Density Operator [lam1]

The most general specification of quantum states employs density operators. They are equally useful for pure states and mixed states.

Pure states:

Pure quantum states expanded in an orthonormal basis have equivalent representations as a state vector or as a density operator:

- State vector: $|\psi\rangle = \sum_n c_n |n\rangle$.
- Expansion coefficients: $c_n = \langle n|\psi\rangle$.
- Normalization: $\langle\psi|\psi\rangle = \sum_n c_n^* c_n = \sum_n |c_n|^2 = 1$.
- Density operator: $\rho = |\psi\rangle\langle\psi| = \sum_{nm} \rho_{nm} |n\rangle\langle m|$.
- Matrix elements: $\rho_{nm} = \langle n|\rho|m\rangle = \langle n|\psi\rangle\langle\psi|m\rangle = c_n c_m^* = \rho_{mn}^*$,

  populations: ρ_{nn} (diagonal),

  coherences: $\rho_{nm} = r_n r_m e^{\imath(\varphi_n - \varphi_m)}$ (off-diagonal).
- Trace: $\mathrm{Tr}[\rho] = \sum_n \rho_{nn} = \sum_n |c_n|^2 = 1$.
- Diagonal and off-diagonal matrix elements:

$$\rho_{nm}\rho_{mn} = |\rho_{mn}|^2 = c_n c_m^* c_m c_n^* = |c_n|^2 |c_m|^2 = \rho_{nn}\rho_{mm}.$$

- Idempotency:[1] $\rho^2 = |\psi\rangle\langle\psi|\psi\rangle\langle\psi| = |\psi\rangle\langle\psi| = \rho$.

Mixed states:

Mixed quantum states are not expressible as state vectors. Density operators are no longer projection operators, now specified by a set of state vectors, $\{|\psi\rangle\}$, which are normalized but not necessarily orthogonal.

- State vectors in the mix: $|\psi\rangle = \sum_n c_n^\psi |n\rangle$, $\langle\psi|\psi\rangle = 1$, $\sum_n |c_n^\psi|^2 = 1$.
- Probabilities of state vectors: P_ψ, $0 \leq P_\psi \leq 1$, $\sum_\psi P_\psi = 1$.

[1]General attribute of projection operators.

– Density operator:

$$\rho = \sum_{\psi} P_{\psi} |\psi\rangle\langle\psi| = \sum_{\psi} \sum_{nm} P_{\psi} c_n^{\psi} c_m^{\psi *} |n\rangle\langle m| = \sum_{nm} \rho_{nm} |n\rangle\langle m|.$$

– Matrix elements: $\rho_{nm} = \sum_{\psi} P_{\psi} \rho_{nm}^{\psi}, \quad \rho_{nm}^{\psi} = c_n^{\psi} c_m^{\psi *}.$

– Trace: $\mathrm{Tr}[\rho] = \sum_{n} \rho_{nn} = \sum_{\psi} P_{\psi} \sum_{n} |c_n^{\psi}|^2 = 1.$

– Diagonal and off-diagonal matrix elements:

$$\begin{aligned} \rho_{nm}\rho_{mn} &= \sum_{\psi} \sum_{\psi'} P_{\psi} P_{\psi'} c_n^{\psi} c_m^{\psi *} c_m^{\psi'} c_n^{\psi' *} \\ &\neq \rho_{nn}\rho_{mm} = \sum_{\psi} \sum_{\psi'} P_{\psi} P_{\psi'} |c_n^{\psi}|^2 |c_m^{\psi'}|^2. \end{aligned}$$

Expectation values:

Expectation value of observable A (Hermitian operator):

$$\langle A \rangle = \mathrm{Tr}[\rho A] = \sum_{nm} \rho_{nm} A_{mn}.$$

The sum over m represents a matrix multiplication for the diagonal elements of the product matrix. The sum over n performs the trace.

Expectation value for a pure quantum state:

$$\langle A \rangle = \sum_{nm} \rho_{nm} A_{mn} = \sum_{nm} \rho_{nm} \langle m|A|n\rangle = \sum_{nm} c_m^{*} c_n \langle m|A|n\rangle = \langle \psi|A|\psi\rangle.$$

Expectation value for a mixed quantum state:

$$\begin{aligned} \langle A \rangle = \sum_{nm} \rho_{nm} A_{mn} &= \sum_{\psi} \sum_{nm} P_{\psi} \rho_{nm}^{\psi} A_{mn} \\ &= \sum_{\psi} \sum_{nm} P_{\psi} c_m^{\psi *} c_n^{\psi} \langle m|A|n\rangle = \sum_{\psi} P_{\psi} \langle \psi|A|\psi\rangle. \end{aligned}$$

Interacting subsystems:

Basis vectors: $|n_a, n_b\rangle = |n_a\rangle \otimes |n_b\rangle$ (tensor product).

