$  in the mixed state is:

$$P(\lambda_n) = \text{Tr}(\hat{\rho} \hat{P}_n)$$

#### Normalization of the Density Operator

The normalization of the density operator ensures that For a *pure state*, the trace of  $\hat{\rho}_k$  is always 1: the total probability sums to 1.  $\text{Tr}(\hat{\rho}_k) = 1$  For a *mixed state*, the total density operator is:  $\hat{\rho} = \sum_k p_k \hat{\rho}_k$ . We can check the trace of  $\hat{\rho}$ :

$$\text{Tr}(\hat{\rho}) = \text{Tr} \left( \sum_k p_k \hat{\rho}_k \right) = \sum_k p_k \text{Tr}(\hat{\rho}_k) = \sum_k p_k = 1$$

Thus, the normalization condition is satisfied for both pure and mixed states.

### Expectation Values

Consider an observable  $\hat{A}$  with eigenvalue decomposition:

$$\hat{A} = \sum_n \lambda_n \hat{P}_n$$

where  $\hat{P}_n = |u_n\rangle\langle u_n|$  is the projection operator onto the eigenstate  $|u_n\rangle$ , and  $\lambda_n$  is the eigenvalue associated with  $\hat{P}_n$ . For a *pure state*  $|\psi_k\rangle$ , the expectation value of  $\hat{A}$  is:  $\langle \hat{A} \rangle = \text{Tr}(\hat{\rho}_k \hat{A})$ . For a *mixed state*, the expectation value of  $\hat{A}$  is:

$$\langle \hat{A} \rangle = \sum_n \lambda_n P(\lambda_n) = \sum_n \lambda_n \text{Tr}(\hat{\rho} \hat{P}_n) = \text{Tr} \left( \hat{\rho} \left( \sum_n \lambda_n \hat{P}_n \right) \right)$$

which simplifies to:

$$\langle \hat{A} \rangle = \text{Tr}(\hat{\rho} \hat{A})$$

Thus, for both pure and mixed states, the expectation value of an observable is given by the trace of the product of the density operator and the observable.

### Time Evolution

The time evolution of the density operator is governed by the Hamiltonian  $\hat{H}(t)$ . For a *mixed state*, the total density operator  $\hat{\rho}(t)$  evolves according to:

$$\frac{d}{dt} \hat{\rho}(t) = \frac{1}{i\hbar} [\hat{H}(t), \hat{\rho}(t)]$$

This result follows from the fact that the total density operator is a weighted sum of the pure state density operators, and the time evolution of the mixed state density operator is the same as for the pure state, with the weights  $p_k$  preserved.

### Distinction Between Pure and Mixed States

Let's emphasize a key difference between pure and mixed states. A pure state density operator  $\hat{\rho}_k$  satisfies:

$$\hat{\rho}_k^2 = \hat{\rho}_k \quad \text{and} \quad \text{Tr}(\hat{\rho}_k^2) = 1$$

However, for a *mixed state*:

$$\hat{\rho} = \sum_k p_k \hat{\rho}_k$$

We find that:

$$\hat{\rho}^2 = \sum_{k,l} p_k p_l \hat{\rho}_k \hat{\rho}_l \neq \hat{\rho}$$

This implies that the density operator of a mixed state is *not* a projection operator. Moreover, the trace of the square of the density operator is less than 1:

$$\text{Tr}(\hat{\rho}^2) = \sum_k p_k^2 \text{Tr}(\hat{\rho}_k) = \sum_k p_k^2 < 1$$

This result is a crucial signature of mixed states:  $\text{Tr}(\hat{\rho}^2)$  is strictly less than 1.

$\gamma = \text{Tr}(\hat{\rho}^2)$  is a measure of the *purity* of a mixed state. The purity serves as an indicator of how much the state deviates from being purely quantum (a pure state). A high purity indicates a state that is almost a pure state, while a low purity suggests a highly mixed or disordered state.

## 4 Examples

### Example 1: Pure State

Consider a quantum system in a pure state  $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$ , where  $\alpha$  and  $\beta$  are complex coefficients and  $|0\rangle$  and  $|1\rangle$  are basis states. The density operator for this pure state is:

$$\hat{\rho} = |\psi\rangle\langle\psi| = (\alpha|0\rangle + \beta|1\rangle)(\alpha^*\langle 0| + \beta^*\langle 1|)$$

This expands to:

$$\hat{\rho} = |\alpha|^2|0\rangle\langle 0| + \alpha\beta^*|0\rangle\langle 1| + \alpha^*\beta|1\rangle\langle 0| + |\beta|^2|1\rangle\langle 1|$$

This is a  $2 \times 2$  matrix (if we assume the basis  $\{|0\rangle, |1\rangle\}$ ):

$$\rho = \begin{pmatrix} |\alpha|^2 & \alpha\beta^* \\ \alpha^*\beta & |\beta|^2 \end{pmatrix}$$

### Example 2: Mixed State

Suppose we have a system that can be in one of two pure states,  $|\psi_1\rangle$  with probability  $p_1$  and  $|\psi_2\rangle$  with probability  $p_2$ . The density operator for the mixed state is:

$$\hat{\rho} = p_1|\psi_1\rangle\langle\psi_1| + p_2|\psi_2\rangle\langle\psi_2|$$

For example, if  $|\psi_1\rangle = |0\rangle$  and  $|\psi_2\rangle = |1\rangle$ , the density matrix becomes:

$$\hat{\rho} = p_1|0\rangle\langle 0| + p_2|1\rangle\langle 1|$$

which, in matrix form, would be:

$$\rho = \begin{pmatrix} p_1 & 0 \\ 0 & p_2 \end{pmatrix}$$

This is a diagonal matrix, which indicates that the system has no coherence between the states  $|0\rangle$  and  $|1\rangle$ .

