Multiple systems, the tensor-product space, and the partial trace
Carlton M. Caves
2005 September 15

Consider two quantum systems, A and B. System A is described by a d_A-dimensional Hilbert space $\mathcal{H}_A$, and system B is described by a d_B-dimensional Hilbert space $\mathcal{H}_B$. What we want to do is to construct the Hilbert space that describes the composite system consisting of both A and B.

The composite space certainly must have a way of describing the situation where A has the (pure) state $|\psi\rangle$ and B has the (pure) state $|\phi\rangle$. We denote the corresponding composite state by $|\psi\rangle \otimes |\phi\rangle$, and we call such a state a *product state*. For the present, the product symbol $\otimes$, read as "o-times," is simply a way of separating the state of A from the state of B, with the state of A on the left and the state of B on the right. More generally, of course, we can apply this product to unnormalized vectors from A and B, and we do so freely in what follows without paying much attention to whether we are talking about normalized or unnormalized vectors. The set of all product states is not a vector space; it is the *Cartesian product* of $\mathcal{H}_A$ and $\mathcal{H}_B$, i.e., the set of all ordered pairs consisting of a vector from $\mathcal{H}_A$ and a vector from $\mathcal{H}_B$.

Now suppose we write $|\psi\rangle$ as a superposition of two other states of A, i.e., $|\psi\rangle = a|\chi\rangle + b|\xi\rangle$. It is certainly reasonable to write

$$|\psi\rangle \otimes |\phi\rangle = (a|\chi\rangle + b|\xi\rangle) \otimes |\phi\rangle = a|\chi\rangle \otimes |\phi\rangle + b|\xi\rangle \otimes |\phi\rangle \ , \tag{1}$$

since all this is saying is that superposing two states of A and then saying B has state $|\phi\rangle$ is the same as saying B has state $|\phi\rangle$ and then superposing the corresponding two composite states. This innocuous assumption, along with the same considerations for B, already says, however, that the o-times product is bilinear in both its inputs.

We can see that the Cartesian product is not a vector space by noting that a linear combination of two product vectors,

$$a|\psi\rangle \otimes |\phi\rangle + b|\chi\rangle \otimes |\xi\rangle \ , \tag{2}$$

is not generally a product vector. It being a general principle of quantum mechanics that systems are described by complex vector spaces, we now assume, in accordance with this principle, that the appropriate state space for the composite system is not just the Cartesian product, but rather the entire vector space spanned by the product states. This is a fateful assumption, because it leads to the phenomenon of *quantum entanglement*, entangled pure states being precisely the composite states that are not product states. The vector space spanned by the product states, denoted by $\mathcal{H}_A \otimes \mathcal{H}_B = \mathcal{H}_{AB}$, is called the *tensor product* of $\mathcal{H}_A$ and $\mathcal{H}_B$. The o-times symbol is now read as "tensor product." The inner product on $\mathcal{H}_{AB}$ is defined by defining the inner product of two product vectors as

$$(\langle\psi| \otimes \langle\phi|)(|\chi\rangle \otimes |\xi\rangle) = \langle\psi|\chi\rangle\langle\phi|\xi\rangle \tag{3}$$

and extending this definition to all vectors in $\mathcal{H}_{AB}$ by the complex bilinearity of the inner product.

We often use capital letters to denote vectors in the tensor-product space, as in $|\Psi\rangle$, and when confusion threatens, we use subscripts (or superscripts) to indicate to which system a vector belongs, as in $|\psi_A\rangle$ for a vector in $\mathcal{H}_A$ or $|\Psi_{AB}\rangle$ for a vector in $\mathcal{H}_{AB}$.

