Ph195a lecture notes for 10/17/01

One more thing about density operators...

Recall from our last lecture that the probability of a measurement outcome x is given by

$$\Pr(x) = \mathrm{Tr}[\boldsymbol{\rho}\mathbf{P}_x], \tag{1}$$

where $\mathbf{P}_x$ is the projector corresponding to x.

From this, we can easily derive an expression for the expectation value of an observable $\mathbf{O}_q$ with respect to the mixed state $\boldsymbol{\rho}$:

$$\begin{aligned} \langle \mathbf{O}_q \rangle &= \sum_i \lambda_i^q \Pr(i^q) \\ &= \sum_i \lambda_i^q \mathrm{Tr}[\boldsymbol{\rho}\mathbf{P}_i^q] \\ &= \mathrm{Tr}\left[\boldsymbol{\rho} \sum_i \lambda_i^q \mathbf{P}_i^q\right] \\ &= \mathrm{Tr}\left[\boldsymbol{\rho}\mathbf{O}_q\right]. \end{aligned} \tag{2}$$

Higher moments of $\mathbf{O}_q$ can be represented in the same fashion.

Joint state space for two subsystems

Suppose we have two *independent* quantum systems. It seems clear that we can separately consider the representation of their physical states in two independent Hilbert spaces. Labelling the systems A and B, we can simply chose state vectors

$$|\Psi_A\rangle \in H_A, \tag{3}$$

and

$$|\Psi_B\rangle \in H_B. \tag{4}$$

What if we need to bring these systems together and let them interact?

The joint state space for two such systems corresponds to the ***tensor product*** of H_A and H_B, denoted $H_{AB} = H_A \otimes H_B$.

Let N_A be the dimension of H_A, and N_B the dimension of H_B. If $\{|1_A\rangle, |2_A\rangle, |3_A\rangle, \ldots\}$ is a complete orthonormal basis for H_A and $\{|1_B\rangle, |2_B\rangle, |3_B\rangle, \ldots\}$ is a complete orthonormal basis for H_B, then $H_A \otimes H_B$ is the Hilbert space of dimension $N_{AB} = N_A N_B$ spanned by the vectors of the form $|i_A\rangle \otimes |j_B\rangle$.

Hence arbitrary states in H_{AB} have the form

$$|\Psi_{AB}\rangle = \sum_{i=1}^{N_A}\sum_{j=1}^{N_B} c_{ij}\,|i_A\rangle \otimes |j_B\rangle. \qquad 5$$

As long as we fix an ordering for the new basis states $|i_A\rangle \otimes |j_B\rangle$, the set of $N_A N_B$ complex coefficients can be used as a vector representation for kets in H_{AB}.

The tensor product operation between vectors has the following properties:

1. Linearity: $(\alpha|\Psi_A\rangle) \otimes |\Psi_B\rangle = \alpha(|\Psi_A\rangle \otimes |\Psi_B\rangle)$, where α is a complex number
2. Distributivity: $|\Psi_A\rangle \otimes (|\Psi_B^1\rangle + |\Psi_B^2\rangle) = |\Psi_A\rangle \otimes |\Psi_B^1\rangle + |\Psi_A\rangle \otimes |\Psi_B^2\rangle$.
3. ‘Commutativity’: formally, $|\Psi_A\rangle \otimes |\Psi_B\rangle$ is the same as $|\Psi_B\rangle \otimes |\Psi_A\rangle$. In practice however, it is wise to use consistent ordering.
4. Adjoint: $(|\Psi_A\rangle \otimes |\Psi_B\rangle)^\dagger = \langle\Psi_A| \otimes \langle\Psi_B|$.
5. Scalar product: $(\langle\Psi_A^1| \otimes \langle\Psi_B^1|)(|\Psi_A^2\rangle \otimes |\Psi_B^2\rangle) = \langle\Psi_A^1|\Psi_A^2\rangle\langle\Psi_B^1|\Psi_B^2\rangle$.

It is important to note that basis kets $|i_A\rangle \otimes |j_B\rangle \in H_{AB}$ thus inherit orthogonality from their ‘factors’ in H_A and H_B.