### Example 3: Mixed State

Let the system be in a mixed state, which is a statistical mixture of two pure states  $|\psi_1\rangle$  and  $|\psi_2\rangle$ , each occurring with probabilities  $p_1$  and  $p_2$ , respectively. Each pure state is a superposition of the basis states  $|0\rangle$  and  $|1\rangle$ :

$$|\psi_1\rangle = \alpha_1|0\rangle + \beta_1|1\rangle$$

$$|\psi_2\rangle = \alpha_2|0\rangle + \beta_2|1\rangle$$

where  $\alpha_1, \beta_1, \alpha_2, \beta_2$  are complex coefficients satisfying the normalization conditions  $|\alpha_1|^2 + |\beta_1|^2 = 1$  and  $|\alpha_2|^2 + |\beta_2|^2 = 1$ . The density operator for the mixed state is given by:

$$\hat{\rho} = p_1|\psi_1\rangle\langle\psi_1| + p_2|\psi_2\rangle\langle\psi_2|$$

First, we compute the outer products  $|\psi_1\rangle\langle\psi_1|$  and  $|\psi_2\rangle\langle\psi_2|$ . For  $|\psi_1\rangle = \alpha_1|0\rangle + \beta_1|1\rangle$ , we have:

$$\begin{aligned} |\psi_1\rangle\langle\psi_1| &= (\alpha_1|0\rangle + \beta_1|1\rangle)(\alpha_1^*\langle 0| + \beta_1^*\langle 1|) \\ &= |\alpha_1|^2|0\rangle\langle 0| + \alpha_1\beta_1^*|0\rangle\langle 1| + \alpha_1^*\beta_1|1\rangle\langle 0| + |\beta_1|^2|1\rangle\langle 1| \end{aligned}$$

Similarly, for  $|\psi_2\rangle = \alpha_2|0\rangle + \beta_2|1\rangle$ , we have:

$$\begin{aligned} |\psi_2\rangle\langle\psi_2| &= (\alpha_2|0\rangle + \beta_2|1\rangle)(\alpha_2^*\langle 0| + \beta_2^*\langle 1|) \\ &= |\alpha_2|^2|0\rangle\langle 0| + \alpha_2\beta_2^*|0\rangle\langle 1| + \alpha_2^*\beta_2|1\rangle\langle 0| + |\beta_2|^2|1\rangle\langle 1| \end{aligned}$$

Now, we calculate the total density matrix  $\rho$  by summing the outer products weighted by the probabilities  $p_1$  and  $p_2$ :

$$\rho = p_1|\psi_1\rangle\langle\psi_1| + p_2|\psi_2\rangle\langle\psi_2|$$

Substituting the expanded forms of  $|\psi_1\rangle\langle\psi_1|$  and  $|\psi_2\rangle\langle\psi_2|$ , we get:

$$\begin{aligned} \rho &= p_1 (|\alpha_1|^2|0\rangle\langle 0| + \alpha_1\beta_1^*|0\rangle\langle 1| + \alpha_1^*\beta_1|1\rangle\langle 0| + |\beta_1|^2|1\rangle\langle 1|) \\ &\quad + p_2 (|\alpha_2|^2|0\rangle\langle 0| + \alpha_2\beta_2^*|0\rangle\langle 1| + \alpha_2^*\beta_2|1\rangle\langle 0| + |\beta_2|^2|1\rangle\langle 1|) \end{aligned}$$

Now, we can express the density operator  $\hat{\rho}$  as a  $2 \times 2$  matrix by calculating each element:

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

Thus, the density matrix  $\rho$  is:

$$\rho = \begin{pmatrix} p_1|\alpha_1|^2 + p_2|\alpha_2|^2 & p_1\alpha_1\beta_1^* + p_2\alpha_2\beta_2^* \\ p_1\alpha_1^*\beta_1 + p_2\alpha_2^*\beta_2 & p_1|\beta_1|^2 + p_2|\beta_2|^2 \end{pmatrix}$$

This density matrix fully encapsulates the mixed state, accounting for both the probabilistic mixture of the two pure states and the coherence between the basis states in each pure state.



## 5 Applications of Density Operators

Density operators are widely used in various fields of quantum mechanics and quantum information science. Some key applications include:

### Quantum Measurement

The density operator allows us to calculate the expectation value of an observable  $\hat{A}$  in a quantum state  $\hat{\rho}$  as:

$$\langle \hat{A} \rangle = \text{Tr}(\hat{\rho}\hat{A})$$

This is especially useful for mixed states, where we don't have a single state vector to work with.

### Quantum Entanglement and Decoherence

Density matrices are essential for studying *quantum entanglement* and *decoherence*. For entangled systems, the density operator describes the global state of the system. Decoherence can be modeled by tracing out the environmental degrees of freedom from a larger system-environment density operator.

### Quantum Statistical Mechanics

In statistical mechanics, the density operator formalism is used to describe ensembles of quantum systems in equilibrium, especially in the context of *thermal states*. The canonical ensemble, for example, uses the density operator:

$$\hat{\rho} = \frac{1}{Z} e^{-\beta \hat{H}}$$

where  $\beta = 1/k_B T$  and  $Z$  is the partition function.

### Quantum Information Theory

In quantum computing and quantum information theory, the density operator is used to describe mixed states, which are crucial for understanding processes like quantum measurement, noise, and error correction.

## 6 Conclusion

In summary, the **density operator** is a powerful tool in quantum mechanics that provides a comprehensive framework for describing both pure and mixed states. It generalizes the concept of the state vector and is particularly useful in situations involving incomplete information or statistical ensembles. The density operator formalism plays a central role in quantum statistical mechanics, quantum computing, quantum information theory, and the study of decoherence and entanglement.