APPPHYS383 Tuesday 2 February 2010

Background material on tensor products and partial traces

(from AP225, 10/21 and 10/23 class notes)

Density matrix representation of mixed quantum states

Generally speaking, valid density operators must be Hermitian and have the property

$$\mathrm{Tr}[\rho] = 1.$$

Here Tr denotes the 'trace' operation

$$\mathrm{Tr}[\rho] = \sum_k \langle k|\rho|k\rangle,$$

where $\{|k\rangle\}$ is ***any*** orthonormal basis for the Hilbert space – the numerical result is independent of choice of basis. In particular, since ρ is Hermitian we can chose to take the trace in its own eigenbasis, which makes it clear that

$$\mathrm{Tr}[\rho] = \sum_i \lambda_i^\rho,$$

where λ_i^ρ are the eigenvalues of ρ. Note that if ρ happens to be available in matrix form, we can further make use of the fact that the sum of the eigenvalues of a matrix is equal to the sum of its diagonal elements.

We can easily derive some of the important properties of the eigenvalues and trace of a density operator in the case where it happens to represent a given mixed ensemble,

$$\rho = \sum_k p_k|\Psi_k\rangle\langle\Psi_k| = \sum_k p_k \mathbf{P}_k.$$

(Note however that the properties must hold for density matrices of arbitrary 'origin.') Here $\mathbf{P}_k$ is the projector onto $|\Psi_k\rangle$, which itself is a normalized pure state that occurs in the ensemble with relative probability p_k. For any arbitrary normalized state $|\Phi\rangle$ in the entire Hilbert space,

$$\langle\Phi|\rho|\Phi\rangle = \sum_k p_k\langle\Phi|\mathbf{P}_k|\Phi\rangle.$$

Since all of the p_k and $\langle\Phi|\mathbf{P}_k|\Phi\rangle$ must be between 0 and 1, it follows that

$$0 \le \langle\Phi|\rho|\Phi\rangle \le 1$$

for absolutely any (normalized) choice of the state $|\Phi\rangle$. This includes, in particular, the eigenstates of ρ, for which we have the deduction

$$\rho|\psi_j\rangle = \lambda_j|\psi_j\rangle,$$
$$\langle\psi_j|\rho|\psi_j\rangle = \lambda_j,$$
$$0 \le \lambda_j \le 1.$$

If we furthermore consider the trace for a density matrix representing a mixed ensemble,

$$\begin{aligned}
\mathrm{Tr}[\rho] &= \sum_k \langle k|\rho|k\rangle = \sum_k \langle k|\left(\sum_j p_j|\Psi_j\rangle\langle\Psi_j|\right)|k\rangle \\
&= \sum_k\sum_j p_j\langle k|\Psi_j\rangle\langle\Psi_j|k\rangle \\
&= \sum_k\sum_j p_j\langle\Psi_j|k\rangle\langle k|\Psi_j\rangle \\
&= \sum_j p_j\langle\Psi_j|\left(\sum_k |k\rangle\langle k|\right)|\Psi_j\rangle = \sum_j p_j\langle\Psi_j|\Psi_j\rangle = \sum_j p_j = 1.
\end{aligned}$$

Density operators can represent either pure states,

$$\rho = |\Psi\rangle\langle\Psi|,$$

or mixed states

$$\rho = \sum_i p_i|\Psi_i\rangle\langle\Psi_i|$$

where there is more than one $p_i > 0$. Note that in the former (pure state) case ρ is a true projection operator, so

$$\text{pure}: \quad \boldsymbol{\rho}^2 = \boldsymbol{\rho}.$$

In particular, $\mathrm{Tr}\,\boldsymbol{\rho}^2 = 1$ for a pure state.

For a mixed state, however, we can use the spectral decomposition to show that $\mathrm{Tr}\,\boldsymbol{\rho}^2 < 1.$ We start by writing

$$\boldsymbol{\rho}^2 = \left(\sum_i \lambda_i^\rho \mathbf{P}_i^\rho\right)^2 = \sum_i (\lambda_i^\rho)^2 \mathbf{P}_i^\rho,$$

and note that since $\mathrm{Tr}\,\boldsymbol{\rho} = \sum_i \lambda_i^\rho = 1,$ each of the λ_i^ρ must be strictly less than one for a mixed state. Hence the eigenvalues of $\boldsymbol{\rho}^2,$ which are equal to the $(\lambda_i^\rho)^2,$ must add up to *less than* one.