Entanglement

The most profound consequence of this mathematical rule for representation of joint states is that there exist $|\Psi_{AB}\rangle \in H_{AB}$ that cannot be expressed the tensor product of a state $|\Psi_A\rangle \in H_A$ with a state $|\Psi_B\rangle \in H_B$. Such ‘nonfactorizable’ states are said to be ***entangled***.

For example, let’s consider two two-dimensional systems. Say we have chosen orthonormal bases $\{|0_A\rangle, |1_A\rangle\}$ for H_A and $\{|0_B\rangle, |1_B\rangle\}$ for H_B. Then H_{AB} is spanned by the four states

$$|0_A\rangle \otimes |0_B\rangle, \quad |0_A\rangle \otimes |1_B\rangle, \quad |1_A\rangle \otimes |0_B\rangle, \quad |1_A\rangle \otimes |1_B\rangle. \qquad 6$$

Factorizable (nonentangled) states in H_{AB} are all of the form

$$\begin{aligned} |\Psi_{AB}^{fac}\rangle &= (c_0^A|0_A\rangle + c_1^A|1_A\rangle) \otimes (c_0^B|0_B\rangle + c_1^B|1_B\rangle) \\ &= c_0^A c_0^B|0_A\rangle \otimes |0_B\rangle + c_0^A c_1^B|0_A\rangle \otimes |1_B\rangle \\ &\quad + c_1^A c_0^B|1_A\rangle \otimes |0_B\rangle + c_1^A c_1^B|1_A\rangle \otimes |1_B\rangle. \end{aligned} \qquad 7$$

That is, a certain relationship exists between the coefficients of the four basis states in H_{AB}.

A simple example of an entangled state, whose coefficients do not exhibit the above relationship, is

$$\begin{aligned} |\Psi_{AB}\rangle &= \frac{1}{\sqrt{2}}(|0_A\rangle \otimes |0_B\rangle + |1_A\rangle \otimes |1_B\rangle) \\ &\neq |\Psi_A\rangle \otimes |\Psi_B\rangle. \end{aligned} \qquad 8$$

When the joint state of two subsystems is entangled, ***there is no way to assign a pure quantum state to either subsystem alone***. As we shall see below, it is possible to ascribe *mixed* quantum states to each of the subsystems considered alone, but first we’ll need to have a look at operators on H_{AB}.

Tensor products of operators

If **A** is an operator on H_A and **B** is an operator on H_B, then

$$\mathbf{A} \otimes \mathbf{B} \tag{9}$$

is a valid operator on H_{AB}. Its action on an arbitrary state

$$|\Psi_{AB}\rangle = \sum_{i,j} c_{ij} |i_A\rangle \otimes |j_B\rangle \tag{10}$$

is defined by

$$(\mathbf{A} \otimes \mathbf{B})|\Psi_{AB}\rangle = \sum_{i,j} c_{ij} (\mathbf{A}|i_A\rangle) \otimes (\mathbf{B}|j_B\rangle). \tag{11}$$

In the case where **A** and **B** are both normal, we may also write

$$\begin{aligned} \mathbf{A} \otimes \mathbf{B} &= \left(\sum_i \lambda_i^A \mathbf{P}_i^A\right) \otimes \left(\sum_j \lambda_j^B \mathbf{P}_j^B\right) \\ &= \sum_{ij} \lambda_i^A \lambda_j^B \mathbf{P}_i^A \otimes \mathbf{P}_j^B. \end{aligned} \tag{12}$$

Note that the usual relationship holds between projectors on the joint state space and outer-products of joint state vectors:

$$\begin{aligned} (|\Psi_A\rangle \otimes |\Psi_B\rangle)(\langle\Psi_A| \otimes \langle\Psi_B|) &= |\Psi_A\rangle\langle\Psi_A| \otimes |\Psi_B\rangle\langle\Psi_B| \\ &= \mathbf{P}_A \otimes \mathbf{P}_B. \end{aligned} \tag{13}$$

Hence any complete set of joint projectors (summing to the identity operator on H_{AB}) specifies a complete measurement.