Expectation values (in general):

$$\langle \mathcal{O} \rangle = \mathrm{Tr}[\rho\, \mathcal{O}] = \sum_{n_a,n_b} \langle n_a, n_b|\rho\, \mathcal{O}|n_a n_b\rangle$$
$$= \sum_{m_a,m_b} \sum_{n_a,n_b} \langle n_a, n_b|\rho|m_a, m_b\rangle\langle m_a, m_b|\mathcal{O}|n_a, n_b\rangle$$

The first sum calculates the diagonal element of a matrix product, the second sum evaluates the trace.

Density operator: $\rho = \sum_{n_a,n_b} \sum_{m_a,m_b} |n_a, n_b\rangle \rho_{n_a,n_b;m_a,m_b} \langle m_a, m_b|$.

Consider an operator $\mathcal{A}$ which acts in subspace a only:

Matrix element: $\langle m_a, m_b|\mathcal{A}|n_a, n_b\rangle = \langle m_a|\mathcal{A}|n_a\rangle\langle m_b|n_b\rangle = \langle m_a|\mathcal{A}|n_a\rangle\delta_{m_b,n_b}$.

Reduced density operator (with action in subspace a):

$$\rho_a \doteq \sum_{n_b} \langle n_b|\rho|n_b\rangle = \mathrm{Tr}_b[\rho] = \sum_{m_a,m_b} \sum_{n_b} |n_a\rangle \rho_{n_a,n_b;m_a,n_b} \langle m_a|.$$

Expectation value of operator $\mathcal{A}$:

$$\langle \mathcal{A} \rangle \doteq \mathrm{Tr}[\rho\, \mathcal{A}] = \sum_{m_a,m_b} \sum_{n_a,n_b} \langle n_a, n_b|\rho|m_a, m_b\rangle \underbrace{\langle m_a, m_b|\mathcal{A}|n_a, n_b\rangle}_{\langle m_a|\mathcal{A}|n_a\rangle\delta_{m_b,n_b}}$$
$$= \sum_{m_a} \sum_{n_a,n_b} \langle n_a, n_b|\rho|m_a, n_b\rangle\langle m_a|\mathcal{A}|n_a\rangle$$
$$= \sum_{m_a} \sum_{n_a} \langle n_a|\rho_a|m_a\rangle\langle m_a|\mathcal{A}|n_a\rangle = \mathrm{Tr}_a[\rho_a \mathcal{A}].$$

Entanglement:

We have learned that density operators are projection operators only for pure quantum states. Next we show that reduced density operators of pure quantum states are not, in general, projection operators.

Pure quantum system in combined subsystems a and b: $|\Phi\rangle$.

Density operator in full system: $\rho = |\Phi\rangle\langle\Phi|$.

Reduced density operator generally represents a mixed state in subsystem a:

$$\rho_a = \sum_{n_b} \langle n_b|\Phi\rangle\langle\Phi|n_b\rangle = \sum_{n_b} P_{n_b} |\alpha_{n_b}\rangle\langle\alpha_{n_b}|.$$

Associated probability distribution: $P_{n_b} = \sum_{n_a} |\langle n_a, n_b|\Phi\rangle|^2 \doteq |\langle n_b|\Phi\rangle|^2$.

Vectors of mixed state: $|\alpha_{n_b}\rangle = \frac{1}{\sqrt{P_{n_b}}} \sum_{n_a} \langle n_a, n_b|\Phi\rangle|n_a\rangle \doteq \frac{1}{\sqrt{P_{n_b}}} \langle n_b|\Phi\rangle$.

Special case of a pure product state: $|\Phi\rangle \doteq |\psi_a\rangle \otimes |\psi_b\rangle$.

Reduced density operator remains a pure state:

$$\rho_a = \sum_{n_b} \langle n_b|\psi_b\rangle\langle\psi_b|n_b\rangle\, |\psi_a\rangle\langle\psi_a| = |\psi_a\rangle\langle\psi_a| \underbrace{\sum_{n_b} P_{n_b}}_{1} .$$

A state $|\Phi\rangle$ which produces more than one nonzero P_{n_b} is entangled.