

## Appendix A

# Combining systems: the tensor product and partial trace

### A.1 Combining two systems

The state of a quantum system is a vector in a complex vector space. (Technically, if the dimension of the vector space is infinite, then it is a separable Hilbert space). Here we will always assume that our systems are finite dimensional. We do this because everything we will discuss transfers without change to infinite dimensional systems. Further, when one actually simulates a system on a computer, one must always truncate an infinite dimensional space so that it is finite.

Consider two separate quantum systems. Now consider the fact that if we take them together, then we should be able to describe them as one big quantum system. That is, instead of describing them by two separate state-vectors, one for each system, we should be able to represent the states of both of them together using one single state-vector. (This state vector will naturally need to have more elements in it than the separate state-vectors for each of the systems, and we will work out exactly how many below.) In fact, in order to describe a situation in which the two systems have affected each other — by interacting in some way — and have become correlated with each other as a result of this interaction, we will *need* to go beyond using a separate state vector for each. If each system is in a pure state, described by a state-vector for it alone, then there are no correlations between the two systems. Using a single state-vector to describe the joint state of the two systems is the natural way to describe all possible states that the two systems could be in (correlated or uncorrelated). We now show how this is done.

Let us say we have two quantum systems, A and B, both of which are two-dimensional. These could be, for example, the spins of two spin-1/2 particles. Let us denote the basis states of A by  $|A_0\rangle$  and  $|A_1\rangle$ , and those of B as  $|B_0\rangle$  and  $|B_1\rangle$ . We need to determine a vector-space that will describe both systems together. First, let us determine a set of basis vectors for this space. We know that each of the two systems can be in one of two mutually orthogonal (distinguishable) states. This means that the systems together can be in one of four possible distinguishable states: for each state of system A there are two possible states of system B, and  $2 \times 2 = 4$ . So these states must be a set of basis states for the combined

system. Let us denote these four basis states as

$$\begin{aligned} |C_{00}\rangle &= |A_0\rangle|B_0\rangle, \\ |C_{01}\rangle &= |A_0\rangle|B_1\rangle, \\ |C_{10}\rangle &= |A_1\rangle|B_0\rangle, \\ |C_{11}\rangle &= |A_1\rangle|B_1\rangle. \end{aligned} \quad (\text{A.1})$$

A state of the combined system is thus a 4-dimensional vector, being a complex linear combination of the four basis states. Let us denote the state of the combined system as

$$|\psi_C\rangle = \sum_{ij} c_{ij} |C_{ij}\rangle, \quad (\text{A.2})$$

and write it as

$$|\psi_C\rangle = \begin{pmatrix} c_{00} \\ c_{01} \\ c_{10} \\ c_{11} \end{pmatrix}. \quad (\text{A.3})$$

The next question we need to ask is, if A has been prepared in state  $|\psi_A\rangle = a_0|A_0\rangle + a_1|A_1\rangle$ , and B has been separately prepared in state  $|\psi_B\rangle = b_0|B_0\rangle + b_1|B_1\rangle$ , what is the state-vector that describes the combined system? To work this out we first note that in this case, because A and B have been prepared separately, they are uncorrelated. That is, the state of A in no way depends on the state of B. In particular, the probabilities that A is in either of its basis states does not depend on which basis state B is in, and vice versa. We next note that the state of the combined system that we seek, must give the same probabilities for the basis states of A and B as do the individual states of A and B. If we denote the probabilities for the A basis states as  $P(A_i)$ , and those of the B basis states as  $P(B_j)$ , then  $P(A_i) = |a_i|^2$  and  $P(B_j) = |b_j|^2$ . Because the states of A and B are *uncorrelated*, the joint probability distribution for the basis states of A and B is just the product of the distributions for each. That is

$$P(A_i, B_j) = P(A_i)P(B_j) = |a_i|^2|b_j|^2 = |a_i b_j|^2. \quad (\text{A.4})$$