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

$$|\Psi_A\rangle \in H_A,$$

and

$$|\Psi_B\rangle \in H_B.$$

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

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

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

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

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

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

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

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

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 $\mathbf{A}$ is an operator on H_A and $\mathbf{B}$ is an operator on H_B, then

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

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

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

is defined by

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

In the case where $\mathbf{A}$ and $\mathbf{B}$ are both normal, we may also write

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

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

$$(|\Psi_A\rangle \otimes |\Psi_B\rangle)(\langle\Psi_A| \otimes \langle\Psi_B|) = |\Psi_A\rangle\langle\Psi_A| \otimes |\Psi_B\rangle\langle\Psi_B|$$
$$= \mathbf{P}_A \otimes \mathbf{P}_B.$$

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}:

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

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

Given subsystem density operators ρ_A and ρ_B, we can form a tensor-product density operator that describes a mixed ensemble of states in H_{AB}:

$$\rho_{AB} = \rho_A \otimes \rho_B.$$

In general, one can form convex combinations of such ρ_{AB} to construct new joint density operators.

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

$$|\Psi_{AB}\rangle = \frac{1}{\sqrt{2}}[|0_A\rangle \otimes |0_B\rangle + |1_A\rangle \otimes |1_B\rangle]$$
$$\rho_{AB} = |\Psi_{AB}\rangle\langle\Psi_{AB}|$$
$$= \frac{1}{2}\begin{bmatrix} |0_A\rangle\langle 0_A| \otimes |0_B\rangle\langle 0_B| + |0_A\rangle\langle 1_A| \otimes |0_B\rangle\langle 1_B| \\ +|1_A\rangle\langle 0_A| \otimes |1_B\rangle\langle 0_B| + |1_A\rangle\langle 1_A| \otimes |1_B\rangle\langle 1_B| \end{bmatrix},$$

and in general

$$\rho_{AB} = \sum_i p_i |\Psi_{AB}^i\rangle\langle\Psi_{AB}^i|.$$

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

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

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

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

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

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

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

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

Working with tensor products

Let's work with our favorite example of two two-dimensional Hilbert spaces H_A and H_B, with given complete orthonormal bases $\{|0_A\rangle, |1_A\rangle\}$ and $\{|0_B\rangle, |1_B\rangle\}$. Let's also choose the simple tensor-product basis for H_{AB}, $\{|0_A 0_B\rangle, |0_A 1_B\rangle, |1_A 0_B\rangle, |1_A 1_B\rangle\}$.

Suppose we are given vectors $|\Psi_A\rangle \in H_A$ and $|\Psi_B\rangle \in H_B$:

$$|\Psi_A\rangle = a_0|0_A\rangle + a_1|1_A\rangle \leftrightarrow \begin{pmatrix} a_0 \\ a_1 \end{pmatrix},$$

$$|\Psi_B\rangle = b_0|0_B\rangle + b_1|1_B\rangle \leftrightarrow \begin{pmatrix} b_0 \\ b_1 \end{pmatrix}.$$

Then $|\Psi_A\Psi_B\rangle \in H_{AB}$ has the vector representation

$$\begin{aligned} |\Psi_A\rangle \otimes |\Psi_B\rangle &= (a_0|0_A\rangle + a_1|1_A\rangle) \otimes (b_0|0_B\rangle + b_1|1_B\rangle) \\ &= a_0 b_0 |0_A 0_B\rangle + a_0 b_1 |0_A 1_B\rangle + a_1 b_0 |1_A 0_B\rangle + a_1 b_1 |1_A 1_B\rangle \\ &\leftrightarrow \begin{pmatrix} a_0 b_0 \\ a_0 b_1 \\ a_1 b_0 \\ a_1 b_1 \end{pmatrix}. \end{aligned}$$

Likewise,

$$\langle \Psi_A \Psi_B| \leftrightarrow \begin{pmatrix} a_0^* b_0^* & a_0^* b_1^* & a_1^* b_0^* & a_1^* b_1^* \end{pmatrix}.$$