Any vector $|\Psi\rangle$ in $\mathcal{H}_{AB}$ can be written as a linear combination of product vectors, all the vectors in the products can be expanded in orthonormal bases, $|e_j\rangle$, $j = 1, \ldots, d_A$, for A and $|f_k\rangle$, $k = 1, \ldots, d_B$, for B, and the bilinearity of the tensor product can then be used to write $|\Psi\rangle$ as a linear combination of the orthonormal product vectors $|e_j\rangle \otimes |f_k\rangle$, showing that these product vectors are a basis for $\mathcal{H}_{AB}$. The number of these vectors is $d_A d_B$, which means that the dimension of the tensor-product space is $d_A d_B$. We often leave out the inner-product symbol in these basis vectors, writing, in increasing order of omitting redundancies, such things as

$$|e_j\rangle \otimes |f_k\rangle = |e_j\rangle|f_k\rangle = |e_j, f_k\rangle = |j,k\rangle = |jk\rangle \; . \tag{4}$$

The expansion of an arbitrary vector in $\mathcal{H}_{AB}$ looks like

$$|\Psi\rangle = \sum_{j,k} |e_j, f_k\rangle\langle e_j, f_k|\Psi\rangle = \sum_{j,k} c_{jk}|e_j, f_k\rangle = \sum_{j,k} c_{jk}|e_j\rangle \otimes |f_k\rangle \; . \tag{5}$$

The expansion coefficients $c_{jk} = \langle e_j, f_k|\Psi\rangle$ can be written as a matrix, or in accord with our usual notation for representations of vectors, they can be written as a column vector:

$$|\Psi\rangle \to \begin{pmatrix} c_{11} \\ \vdots \\ c_{1d_B} \\ c_{21} \\ \vdots \\ c_{2d_B} \\ c_{d_A 1} \\ \vdots \\ c_{d_A d_B} \end{pmatrix} = \begin{pmatrix} \vec{c}_1 \\ \vdots \\ \vec{c}_{d_A} \end{pmatrix} \; . \tag{6}$$

In the second form, we introduce d_B-dimensional column vectors

$$\vec{c}_j = \begin{pmatrix} c_{j1} \\ \vdots \\ c_{jd_B} \end{pmatrix} \; , \tag{7}$$

thus showing how we can think of a vector in the tensor-product space as a d_A-dimensional vector whose components are themselves d_B-dimensional vectors. One should recognize that Eqs. (6) and (7) are simply the column-vector version of the following way of writing $|\Psi\rangle$:

$$|\Psi\rangle = \sum_j |e_j\rangle \otimes \left(\sum_k c_{jk}|f_k\rangle \right) \; . \tag{8}$$

The expansion coefficients of a product vector $|\psi\rangle \otimes |\phi\rangle$ are the outer product of the expansion coefficients for $|\psi\rangle = \sum_j a_k |e_k\rangle$ and $|\phi\rangle = \sum_k b_k |f_k\rangle$, i.e.,

$$c_{jk} = \langle e_j, f_k|(|\psi\rangle \otimes |\phi\rangle) = \langle e_j|\psi\rangle\langle f_k|\phi\rangle = a_j b_k \;, \tag{9}$$

which means that the column vectors in Eq. (7) are A-dependent multiples of the column vector for $|\phi\rangle$:

$$\vec{c}_j = a_j \begin{pmatrix} b_1 \\ \vdots \\ b_{d_B} \end{pmatrix} \;. \tag{10}$$

Once we have the tensor product under our belt, we realize that we can make sense of what might be called the "partial inner product," $\langle \phi_B|\Psi_{AB}\rangle$. This is defined to be the ket in $\mathcal{H}_A$ whose inner product with any vector $|\psi_A\rangle$ in $\mathcal{H}_A$ is the same as the complete inner product of $|\psi_A\rangle \otimes |\phi_B\rangle$ with $|\Psi_{AB}\rangle$, i.e.,

$$\langle \psi_A|\big(\langle \phi_B|\Psi_{AB}\rangle\big) = (\langle \psi_A| \otimes \langle \phi_B|)|\Psi_{AB}\rangle \;. \tag{11}$$

Working this out explicitly in the product basis $|e_j, f_k\rangle$, we get

$$\langle \phi_B|\Psi_{AB}\rangle = \sum_{j,k} c_{jk}|e_j\rangle\langle \phi_B|f_k\rangle = \sum_j |e_j\rangle \left(\sum_k b_k^* c_{jk}\right) \;. \tag{12}$$