The probability distribution for the states of A and B as determined by  $|\psi_C\rangle$  is

$$P(A_i, B_j) = |c_{ij}|^2. \quad (\text{A.5})$$

Equating Eqs.(A.4) and (A.5) we see that we require  $|c_{ij}|^2 = |a_i b_j|^2$ , and we can satisfy this by choosing

$$c_{ij} = a_i b_j. \quad (\text{A.6})$$

Using this relation the state of the joint system is

$$|\psi_C\rangle = \begin{pmatrix} a_0 b_0 \\ a_0 b_1 \\ a_1 b_0 \\ a_1 b_1 \end{pmatrix} = \begin{pmatrix} a_0 \begin{pmatrix} b_0 \\ b_1 \end{pmatrix} \\ a_1 \begin{pmatrix} b_0 \\ b_1 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} a_0 |\psi_B\rangle \\ a_1 |\psi_B\rangle \end{pmatrix} \quad (\text{A.7})$$

So to form the vector for the combined system, we have multiplied the vector for B by each of the elements of the vector for A, and stacked the resulting vectors end-to-end. This operation is called “taking the tensor product of the vectors of A and B”, and denoted by “ $\otimes$ ”. We write

$$|\psi_C\rangle = |\psi_A\rangle \otimes |\psi_B\rangle. \quad (\text{A.8})$$

Naturally the density matrix for the combined system is  $\rho^C = |\psi_C\rangle\langle\psi_C|$ . If we denote the density matrix of A by  $\rho = |\psi_A\rangle\langle\psi_A|$  and that of B by  $\sigma = |\psi_B\rangle\langle\psi_B|$ , then a little calculation shows that (this is a good exercise)

$$\rho^C = \begin{pmatrix} \rho_{11} \begin{pmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{21} & \sigma_{22} \end{pmatrix} & \rho_{12} \begin{pmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{21} & \sigma_{22} \end{pmatrix} \\ \rho_{21} \begin{pmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{21} & \sigma_{22} \end{pmatrix} & \rho_{22} \begin{pmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{21} & \sigma_{22} \end{pmatrix} \end{pmatrix} = \begin{pmatrix} \rho_{11} \sigma & \rho_{12} \sigma \\ \rho_{21} \sigma & \rho_{22} \sigma \end{pmatrix} \quad (\text{A.9})$$

where the  $\rho_{ij}$  are the elements of the density matrix of A. We see that to form the density matrix of the combined system we multiply the density matrix of B with each of the elements of the density matrix of A. This is the same operation that we used to obtain the state-vector for the combined system, but now generalized for matrices. We write it as

$$\rho^C = \rho \otimes \sigma. \quad (\text{A.10})$$

We know now how to determine the state of the total system, when each of the subsystems is in a separate state, independent of the other. Next we need to know how to write the (two-dimensional) operators for each system as operators in the (4-dimensional) combined space. Let us consider first an operator  $U_B$  acting on B. We know that for a state such as  $|\psi_C\rangle$  above, in which each system is in its "own" state, uncorrelated with the other system, the operator  $U_B$  must change the state of B, but leave the state of A alone. This means that  $U_B$  must change the coefficients  $b_0$  and  $b_1$  appearing in  $|\psi^C\rangle$ , while leaving the coefficients  $a_0$  and  $a_1$  unchanged. This is precisely the action of the operator

$$U_{\text{full}}^B = \begin{pmatrix} U^B & \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \\ \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} & U^B \end{pmatrix} = I_2 \otimes U^B, \quad (\text{A.11})$$

where  $I_2$  is the 2-dimensional identity operator. Using the same argument, an operator for system A must take the form

$$U_{\text{full}}^A = \begin{pmatrix} U_{11}^A \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} & U_{12}^A \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\ U_{21}^A \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} & U_{22}^A \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \end{pmatrix} = U^A \otimes I_2, \quad (\text{A.12})$$

where the  $U_{ij}^A$  are the matrix elements of  $U^A$ .