Moving on to operators, let's compute a matrix representation for $\boldsymbol{\sigma}_x^A \otimes \boldsymbol{\sigma}_x^B$, where $\boldsymbol{\sigma}_x = |0\rangle\langle 1| + |1\rangle\langle 0|$. So

$$\begin{aligned} \boldsymbol{\sigma}_x^A \otimes \boldsymbol{\sigma}_x^B &= (|0_A\rangle\langle 1_A| + |1_A\rangle\langle 0_A|) \otimes (|0_B\rangle\langle 1_B| + |1_B\rangle\langle 0_B|) \\ &= |0_A 0_B\rangle\langle 1_A 1_B| + |0_A 1_B\rangle\langle 1_A 0_B| + |1_A 0_B\rangle\langle 0_A 1_B| + |1_A 1_B\rangle\langle 0_A 0_B| \\ &\leftrightarrow \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}. \end{aligned}$$

Given the ordering we have chosen for the basis of H_{AB}, we could have also used

$$\mathbf{A} \otimes \mathbf{B} \leftrightarrow \begin{pmatrix} a_{00}B & a_{01}B \\ a_{10}B & a_{11}B \end{pmatrix},$$

where in this case

$$A = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad B = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\mathbf{A} \otimes \mathbf{B} \leftrightarrow \begin{pmatrix} 0\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} & 1\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ 1\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} & 0\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}.$$

Partial projections

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

$$\mathbf{1}^A \otimes \mathbf{P}_j^B$$

and

$$\mathbf{P}_i^A \otimes \mathbf{1}^B,$$

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

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

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

$$(\mathbf{1}^A \otimes \mathbf{P}_k^B)|\Psi_{AB}\rangle = (\mathbf{1}^A \otimes \mathbf{P}_k^B)\sum_{ij} c_{ij}|i_A\rangle \otimes |j_B\rangle$$

$$= \sum_{ij} c_{ij}|i_A\rangle \otimes \mathbf{P}_k^B|j_B\rangle = \sum_i c_{ik}|i_A\rangle \otimes |k_B\rangle = |\Psi_A^k\rangle \otimes |k_B\rangle.$$

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

$$|\Psi_{AB}\rangle = |\Psi_A\rangle \otimes |\Psi_B\rangle,$$

$$|\Psi_B\rangle = \sum_{j=1}^{N_B} c_j^B|j_B\rangle,$$

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

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

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

$$|\Psi_{AB}\rangle = c_1|\Psi_A^1\rangle \otimes |1_B\rangle + c_2|\Psi_A^2\rangle \otimes |2_B\rangle,$$

$$\langle\Psi_A^1|\Psi_A^2\rangle \neq 1,$$

then

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

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

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

$$\sum_{j=1}^{N_B} \mathbf{1}^A \otimes \mathbf{P}_j^B = \mathbf{1}^A \otimes \mathbf{1}^B = \mathbf{1}^{AB},$$

$$\sum_{i=1}^{N_A} \mathbf{P}_i^A \otimes \mathbf{1}^B = \mathbf{1}^A \otimes \mathbf{1}^B.$$

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

$$\{\mathbf{1}^A \otimes \mathbf{P}_0^B, \mathbf{1}^A \otimes \mathbf{P}_1^B, \dots\}$$

or

$$\{\mathbf{P}_0^A \otimes \mathbf{1}^B, \mathbf{P}_1^A \otimes \mathbf{1}^B, \dots\}.$$

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:

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

or

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

But as noted above, the post-measurement state of both subsystems will generally be affected by the outcome, since (for conditioning via the projection postulate)

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

or

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

The usual generalization holds for joint density operators.

Exercise: Suppose systems A and B are initially prepared in the joint pure state

$$|\Psi_{AB}\rangle = \frac{1}{\sqrt{2}}(|0_A\rangle \otimes |0_B\rangle + |1_A\rangle \otimes |1_B\rangle),$$

and we perform a measurement of the A-system observable

$$\mathbf{S}_{xA} \otimes \mathbf{1}^B = \frac{\hbar}{2}\mathbf{P}_{x+}^A \otimes \mathbf{1}^B - \frac{\hbar}{2}\mathbf{P}_{x-}^A \otimes \mathbf{1}^B,$$

$$\mathbf{P}_{x+} \equiv |x_+\rangle\langle x_+|, \quad |x_+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle),$$

$$\mathbf{P}_{x-} \equiv |x_-\rangle\langle x_-|, \quad |x_-\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle).$$

What are the possible post-measurement states? What if the initial preparation is the following mixed state?

$$\rho_{AB} = \frac{1}{2}(|0_A 0_B\rangle\langle 0_A 0_B| + |1_A 1_B\rangle\langle 1_A 1_B|).$$

Partial trace and reduced density operators

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

$$\rho_{AB} = \sum_{ijkl} \rho_{ijkl} |i_A\rangle \otimes |j_B\rangle\langle k_A| \otimes \langle l_B|,$$

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

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

We define the partial trace of ρ_{AB} over the B subsystem to be

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

Here $\tilde{\rho}_A$ 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.