As was the case with state vectors, linear combinations of tensor-product operators are also valid opeators on H_{AB}:

$$\mathbf{O}_{AB} = \sum_m c_m \mathbf{A}_m \otimes \mathbf{B}_m. \tag{14}$$

Hence, not all operators on a joint state space are factorizable.

Given subsystem density operators $\boldsymbol{\rho}_A$ and $\boldsymbol{\rho}_B$, we can form a tensor-product density operator that describes a mixed ensemble of states in H_{AB}:

$$\boldsymbol{\rho}_{AB} = \boldsymbol{\rho}_A \otimes \boldsymbol{\rho}_B. \tag{15}$$

In general, one can form convex combinations of such $\boldsymbol{\rho}_{AB}$ to construct new joint density operators, which may or may not be factorizable.

One can also construct joint density operators directly from ensembles of pure states in H_{AB}. For instance, the density operator corresponding to the entangled state described above is

$$\begin{aligned} |\Psi_{AB}\rangle &= \frac{1}{\sqrt{2}}[|0_A\rangle \otimes |0_B\rangle + |1_A\rangle \otimes |1_B\rangle] \\ \boldsymbol{\rho}_{AB} &= |\Psi_{AB}\rangle\langle\Psi_{AB}| \\ &= \frac{1}{2}\begin{bmatrix} |0_A\rangle\langle 0_A| \otimes |0_B\rangle\langle 0_B| + |0_A\rangle\langle 1_A| \otimes |0_B\rangle\langle 1_B| \\ +|1_A\rangle\langle 0_A| \otimes |1_B\rangle\langle 0_B| + |1_A\rangle\langle 1_A| \otimes |1_B\rangle\langle 1_B| \end{bmatrix}, \end{aligned} \qquad 16$$

and in general

$$\boldsymbol{\rho}_{AB} = \sum_i p_i |\Psi^i_{AB}\rangle\langle\Psi^i_{AB}|. \qquad 17$$

Note that operators on a tensor-product space can be expressed as complex matrices o_{kl}:

$$\mathbf{O}_{AB} = \sum_{kl} o_{kl} |k_{AB}\rangle\langle l_{AB}|, \qquad 18$$

where the summations both run over a complete set of N_{AB} basis vectors.

Given matrix representations for subsystem operators **A** and **B**, it is customary to choose an ordering for the basis states of the joint space such that

$$\mathbf{A} \otimes \mathbf{B} \leftrightarrow \begin{pmatrix} a_{11}B & a_{12}B & a_{13}B & \\ a_{21}B & a_{22}B & a_{23}B & \cdots \\ a_{31}B & a_{32}B & a_{33}B & \\ & \vdots & & \ddots \end{pmatrix}. \qquad 19$$

For example if $\{|1_A\rangle, |2_A\rangle, \ldots\}$ is the orthnormal basis for H_A used in defining the matrix representation of A, and similarly for H_B, then

$$\begin{aligned} |1_{AB}\rangle &\leftrightarrow |1_A\rangle \otimes |1_B\rangle, \\ |2_{AB}\rangle &\leftrightarrow |1_A\rangle \otimes |2_B\rangle, \\ |3_{AB}\rangle &\leftrightarrow |1_A\rangle \otimes |3_B\rangle, \\ &\vdots \\ |(N_B+1)_{AB}\rangle &\leftrightarrow |2_A\rangle \otimes |1_B\rangle, \\ &\vdots \end{aligned} \qquad 20$$

As a result, the common class of operators $\mathbf{1}^A \otimes \mathbf{B}$ will have block-diagonal representations.

Partial projections

A particularly useful class of tensor-product operators are the partial projectors,

$$\mathbf{1}^A \otimes \mathbf{P}^B_j \qquad 21$$

and

$$\mathbf{P}^A_i \otimes \mathbf{1}^B, \qquad 22$$

where $\mathbf{P}_j^B$ is a projector onto some state in H_B and likewise for $\mathbf{P}_i^A$. Note that such operators are themselves projectors according to the usual definition, since

$$(\mathbf{A}_1 \otimes \mathbf{B}_1)(\mathbf{A}_2 \otimes \mathbf{B}_2) = \mathbf{A}_1\mathbf{A}_2 \otimes \mathbf{B}_1\mathbf{B}_2.$$

Clearly, observables such as

$$\mathbf{O}_q^A \otimes \mathbf{1}^B \tag{23}$$

can be spectrally decomposed using partial projectors.