An interaction between systems A and B is described by a term in the Hamiltonian that depends jointly upon physical observables of both systems. As an example, the total energy of the combined system may contain a term that is the product of the values of the  $z$ -component of spin for the two systems. We can determine the 4-dimensional operator that correspond to this product by working in the basis in which the operators for the  $z$ -components of spin for the two systems are diagonal (the eigenbasis of both operators). Let us denote the  $\sigma_z$  operator for A by  $\sigma_z^A$ , and that for B by  $\sigma_z^B$ . Let us denote the respective eigenstates of these operators as  $|\pm\rangle_A$  and  $|\pm\rangle_B$ , so that

$$\sigma_z^A |\alpha\rangle_A = \alpha |\alpha\rangle_A, \quad \text{where } \alpha = \pm 1, \quad (\text{A.13})$$

$$\sigma_z^B |\beta\rangle_B = \beta |\beta\rangle_B, \quad \text{where } \beta = \pm 1, \quad (\text{A.14})$$

If we denote the operator that corresponds to the product of  $\sigma_z^A$  and  $\sigma_z^B$  as  $\sigma_z^A \sigma_z^B$ , then it must have the property that

$$\sigma_z^A \sigma_z^B |n\rangle_A |m\rangle_B = \alpha \beta |\alpha\rangle_A |\beta\rangle_B. \quad (\text{A.15})$$

By writing the basis states of the joint system as products of the bases  $\{|\pm\rangle_A\}$  and  $\{|\pm\rangle_B\}$ , it is clear that  $\sigma_z^A \sigma_z^B$  is given by

$$\sigma_z^A \sigma_z^B = \sigma_z^A \otimes \sigma_z^B. \quad (\text{A.16})$$

It is important to note that when a joint system evolves under a Hamiltonian that includes interactions between the subsystems, the resulting state of the joint system can, in general, no longer be written as a tensor product of states of each of the subsystems. When two systems interact their states becomes correlated. This means that the joint probability distribution giving the probabilities that each of them are in either of two basis states no longer factors into the respective probability distributions for each subsystem. Further, the state of the two systems will, in general, become *entangled*, such that the correlations between observables of both subsystems can no longer be described by classical correlations. In this book we do not deal with the properties of entanglement — this interesting subject is discussed in detail in, e.g. [25, 228–230].

Note that if we reorder the basis states of the combined system we can swap the roles of system A and B in our representation. That is, we can alternatively use the convention

$$\rho^C = \begin{pmatrix} \sigma_{11} \rho & \sigma_{12} \rho \\ \sigma_{21} \rho & \sigma_{22} \rho \end{pmatrix} \equiv \rho \otimes \sigma \quad (\text{A.17})$$

for the density matrix of the combined system, and similarly for other operators.

There are certain shorthand notations that are useful when dealing with combined systems. We have, in fact, already used one: now that we have defined the tensor product, we see that  $|a_0\rangle|b_0\rangle$  is actually a shorthand notation for  $|a_0\rangle \otimes |b_0\rangle$ . Since operators in the combined space consist of a matrix of sub-blocks of operators that act in one of the spaces alone, it is useful to have a ket-style notation for these sub-blocks. Consider a general operator in the full space given by

$$V = \sum_{nn'jj'} v_{nj,n'j'} |c_{nj}\rangle \langle c_{n'j'}| = \sum_{nn'jj'} v_{nj,n'j'} |a_n\rangle |b_j\rangle \langle a_{n'}| \langle b_{j'}|. \quad (\text{A.18})$$

Here the numbers  $v_{nj,n'j'}$  are the matrix elements of  $V$ . If we sandwich  $V$  between the basis states  $|a_n\rangle|b_j\rangle$  and  $\langle a_{n'}| \langle b_{j'}|$ , then we pick out one of its elements:

$$\langle a_n| \langle b_j| V |a_{n'}\rangle |b_{j'}\rangle = v_{nj,n'j'}. \quad (\text{A.19})$$

It is convenient to define  $\langle a_n| V |a_{n'}\rangle$  as the sub-block of  $V$  corresponding to the  $(n, n')$  element of system A. That is

$$\langle a_n| V |a_{n'}\rangle \equiv \sum_{jj'} v_{nj,n'j'} |b_j\rangle \langle b_{j'}|, \quad (\text{A.20})$$

and this is an operator acting in the two-dimensional space of system B alone. This is handy notation because it means that we can write

$$\begin{aligned} v_{nj,n'j'} &= \langle b_j| \langle a_n| V |b_{j'}\rangle |a_{n'}\rangle \\ &= \langle b_j| (\langle a_n| V |a_{n'}\rangle) |b_{j'}\rangle \\ &= \langle b_j| \left( \sum_{kk'} v_{nk,n'k'} |b_k\rangle \langle b_{k'}| \right) |b_{j'}\rangle. \end{aligned} \quad (\text{A.21})$$

