

Fundamentals of Quantum Technology

Week 3: The Density Operator

Recommended literature: Gerry, Knight (Appendix A)

1 The density operator

The density operator generalizes the notion of a quantum state that we used to work with until now. Consider a $\frac{1}{2}$ -spin particle; isolated from any environment, its state can be written as a vector which is a superposition of basis vectors,

$$|\psi\rangle = c_1 |\uparrow\rangle + c_2 |\downarrow\rangle.$$

But a system comprised of two $\frac{1}{2}$ -spin particles can be, for example, in the state

$$|\Psi\rangle = \frac{1}{\sqrt{2}} [|\uparrow\rangle_1 |\downarrow\rangle_2 - |\downarrow\rangle_1 |\uparrow\rangle_2].$$

The state of the full two-particle system is written in the usual form: a coherent superposition of basis vectors. But what is the state of, say, particle 1? We might think about finding a different basis for the representation of the state of particle 1, but there is actually *no* basis in which the above two-particle state can be written in the form

$$|\Psi\rangle = |\text{spin } 1\rangle |\text{spin } 2\rangle. \quad (\text{wrong!})$$

We say that the full two-particle system is in a *pure* state, as it can be written as a state vector. Each particle on its own is in a *mixed* state, since its state cannot be described using state vectors. Let us discuss this distinction more generally.

1.1 Definition: Density operator

Let $\{|\psi_i\rangle\}$ be a set of state vectors which can describe a certain system (they need not be orthogonal with respect to each other); we refer to this set as the *ensemble*. With each state $|\psi_i\rangle$ we associate a probability $0 \leq p_i \leq 1$, and these probabilities must obviously satisfy

$$\sum_i p_i = 1.$$

We define a **density operator** as

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

This is a sum of projection operators over the ensemble, where the operators are weighted by the corresponding probabilities. Note that $\hat{\rho}$ is Hermitian.

We say that $\hat{\rho}$ represents a **pure state** if $p_j = 1$ for some j (and thus $p_i = 0$ for all $i \neq j$),

$$\hat{\rho} = |\psi_j\rangle \langle\psi_j|.$$

Otherwise – that is, if there are at least two different i 's for which $0 < p_i < 1$ – we say that $\hat{\rho}$ represents a **mixed state**.

Choosing some complete orthonormal basis $\{|\varphi_n\rangle\}$, we can define a **density matrix**, the elements of which are given by $\rho_{mn} = \langle\varphi_m|\hat{\rho}|\varphi_n\rangle$.

Exercise

Construct a density matrix corresponding to the pure state

$$|\psi\rangle = \frac{1}{\sqrt{2}} (|\uparrow\rangle + e^{i\phi} |\downarrow\rangle)$$

of a single $\frac{1}{2}$ -spin.

Solution

The density operator is given by

$$\hat{\rho} = |\psi\rangle\langle\psi| = \frac{1}{2} [|\uparrow\rangle\langle\uparrow| + e^{i\phi} |\downarrow\rangle\langle\uparrow| + e^{-i\phi} |\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\downarrow|],$$

and this directly gives us the form of the density matrix in the $\{|\uparrow\rangle, |\downarrow\rangle\}$ basis:

$$\hat{\rho}_{\text{pure}} = \frac{1}{2} \begin{pmatrix} 1 & e^{-i\phi} \\ e^{i\phi} & 1 \end{pmatrix}.$$

Alternatively, we can choose the basis $\{|\psi\rangle, |\psi^\perp\rangle\}$ with

$$|\psi^\perp\rangle = \frac{1}{\sqrt{2}} (|\uparrow\rangle - e^{i\phi} |\downarrow\rangle),$$

yielding the density matrix

$$\hat{\rho}'_{\text{pure}} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}.$$

As an example for a mixed state of a single $\frac{1}{2}$ -spin particle, we may look at an equal mixture of its two orthogonal states,

$$\hat{\rho}_{\text{mixed}} = \frac{1}{2} [|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|] = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

Note the disappearance of the off-diagonal terms, the **coherence terms**.

1.2 Properties of the density matrix

Exercise

Show that the density matrix always obeys $\text{Tr}\hat{\rho} = 1$.