If $\mathbf{P}_k^B = |k_B\rangle\langle k_B|$ (where $|k_B\rangle$ is a basis vector), then

$$\begin{aligned}\left(\mathbf{1}^A \otimes \mathbf{P}_k^B\right)|\Psi_{AB}\rangle &= \left(\mathbf{1}^A \otimes \mathbf{P}_k^B\right)\sum_{ij} c_{ij}|i_A\rangle \otimes |j_B\rangle \\ &= \sum_{ij} c_{ij}|i_A\rangle \otimes \mathbf{P}_k^B|j_B\rangle \\ &= \sum_{i} c_{ik}|i_A\rangle \otimes |k_B\rangle \\ &= |\Psi_A^k\rangle \otimes |k_B\rangle.\end{aligned} \tag{24}$$

Hence the effect of a partial projector on a joint state in H_{AB} is to knock out all terms in the superposition that are not consistent with subsystem B being in the k^{th} basis state.

It is very important to appreciate that the action of a partial projector will in general 'affect' the state of both subsystems, *unless* the joint state is factorizable. For example, if

$$\begin{aligned}|\Psi_{AB}\rangle &= |\Psi_A\rangle \otimes |\Psi_B\rangle, \\ |\Psi_B\rangle &= \sum_{j=1}^{N_B} c_j^B|j_B\rangle,\end{aligned} \tag{25}$$

then under $\mathbf{1}^A \otimes \mathbf{P}_k^B$

$$|\Psi_{AB}\rangle \mapsto |\Psi_A\rangle \otimes c_k^B|k_B\rangle. \tag{26}$$

If on the other hand $|\Psi_{AB}\rangle$ is *entangled*, e.g.

$$\begin{aligned}|\Psi_{AB}\rangle &= c_1|\Psi_A^1\rangle \otimes |1_B\rangle + c_2|\Psi_A^2\rangle \otimes |2_B\rangle, \\ \langle\Psi_A^1|\Psi_A^2\rangle &\neq 1,\end{aligned} \tag{27}$$

then

$$\mathbf{1}^A \otimes \mathbf{P}_2^B|\Psi_{AB}\rangle = c_2|\Psi_A^2\rangle \otimes |2_B\rangle. \tag{28}$$

Hence even quantities such as $\left\langle \mathbf{O}_q^A \otimes \mathbf{1}^B \right\rangle$ will be changed.

Note that if $\sum_j \mathbf{P}_j^B = \mathbf{1}^B$ (and likewise for the $\left\{\mathbf{P}_i^A\right\}$)

$$\begin{aligned}\sum_{j=1}^{N_B} \mathbf{1}^A \otimes \mathbf{P}_j^B &= \mathbf{1}^A \otimes \mathbf{1}^B = \mathbf{1}^{AB}, \\ \sum_{i=1}^{N_A} \mathbf{P}_i^A \otimes \mathbf{1}^B &= \mathbf{1}^A \otimes \mathbf{1}^B.\end{aligned} \tag{29}$$

Hence one can speak of a 'complete' set of *partial* projectors (with respect to either H_A or H_B), given by

$$\left\{\mathbf{1}^A \otimes \mathbf{P}_0^B, \mathbf{1}^A \otimes \mathbf{P}_1^B, \ldots\right\} \tag{30}$$

or

$$\left\{\mathbf{P}_0^A \otimes \mathbf{1}^B, \mathbf{P}_1^A \otimes \mathbf{1}^B, \ldots\right\}. \qquad 31$$

Such sets of operators specify standard measurements on H_{AB} – the projectors in the set are mutually orthogonal and sum to the identity. In essence, this type of measurement probes the state of one subsystem without regard for the other:

$$\Pr(j) = \left\langle \mathbf{1}^A \otimes \mathbf{P}_j^B \right\rangle, \qquad 32$$

or

$$\Pr(i) = \left\langle \mathbf{P}_i^A \otimes \mathbf{1}^B \right\rangle. \qquad 33$$