The above notation is also useful for describing von Neumann measurements on one of the subsystems. A von Neumann measurement projects a system onto one of a set of basis states (see sections 1.2.1 and 1.2.3). Let us say that our system is in the state  $|\psi\rangle = \sum_n c_n |n\rangle$  (where  $\{|n\rangle\}$  is an orthonormal basis), so that the density matrix is  $\rho = |\psi\rangle\langle\psi|$ . A von Neumann measurement in the basis  $\{|n\rangle\}$  will project the system onto the state

$$\tilde{\rho}_n = |n\rangle\langle n| = \frac{1}{\mathcal{N}} (|n\rangle\langle n|) \rho (|n\rangle\langle n|), \quad (\text{A.22})$$

(where  $\mathcal{N}$  is chosen so that the resulting state is normalized) and this occurs with probability

$$|c_n|^2 = \langle n|\rho|n\rangle. \quad (\text{A.23})$$

So how do we describe a von Neumann measurement on system A in the combined space of A and B? If the von Neumann measurement tells us that the state of system A is  $|a_0\rangle$ , then since the measurement must not have any direct action on system B, the state of system B must simply be the sub-block of the density matrix that corresponds to  $|a_0\rangle$ . So the state of system B after the measurement is, in our convenient notation,

$$\rho^B = \frac{1}{\mathcal{N}} \langle a_0|\rho^C|a_0\rangle. \quad (\text{A.24})$$

The state of the joint system after the measurement is

$$\frac{1}{\mathcal{N}} (|a_0\rangle\langle a_0|) \rho^C (|a_0\rangle\langle a_0|) = |a_0\rangle\langle a_0| \otimes \rho^B. \quad (\text{A.25})$$

The probability of getting this result is the sum over all the diagonal elements of  $\rho^C$  that correspond to system A being in state  $|a_0\rangle$ . This is

$$P(|a_0\rangle) = \text{Tr}[\langle a_0|\rho^C|a_0\rangle] = \mathcal{N}. \quad (\text{A.26})$$

## A.2 The partial trace

Now that we understand how to represent the states and operators of two systems in a joint space, another question arises: how do we retrieve the state of one of the subsystems from the state of the joint system? To answer this, first we must explain what we mean by “the state of one system”. If the two systems are together in a pure state, but this state is *correlated*, meaning that measurements on one system will in general be correlated with measurements on the other, then each of the systems cannot be represented by a pure state.

We can nevertheless define the state of one of the systems alone as an object from which we can determine the probabilities of the outcomes of all measurements on that system alone, and that does not refer to the other system. It turns out that it is possible to obtain such an object, and it is simply a density matrix for the single system. That is, while the state of a single system cannot necessarily be written as a state-vector, it can be written as a density matrix, and this is true for *any* joint state of the combined systems, pure or mixed. We now explain how to calculate the density matrix for a single system, when it is part of a larger system.

First let us consider the trivial case in which each system has been separately have been prepared in its own state. In this case the joint state is simply  $|\psi_C\rangle = |\psi_A\rangle \otimes |\psi_B\rangle$ . Writing the joint state as a density matrix we have

$$\rho^C = \rho \otimes \sigma = \begin{pmatrix} \rho_{11} \sigma & \rho_{12} \sigma \\ \rho_{21} \sigma & \rho_{22} \sigma \end{pmatrix}. \quad (\text{A.27})$$

Because  $\rho_{11} + \rho_{22} = 1$ , we see that we retrieve the density matrix for system B by summing the diagonal sub-blocks corresponding to the states of system A:

$$\rho_{11}\sigma + \rho_{22}\sigma = (\rho_{11} + \rho_{22})\sigma = \text{Tr}[\rho]\sigma = \sigma. \quad (\text{A.28})$$

Summing the diagonal elements of a matrix is called the “trace” operation. Summing the diagonal sub-blocks that correspond to a state of system A, so as to obtain the density matrix of system B, is called taking the “partial trace over system A”. If we take the partial trace over system A, and then take the trace of the resulting density matrix, the result is the same as taking the full trace over the combined system. Similarly we can take the partial trace over system B, to obtain the density matrix for system A. This is

$$\text{Tr}_B[\rho^C] = \begin{pmatrix} \rho_{11} \text{Tr}[\sigma] & \rho_{12} \text{Tr}[\sigma] \\ \rho_{21} \text{Tr}[\sigma] & \rho_{22} \text{Tr}[\sigma] \end{pmatrix} = \begin{pmatrix} \rho_{11} & \rho_{12} \\ \rho_{21} & \rho_{22} \end{pmatrix} = \rho. \quad (\text{A.29})$$