The final form on the right makes clear that the partial inner product is the inner product of b_k with the second (system B) index of c_{jk}, with the first (system A) index left over to form a vector for system A. The partial inner product with a product state is obviously $\langle \xi_B|(|\psi_A\rangle \otimes |\phi_B\rangle) = |\psi_A\rangle\langle \xi_B|\phi_B\rangle$. We can, of course, define in the same way a partial inner product $\langle \psi_A|\Psi_{AB}\rangle$. It is worth noting that the partial inner product $\langle e_j|\Psi_{AB}\rangle = \sum_k c_{jk}|f_k\rangle$ is the vector in $\mathcal{H}_B$ that is represented by the column vector $\vec{c}_j$. Thus another way of thinking of the partial inner product is that it is a way of generating the column vectors $\vec{c}_j$.

We're now ready to go on to operators acting on the tensor-product space. The basic operators are outer products

$$|\psi\rangle \otimes |\phi\rangle\langle \chi| \otimes \langle \xi| = |\psi\rangle\langle \chi| \otimes |\phi\rangle\langle \xi| \;. \tag{13}$$

The first form is in standard outer-product notation in the tensor-product space; we know how to handle this form because we have defined the inner product on the tensor-product space. The second form re-arranges the outer product as a tensor product of an outer-product operators for A and B. This innocuous re-arrangement defines the tensor product of operators. Equation (13) defines the definition of a tensor product of outer products; the definition is extended to the outer product of any two operators by assuming that the operator tensor product is bilinear, i.e.,

$$\begin{aligned} A \otimes B &= \left(\sum_{j,l} A_{jl}|e_j\rangle\langle e_l|\right) \otimes \left(\sum_{k,m} B_{km}|f_k\rangle\langle f_m|\right) \\ &= \sum_{j,k,l,m} A_{jl}B_{km}|e_j\rangle\langle e_l| \otimes |f_k\rangle\langle f_m| \\ &= \sum_{j,k,l,m} A_{jl}B_{km}|e_j, f_k\rangle\langle e_l, f_m| \;. \end{aligned} \tag{14}$$

Once we're working in the tensor-product space, we really should write an operator A acting on $\mathcal{H}_A$ as $A \otimes I_B$, i.e.,

$$A \otimes I_B = \sum_{j,l,k} A_{jl} |e_j\rangle\langle e_l| \otimes |f_k\rangle\langle f_k| = \sum_{j,l,k} A_{jl} |e_j, f_k\rangle\langle e_l, f_k| \, . \tag{15}$$

Likewise, an operator B acting on $\mathcal{H}_B$ should be written as $I_A \otimes B$. We usually ignore this nicety unless doing so causes confusion. It is easy to verify from Eq. (14) that $(A_1 \otimes B_1)(A_2 \otimes B_2) = A_1 A_2 \otimes B_1 B_2$.

An arbitrary operator O acting on the tensor-product space can be expanded as

$$O = \sum_{j,l,k,m} O_{jk,lm} |e_j, f_k\rangle\langle e_l, f_m| = \sum_{j,k,l,m} O_{jk,lm} |e_j\rangle\langle e_l| \otimes |f_k\rangle\langle f_m| \, . \tag{16}$$

Using our usual notation for representing an operator as a matrix, we write

$$O \rightarrow \begin{pmatrix} O_{11,11} & \cdots & O_{11,1d_B} & \cdots & O_{11,d_A 1} & \cdots & O_{11,d_A d_B} \\ \vdots & \ddots & \vdots & \cdots & \vdots & \ddots & \vdots \\ O_{1d_B,11} & \cdots & O_{1d_B,1d_B} & \cdots & O_{1d_B,d_A 1} & \cdots & O_{1d_B,d_A d_B} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ O_{d_A 1,11} & \cdots & O_{d_A 1,1d_B} & \cdots & O_{d_A 1,d_A 1} & \cdots & O_{d_A 1,d_A d_B} \\ \vdots & \ddots & \vdots & \cdots & \vdots & \ddots & \vdots \\ O_{d_A d_B,11} & \cdots & O_{d_A d_B,1d_B} & \cdots & O_{d_A d_B,d_A 1} & \cdots & O_{d_A d_B,d_A d_B} \end{pmatrix} \tag{17}$$