But as noted above, the post-measurement state of both subsystems will generally be affected by the outcome, since

$$|\Psi_{AB}\rangle \mapsto \frac{\mathbf{1}^A \otimes \mathbf{P}_j^B |\Psi_{AB}\rangle}{\sqrt{\left\langle \mathbf{1}^A \otimes \mathbf{P}_j^B \right\rangle}} \qquad 34$$

or

$$|\Psi_{AB}\rangle \mapsto \frac{\mathbf{P}_i^A \otimes \mathbf{1}^B |\Psi_{AB}\rangle}{\sqrt{\left\langle \mathbf{P}_i^A \otimes \mathbf{1}^B \right\rangle}}. \qquad 35$$

The usual generalization holds for joint density operators.

Partial trace and reduced density operators

Having defined partial projectors, we can now define the partial trace operation. Let $\boldsymbol{\rho}_{AB}$ be a density operator on H_{AB}:

$$\boldsymbol{\rho}_{AB} = \sum_{ijkl} \rho_{ijkl} |i_A\rangle \otimes |j_B\rangle\langle k_A| \otimes \langle l_B|, \qquad 36$$

where the summations are take over orthonormal bases for H_A and H_B. Consider the sum of partial projections,

$$\begin{aligned}
&\sum_{m=1}^{N_B} \left(\mathbf{1}^A \otimes \mathbf{P}_m^B\right) \boldsymbol{\rho}_{AB} \left(\mathbf{1}^A \otimes \mathbf{P}_m^B\right) \\
&= \sum_{m=1}^{N_B} \left(\mathbf{1}^A \otimes \mathbf{P}_m^B\right) \left(\sum_{ijkl} \rho_{ijkl} |i_A\rangle \otimes |j_B\rangle\langle k_A| \otimes \langle l_B| \right) \left(\mathbf{1}^A \otimes \mathbf{P}_m^B\right) \\
&= \sum_{m=1}^{N_B} \sum_{i,k=1}^{N_A} \rho_{imkm} |i_A\rangle \otimes |m_B\rangle\langle k_A| \otimes \langle m_B| \\
&= \sum_{m=1}^{N_B} |m_B\rangle\langle m_B| \otimes \sum_{i,k=1}^{N_A} \rho_{imkm} |i_A\rangle\langle k_A|. \qquad \#
\end{aligned}$$

We define the partial trace of $\boldsymbol{\rho}_{AB}$ over the B subsystem to be

$$\begin{aligned}\tilde{\boldsymbol{\rho}}_A &\equiv \mathrm{Tr}_B[\boldsymbol{\rho}_{AB}] \\ &= \sum_{m=1}^{N_B}\sum_{i,k=1}^{N_A} \rho_{imkm}|i_A\rangle\langle k_A| \\ &= \sum_{i,k=1}^{N_A}\left(\sum_{m=1}^{N_B}\rho_{imkm}\right)|i_A\rangle\langle k_A|\end{aligned} \tag{38}$$

Here $\tilde{\boldsymbol{\rho}}_A$ is called the ‘reduced density operator’ for subsystem A. It provides the best possible representation of subsystem A within H_A, when the joint state of A and B is entangled/nonfactorizable.

A notationally more convenient, but mathematically less precise way of computing the partial trace is as follows:

$$\begin{aligned}\mathrm{Tr}_B[\boldsymbol{\rho}_{AB}] &= \sum_{m=1}^{N_B}\langle m_B|\boldsymbol{\rho}_{AB}|m_B\rangle \\ &= \sum_{m=1}^{N_B}\langle m_B|\left(\sum_{ijkl}\rho_{ijkl}|i_A\rangle\otimes|j_B\rangle\langle k_A|\otimes\langle l_B|\right)|m_B\rangle \\ &= \sum_{m=1}^{N_B}\sum_{i,k=1}^{N_A}\rho_{imkm}|i_A\rangle\langle k_A|.\end{aligned} \tag{39}$$