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

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

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

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

Likewise,

$$\mathrm{Tr}[\tilde{\rho}_A \mathbf{P}_i^A] = \mathrm{Tr}\left[\sum_{k,l=1}^{N_A} \left(\sum_{j=1}^{N_B} \rho_{ijkj}\right) |k_A\rangle\langle l_A| \mathbf{P}_i^A\right]$$
$$= \mathrm{Tr}\left[\sum_{k=1}^{N_A} \left(\sum_{j=1}^{N_B} \rho_{ijkj}\right) |k_A\rangle\langle i_A|\right]$$
$$= \sum_{m=1}^{N_A} \langle m_A| \sum_{k=1}^{N_A} \left(\sum_{j=1}^{N_B} \rho_{ijkj}\right) |k_A\rangle\langle i_A| |m_A\rangle$$

$$= \sum_{m=1}^{N_A} \sum_{k=1}^{N_A} \left(\sum_{j=1}^{N_B} \rho_{ijkj} \right) \delta_{mk} \delta_{im}$$

$$= \sum_{j=1}^{N_B} \rho_{ijij}.$$

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

$$\mathrm{Tr}_B[\boldsymbol{\rho}_{AB}] = \sum_{m=1}^{N_B} \langle m_B | \boldsymbol{\rho}_{AB} | m_B \rangle = \sum_{m=1}^{N_B} \langle m_B | \left(\sum_{ijkl} \rho_{ijkl} | i_A \rangle \otimes | j_B \rangle \langle k_A | \otimes \langle l_B | \right) | m_B \rangle$$

$$= \sum_{m=1}^{N_B} \sum_{i,k=1}^{N_A} \rho_{imkm} | i_A \rangle \langle k_A |.$$

It is perhaps useful to see a few examples of this type of manipulation.

Open quantum systems

Suppose we have a composite system $H_{AB} = H_A \otimes H_B$ with Hamiltonian $\mathbf{H}_{AB}$. We know that the overall dynamics is described by the SE

$$i\hbar \frac{d}{dt} |\Psi_{AB}(t)\rangle = \mathbf{H}_{AB} |\Psi_{AB}(t)\rangle.$$

Let's say, however, that H_A corresponds to a small, 'compact' physical system that we are trying to study in the lab, whereas H_B actually represents the degrees of freedom of some environmental reservoir. If we are unable (as is always the case) to completely isolate the system from the environment, then the Hamiltonian will not separate: $\mathbf{H}_{AB} \neq \mathbf{H}_A \otimes \mathbf{1}_B + \mathbf{1}_A \otimes \mathbf{H}_B$, $\mathbf{T}_{AB}(t,0) \neq \mathbf{T}_A(t,0) \otimes \mathbf{T}_B(t,0)$. Hence, even for pure initial states of the system $|\Psi_A(0)\rangle \in H_A$, the above SE *may* (for some initial states) induce evolution into entangled states of the system and environment.

In general we will be unable to perform complete measurements on the joint Hilbert space H_{AB}, because reservoirs are usually infinite-dimensional (hence H_{AB} will be also). So limiting our attention to the system H_A, it appears that we must settle for a density-operator description obtained by tracing over the environmental degrees of freedom:

$$\tilde{\rho}_A(t) = \mathrm{Tr}_B[|\Psi_{AB}(t)\rangle\langle\Psi_{AB}(t)|].$$

From what we have learned about entanglement in previous lectures, we may expect that this type of evolution (formation of entanglements with an unobservable reservoir) will lead to loss of purity for the system state. Such phenomena are generally referred to as 'decoherence.'

Under certain assumptions about the nature of $\mathbf{H}_{AB}$ and of the environment H_B, it is sometimes possible to derive a closed-form evolution equation for the reduced density operator $\tilde{\rho}_A(t)$. In a 'Master Equation' of this type, operators and states for H_B do not appear explicitly because they have been analytically traced-out of the equations of motion. This type of approach is particularly useful for understanding things like dissipation and thermal fluctuations in a quantum-mechanical setting, and the overall field of studying these things has come to be known as the theory of open quantum systems.