$$= \begin{pmatrix} O_{11} & \cdots & O_{1d_A} \\ \vdots & \ddots & \vdots \\ O_{d_A 1} & \cdots & O_{d_A d_A} \end{pmatrix} .$$

In the second form, we introduce $(d_B \times d_B)$-dimensional matrices

$$O_{jl} = \begin{pmatrix} O_{j1,l1} & \cdots & O_{j1,ld_B} \\ \vdots & \ddots & \vdots \\ O_{jd_B,l1} & \cdots & O_{jd_B,ld_B} \end{pmatrix} , \tag{18}$$

thus showing how we can think of a matrix in the tensor-product space as a $(d_A \times d_A)$-dimensional matrix whose components are themselves $(d_B \times d_B)$-dimensional matrices. One should recognize that Eqs. (17) and (18) are simply the matrix version of the following way of writing O:

$$O = \sum_{j,l} |e_j\rangle\langle e_l| \otimes \left(\sum_{k,m} O_{jk,lm} |f_k\rangle\langle f_m| \right) . \tag{19}$$

This realization should cure one of wanting to write the explicit matrix forms ever again, but it is useful to able to look at Eq. (19) and to be able to reconstruct the matrices (17) and (18) in your head.

Using the partial inner product, we can go on to define a "partial matrix element" of a composite operator O,

$$\langle\phi_B|O|\xi_B\rangle = \sum_{j,l} |e_j\rangle\langle e_l| \left(\sum_{k,m} O_{jk,lm} \langle\phi_B|f_k\rangle\langle f_m|\xi_B\rangle \right) , \tag{20}$$

which is an operator acting on system A. It should be obvious that the partial matrix element of a tensor product is $\langle\phi_B|A\otimes B|\xi_B\rangle = A\langle\phi_B|B|\xi_B\rangle$. Nearly as obvious is that $\langle\phi_B|(A\otimes I_B)O|\xi_B\rangle = A\langle\phi_B|O|\xi_B\rangle$ and $\langle\phi_B|O(A\otimes I_B)|\xi_B\rangle = \langle\phi_B|O|\xi_B\rangle A$. In the same way, we can, of course, define a partial matrix element $\langle\psi_A|O|\chi_A\rangle$. It is worth noting that

$$\langle e_j|O|e_l\rangle = \sum_{k,m} O_{jk,lm} |f_k\rangle\langle f_m| \tag{21}$$

is the operator that has the matrix representation (18).

We have all the ingredients now to define the partial trace of a composite operator O. The partial trace of O with respect to system B is an operator on system A:

$$\mathrm{tr}_B(O) = \sum_k \langle f_k|O|f_k\rangle = \sum_{j,l} O_{jk,lk} |e_j\rangle\langle e_k| . \tag{22}$$

The partial trace of O with respect to A is similarly defined as

$$\mathrm{tr}_A(O) = \sum_j \langle e_j|O|e_j\rangle = \sum_{k,m} O_{jk,jm} |f_k\rangle\langle f_m| . \tag{23}$$

Notice that the complete trace can be obtained by doing two partial traces:

$$\mathrm{tr}(O) = \sum_{j,k} O_{jk,jk} = \mathrm{tr}_A\big(\mathrm{tr}_B(O)\big) = \mathrm{tr}_B\big(\mathrm{tr}_A(O)\big) . \tag{24}$$

In the same way as the complete trace, the partial trace is linear and independent of the orthonormal basis used to calculate it. It should be obvious that $\mathrm{tr}_B(A\otimes B) = A\mathrm{tr}(B)$. Nearly as obvious is that $\mathrm{tr}_B\big((A\otimes I_B)O\big) = A\mathrm{tr}_B(O)$ and $\mathrm{tr}_B\big(O(A\otimes I_B)\big) = \mathrm{tr}_B(O)A$.