When would we need such a representation? Suppose systems A and B are allowed to interact, and as a result end up in some entangled state $|\Psi_{AB}^{ent}\rangle$. Then, however, someone comes and removes subsystem B from our lab. Once B becomes unavailable to us, we can only make measurements of the form

$$\left\{\mathbf{P}_0^A\otimes\mathbf{1}^B,\mathbf{P}_1^A\otimes\mathbf{1}^B,\ldots\right\}. \tag{40}$$

The statistics of all such measurements are predicted by the reduced density operator:

$$
\begin{aligned}
\Pr(i) &= \mathrm{Tr}\left[\boldsymbol{\rho}_{AB}\,\mathbf{P}_i^A \otimes \mathbf{1}^B\right] \\
&= \mathrm{Tr}\left[\left(\sum_{j=1}^{N_B}\left(\mathbf{1}^A \otimes \mathbf{P}_j^B\right)\right)\boldsymbol{\rho}_{AB}\left(\sum_{k=1}^{N_B}\left(\mathbf{1}^A \otimes \mathbf{P}_k^B\right)\right)\mathbf{P}_i^A \otimes \mathbf{1}^B\right] \\
&= \mathrm{Tr}\left[\left(\sum_{j=1}^{N_B}\left(\mathbf{1}^A \otimes \mathbf{P}_j^B\right)\boldsymbol{\rho}_{AB}\left(\mathbf{1}^A \otimes \mathbf{P}_j^B\right)\right)\mathbf{P}_i^A \otimes \mathbf{1}^B\right] \\
&= \mathrm{Tr}\left[\left(\sum_{j=1}^{N_B}|j_B\rangle\langle j_B| \otimes \sum_{k,l=1}^{N_A}\rho_{kjlj}|k_A\rangle\langle l_A|\right)\left(\mathbf{P}_i^A \otimes \mathbf{1}^B\right)^2\right] \\
&= \mathrm{Tr}\left[\left(\sum_{j=1}^{N_B}|j_B\rangle\langle j_B| \otimes \sum_{k,l=1}^{N_A}\rho_{kjlj}\mathbf{P}_i^A|k_A\rangle\langle l_A|\mathbf{P}_i^A\right)\right] \\
&= \mathrm{Tr}\left[\left(\sum_{j=1}^{N_B}|j_B\rangle\langle j_B| \otimes \rho_{ijij}|i_A\rangle\langle i_A|\right)\right] \\
&= \sum_{k=1}^{N_B}\sum_{l=1}^{N_A}\langle l_A| \otimes \langle k_B|\left(\sum_{j=1}^{N_B}|j_B\rangle\langle j_B| \otimes \rho_{ijij}|i_A\rangle\langle i_A|\right)|l_A\rangle \otimes |k_B\rangle \\
&= \sum_{j=1}^{N_B}\rho_{ijij}.
\end{aligned} \qquad 41
$$

Likewise,

$$
\begin{aligned}
\mathrm{Tr}\left[\tilde{\boldsymbol{\rho}}_A\mathbf{P}_i^A\right] &= \mathrm{Tr}\left[\sum_{k,l=1}^{N_A}\left(\sum_{j=1}^{N_B}\rho_{ijkj}\right)|k_A\rangle\langle l_A|\mathbf{P}_i^A\right] \\
&= \mathrm{Tr}\left[\sum_{k=1}^{N_A}\left(\sum_{j=1}^{N_B}\rho_{ijkj}\right)|k_A\rangle\langle i_A|\right] \\
&= \sum_{m=1}^{N_A}\langle m_A|\sum_{k=1}^{N_A}\left(\sum_{j=1}^{N_B}\rho_{ijkj}\right)|k_A\rangle\langle i_A\|m_A\rangle && \# \\
&= \sum_{m=1}^{N_A}\sum_{k=1}^{N_A}\left(\sum_{j=1}^{N_B}\rho_{ijkj}\right)\delta_{mk}\delta_{im} && \# \\
&= \sum_{j=1}^{N_B}\rho_{ijij}.
\end{aligned} \qquad 42
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