Solution

The trace is simply the sum of diagonal terms, so

$$\begin{aligned} \text{Tr}\hat{\rho} &= \sum_n \langle\varphi_n|\hat{\rho}|\varphi_n\rangle = \sum_i \sum_n p_i \langle\varphi_n|\psi_i\rangle \langle\psi_i|\varphi_n\rangle \\ &= \sum_i \sum_n p_i \langle\psi_i|\varphi_n\rangle \langle\varphi_n|\psi_i\rangle = \sum_i p_i \langle\psi_i|\left(\sum_n |\varphi_n\rangle\langle\varphi_n|\right)|\psi_i\rangle \\ &= \sum_i p_i \langle\psi_i|\psi_i\rangle = \sum_i p_i = 1. \end{aligned}$$

Here we used the completeness relation $\sum_n |\varphi_n\rangle \langle \varphi_n| = 1$.

At home you will also prove the following statement, giving us a conclusive criterion determining the purity of a state:

$$\begin{aligned}\text{Tr} \hat{\rho}^2 &= 1, \quad \text{for a pure state,} \\ \text{Tr} \hat{\rho}^2 &< 1, \quad \text{for a mixed state.}\end{aligned}$$

Let us check this for the two density matrices we have derived:

$$\begin{aligned}(\hat{\rho}_{\text{pure}})^2 &= \frac{1}{2} \begin{pmatrix} 1 & e^{-i\phi} \\ e^{i\phi} & 1 \end{pmatrix} \longrightarrow \text{Tr} (\hat{\rho}_{\text{pure}})^2 = 1, \\ (\hat{\rho}_{\text{mixed}})^2 &= \frac{1}{4} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \longrightarrow \text{Tr} (\hat{\rho}_{\text{mixed}})^2 = \frac{1}{2}.\end{aligned}$$

2 Entangled states

The formalism of density operators allows us to detect entanglement in a straightforward manner. Consider, for simplicity, a system comprised of two $\frac{1}{2}$ -spin particles. A pure state of the total system is a state vector which is generally a superposition of 4 basis states:

$$|\Psi\rangle = c_{\uparrow\uparrow} |\uparrow\rangle_1 |\uparrow\rangle_2 + c_{\uparrow\downarrow} |\uparrow\rangle_1 |\downarrow\rangle_2 + c_{\downarrow\uparrow} |\downarrow\rangle_1 |\uparrow\rangle_2 + c_{\downarrow\downarrow} |\downarrow\rangle_1 |\downarrow\rangle_2.$$

The corresponding density operator is $\hat{\rho}_{12} = |\Psi\rangle \langle \Psi|$, and it can be written explicitly as a 4×4 density matrix.

We can focus on a certain subsystem by defining a *reduced* density operator. This is done by tracing the density operator of the full system over all the states of all other subsystems. For example, the reduced density operator of particle 1 is defined as

$$\hat{\rho}_1 = \text{Tr}_2 \hat{\rho}_{12} = \langle \uparrow |_2 \hat{\rho}_{12} | \uparrow \rangle_2 + \langle \downarrow |_2 \hat{\rho}_{12} | \downarrow \rangle_2,$$

yielding an operator that acts only on the degrees-of-freedom of particle 1.

Exercise

Compute $\hat{\rho}_1$ for the states

$$\begin{aligned}|\Psi^{(i)}\rangle &= \frac{1}{\sqrt{2}} [|\uparrow\rangle_1 |\downarrow\rangle_2 + e^{i\phi} |\downarrow\rangle_1 |\downarrow\rangle_2], \\ |\Psi^{(ii)}\rangle &= \frac{1}{\sqrt{2}} [|\uparrow\rangle_1 |\downarrow\rangle_2 - |\downarrow\rangle_1 |\uparrow\rangle_2].\end{aligned}$$

Solution

We first write the 4×4 density matrix of the full system pure state, choosing the order of the basis states to be $\{|\uparrow\rangle_1 |\uparrow\rangle_2, |\uparrow\rangle_1 |\downarrow\rangle_2, |\downarrow\rangle_1 |\uparrow\rangle_2, |\downarrow\rangle_1 |\downarrow\rangle_2\}$:

$$\begin{aligned}\hat{\rho}_{12}^{(i)} &= |\Psi^{(i)}\rangle \langle \Psi^{(i)}| = \frac{1}{2} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & e^{-i\phi} \\ 0 & 0 & 0 & 0 \\ 0 & e^{i\phi} & 0 & 1 \end{pmatrix}, \\ \hat{\rho}_{12}^{(ii)} &= |\Psi^{(ii)}\rangle \langle \Psi^{(ii)}| = \frac{1}{2} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.\end{aligned}$$