It is not generally true that $\mathrm{tr}_B(NO) = \mathrm{tr}_B(ON)$, as one discovers by trying to duplicate the proof for the complete trace:

$$\mathrm{tr}_B(NO) = \sum_k \langle f_k|NO|f_k\rangle = \sum_{k,m} \langle f_k|N|f_m\rangle\langle f_m|O|f_k\rangle . \tag{25}$$

When dealing with the complete trace, one can switch the order of the matrix elements, since they are complex numbers, thus changing the order of the product. In contrast, the partial matrix elements in Eq. (25) are *operators* on system A, and these operators generally don't commute. It is true, however, that

$$\mathrm{tr}_B\big((I_A\otimes B)O\big) = \mathrm{tr}_B\big(O(I_A\otimes B)\big) , \tag{26}$$

because in this case the partial matrix element $\langle f_k|I_A \otimes B|f_m\rangle = I_A\langle f_k|B|f_m\rangle$ is a multiple of the unit operator, so it does commute with $\langle f_m|O|f_k\rangle$. In the same way, we can also show that

$$\begin{aligned} \mathrm{tr}_B\big(O(I_A \otimes |\phi_B\rangle\langle\xi_B|)\big) &= \sum_{k,m}\langle f_k|O|f_m\rangle\langle f_m|\phi_B\rangle\langle\xi_B|f_k\rangle \\ &= \sum_{k,m}\langle\xi_B|f_k\rangle\langle f_k|O|f_m\rangle\langle f_m|\phi_B\rangle \\ &= \langle\xi_B|O|\phi_B\rangle \ , \end{aligned} \tag{27}$$

so that the partial trace with respect to B does turn an outer product on B into a partial matrix element with respect to B. The main thing to be alert to in performing these manipulations is which objects are operators and which are complex numbers—in Eq. (27), $\langle f_k|O|f_m\rangle$ is an operator on system A, whereas $\langle f_m|\phi_B\rangle$ and $\langle\xi_B|f_k\rangle$ are complex numbers—since we use the same notation that for a single system, made everything a complex number.

We use the partial trace for a lot of things—we really couldn't do without it—but it receives its main justification from the notion of a marginal density operator for a subsystem of a composite system. If the composite system has the density operator ρ_{AB}, a measurement in the basis $|e_j\rangle$ on system A yields result j with probability

$$p_j = \sum_k p_{jk} = \sum_k \langle e_j, f_k|\rho_{AB}|e_j, f_k\rangle \ , \tag{28}$$

In writing this expression, we imagine that in addition to the measurement in the basis $|e_j\rangle$ on system A, a measurement in an arbitrary basis $|f_k\rangle$ is made on system B. To find the probability for j, we sum the joint probabilities over the results of the measurement on B, in accordance with the rules for classical probabilities The probability for result j can be put in the form

$$p_j = \langle e_j|\Bigg(\underbrace{\sum_k \langle f_k|\rho_{AB}|f_k\rangle}_{=\,\mathrm{tr}_B(\rho_{AB}) = \rho_A}\Bigg)|e_j\rangle = \langle e_j|\rho_A|e_j\rangle \ . \tag{29}$$

where $\rho_A = \mathrm{tr}_B(\rho_{AB})$, obtained by taking the partial trace of ρ_{AB} with respect to B, is called the *marginal* density operator of system A. We use this terminology because as far as measurements on A are concerned, all probabilities are calculated as though ρ_A is the density operator of system A.

We can put p_j in other useful forms through the following manipulations:

$$\begin{aligned}
p_j &= \sum_k \mathrm{tr}\big(\rho_{AB}|e_j, f_k\rangle\langle e_j, f_k|\big) \\
&= \sum_k \mathrm{tr}\big(\rho_{AB}|e_j\rangle\langle e_j| \otimes |f_k\rangle\langle f_k|\big) \\
&= \mathrm{tr}\left(\rho_{AB}|e_j\rangle\langle e_j| \otimes \left(\sum_k |f_k\rangle\langle f_k|\right)\right) \\
&= \mathrm{tr}\big(\rho_{AB}(P_j \otimes I_B)\big) \\
&= \mathrm{tr}_A\Big(\mathrm{tr}_B\big(\rho_{AB}(P_j \otimes I_B)\big)\Big) \\
&= \mathrm{tr}_A\big(\mathrm{tr}_B(\rho_{AB})P_j\big) \\
&= \mathrm{tr}_A(\rho_A P_j)\ .
\end{aligned} \tag{30}$$

In the last form, we get back to Eq. (29). In the middle, we find that when we are working with the composite state ρ_{AB}, the projection operator that goes with a particular result on A is $P_j \otimes I_B = |e_j\rangle\langle e_j| \otimes I_B$, which is a multi-dimensional projector with rank d_B, corresponding to the fact that result j is degenerate, with d_B different possibilities for system B.

Let's put this machinery into action in a particular case. Suppose we have two qubits in the pure state

$$|\Psi_{AB}\rangle = \cos\theta|00\rangle + \sin\theta|11\rangle\ . \tag{31}$$

The corresponding composite density operator is

$$\rho_{AB} = |\Psi_{AB}\rangle\langle\Psi_{AB}| = \cos^2\theta|00\rangle\langle 00| + \sin^2\theta|11\rangle\langle 11| + \cos\theta\sin\theta\big(|00\rangle\langle 11| + |11\rangle\langle 00|\big)\ . \tag{32}$$

A measurement of $Z = |0\rangle\langle 0| - |1\rangle\langle 1|$ yields $+1$ with probability

$$\begin{aligned}
p_{+1} &= \mathrm{tr}\big(\rho_{AB}P_{\mathbf{e}_z} \otimes I_B\big) \\
&= \langle\Psi_{AB}|P_{\mathbf{e}_z} \otimes I_B|\Psi_{AB}\rangle \\
&= \langle\Psi_{AB}|\big(|0\rangle\langle 0| \otimes (|0\rangle\langle 0| + |1\rangle\langle 1|)\big)|\Psi_{AB}\rangle \\
&= \langle\Psi_{AB}|(|00\rangle\langle 00| + |01\rangle\langle 01|)|\Psi_{AB}\rangle \\
&= \cos^2\theta\ .
\end{aligned} \tag{33}$$

We can get the same result by calculating the marginal density operator

$$\begin{aligned}
\rho_A &= \mathrm{tr}_B(\rho_{AB}) \\
&= \cos^2\theta\,\mathrm{tr}_B\big(|00\rangle\langle 00|\big) + \sin^2\theta\,\mathrm{tr}_B\big(|11\rangle\langle 11|\big) \\
&\qquad + \cos\theta\sin\theta\Big(\mathrm{tr}_B\big(|00\rangle\langle 11|\big) + \mathrm{tr}_B\big(|11\rangle\langle 00|\big)\Big) \\
&= \cos^2\theta\,|0\rangle\langle 0|\langle 0|0\rangle + \sin^2\theta\,|1\rangle\langle 1|\langle 1|1\rangle\cos\theta\sin\theta\big(|0\rangle\langle 1|\langle 1|0\rangle + |1\rangle\langle 0|\langle 0|1\rangle\big) \\
&= \cos^2\theta\,|0\rangle\langle 0| + \sin^2\theta\,|1\rangle\langle 1|\ ,
\end{aligned} \tag{34}$$

from which we calculate

$$p_{+1} = \mathrm{tr}_A\big(\rho_A P_{\mathbf{e}_z}\big) = \mathrm{tr}_A\big(\rho_A|0\rangle\langle 0|\big) = \langle 0|\big(\cos^2\theta\,|0\rangle\langle 0| + \sin^2\theta\,|1\rangle\langle 1|\big)|0\rangle = \cos^2\theta\ . \tag{35}$$