We now need to trace out the states of particle 2. The density matrices we wrote are divided to four 2×2 blocks where only the degree-of-freedom of particle 2 changes when we move between rows or columns inside each block. We take the trace of each such block and plug it into a reduced 2×2 matrix:

$$\hat{\rho}_1^{(i)} = \frac{1}{2} \begin{pmatrix} 0+1 & 0+e^{-i\phi} \\ 0+e^{i\phi} & 0+1 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & e^{-i\phi} \\ e^{i\phi} & 1 \end{pmatrix},$$

$$\hat{\rho}_1^{(ii)} = \frac{1}{2} \begin{pmatrix} 0+1 & 0+0 \\ 0+0 & 1+0 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

Note This calculation may also be performed without using an explicit matrix representation. For example, when we write the ket-bra expression for $\hat{\rho}_{12}^{(ii)} = |\Psi^{(ii)}\rangle\langle\Psi^{(ii)}|$, we obtain

$$\hat{\rho}_{12}^{(ii)} = \frac{1}{2} [|\uparrow_1\downarrow_2\rangle\langle\uparrow_1\downarrow_2| - |\downarrow_1\uparrow_2\rangle\langle\uparrow_1\downarrow_2| - |\uparrow_1\downarrow_2\rangle\langle\downarrow_1\uparrow_2| + |\downarrow_1\uparrow_2\rangle\langle\downarrow_1\uparrow_2|].$$

Now, in the partial trace over the states of particle 2, the term $\langle\uparrow|_2 \hat{\rho}_{12}^{(ii)} |\uparrow\rangle_2$ keeps only “ket-bra”s where particle 2 was in the state $|\uparrow\rangle$ both in the “bra” and in the “ket”; note that in the above expression, only the last summand satisfies this requirement. Then we are left with a “ket-bra” that acts only on particle 1, since we projected the operator on a specific state of particle 2:

$$\langle\uparrow|_2 \hat{\rho}_{12}^{(ii)} |\uparrow\rangle_2 = \langle\uparrow|_2 \left[\frac{1}{2} |\downarrow_1\uparrow_2\rangle\langle\downarrow_1\uparrow_2| \right] |\uparrow\rangle_2 = \frac{1}{2} |\downarrow\rangle_1 \langle\downarrow|_1.$$

Similarly, the term $\langle\downarrow|_2 \hat{\rho}_{12}^{(ii)} |\downarrow\rangle_2$ keeps only “ket-bra”s where particle 2 was in the state $|\downarrow\rangle$ both in the “bra” and in the “ket”:

$$\langle\downarrow|_2 \hat{\rho}_{12}^{(ii)} |\downarrow\rangle_2 = \langle\downarrow|_2 \left[\frac{1}{2} |\uparrow_1\downarrow_2\rangle\langle\uparrow_1\downarrow_2| \right] |\downarrow\rangle_2 = \frac{1}{2} |\uparrow\rangle_1 \langle\uparrow|_1.$$

Thus, in total, the reduced density operator for particle 1 is

$$\hat{\rho}_1^{(ii)} = \langle\uparrow|_2 \hat{\rho}_{12}^{(ii)} |\uparrow\rangle_2 + \langle\downarrow|_2 \hat{\rho}_{12}^{(ii)} |\downarrow\rangle_2 = \frac{1}{2} [|\uparrow\rangle_1 \langle\uparrow|_1 + |\downarrow\rangle_1 \langle\downarrow|_1],$$

which of course matches the matrix we got.

So, for the **disentangled** two-particle state we got a reduced density matrix representing a **pure** state, while for the **entangled** two-particle state we got a reduced density matrix representing a **mixed** state. Thus the purity of the reduced density operator signals the entanglement of the original multiparticle state:

$$\begin{aligned} \text{Tr}(\hat{\rho}_1)^2 &= 1, \quad \text{for a disentangled state,} \\ \text{Tr}(\hat{\rho}_1)^2 &< 1, \quad \text{for an entangled state.} \end{aligned}$$

This criterion is independent of the choice of representing basis, and in the case where we examine the entanglement between two complementary subsystems it is independent of the choice of subsystem which we trace out from the density operator (in the two-particle case this means that the same criterion applies to $\hat{\rho}_2 = \text{Tr}_1 \hat{\rho}_{12}$).