While we have only shown that the partial trace gives the correct answer when the subsystems are in separate (unentangled) states, it seems reasonable that this should remain true when they are not. We now present two arguments that show that it does. The first is obtained by noting that the density matrix for system B alone must give the same expectation value for all observables of system B as does the joint density matrix. Because the full trace over the joint system is the same as taking the partial trace over A followed by the trace over system B, this is guaranteed to be true if the density matrix of B is equal to the partial trace over A:

$$\langle X_B \rangle = \text{Tr}[X_B \rho^B] = \text{Tr}[X_B (\text{Tr}_A[\rho^C])] = \text{Tr}[(I \otimes X_B) \rho^C]. \quad (\text{A.30})$$

That the last equality here is true can be easily seen by writing  $\rho^C$  out in terms of its sub-blocks. Since Eq.(A.30) is true for *every* observable of system B,  $\rho^B$  defined as the partial trace  $\text{Tr}_A[\rho^C]$  must be the correct state of system B.

A second way to see that the partial trace  $\text{Tr}_A[\rho^C]$  gives the correct density matrix for system B employs measurements and the resulting states-of-knowledge, and so is very much in the theme of this book. We note that if an observer, who we will call Alice, only has access to system B, then she cannot know what has happened to system A. In particular, she cannot know what measurements have been performed on A. If another observer has made a von Neumann measurement on A, then Alice’s state of knowledge is given by averaging over the possible outcomes of this measurement. If A is measured in the basis  $\{|a_n\rangle\}$ , then the probability of getting the final state

$$\rho_n^B = \frac{1}{\mathcal{N}_n} \langle a_n | \rho^C | a_n \rangle \quad (\text{A.31})$$

is

$$P(n) = \text{Tr}[\langle a_n | \rho^C | a_n \rangle] = \mathcal{N}_n. \quad (\text{A.32})$$

So Alice’s state-of-knowledge is

$$\rho^B = \sum_n P(n) \rho_n^B = \sum_n \langle a_n | \rho^C | a_n \rangle = \text{Tr}_A[\rho^C], \quad (\text{A.33})$$

being precisely the partial trace over A. However, since Alice cannot know what measurement has been made on A, this argument only works (and quantum mechanics is only consistent!) if Alice’s state-of-knowledge is the same for *every* measurement that can be made on A. So if Alice’s state is indeed given by the partial trace, this trace must be derivable by choosing *any* measurement that can be made on A.

In section 1.2.3 we show that all quantum measurements are described by a set of operators  $\{A_n\}$  that satisfy  $\sum_n A_n^\dagger A_n = 1$ . The probability that result  $n$  will occur is  $P(n) = \text{Tr}[A_n^\dagger A_n \rho]$ , where  $\rho$  is the initial density matrix of the measured system. The final state given by result  $n$  is  $\rho_n = A_n \rho A_n^\dagger / P(n)$ . If a general measurement is made on system A, then the state of the combined system, from Alice's point of view, is

$$\rho_{\text{Alice}}^{\text{C}} = \sum_n P(n) \rho_n^{\text{C}} = \sum_n (A_n \otimes I) \rho^{\text{C}} (A_n^\dagger \otimes I). \quad (\text{A.34})$$

Alice's state of knowledge of B is the partial trace over this, which is

$$\begin{aligned} \rho^{\text{B}} &= \text{Tr}_A \left[ \sum_n (A_n \otimes I) \rho^{\text{C}} (A_n^\dagger \otimes I) \right] \\ &= \text{Tr}_A \left[ \sum_n (A_n^\dagger \otimes I) (A_n \otimes I) \rho^{\text{C}} \right] \\ &= \text{Tr}_A \left[ \left( \sum_n A_n^\dagger A_n \otimes I \right) \rho^{\text{C}} \right] \\ &= \text{Tr}_A [(I \otimes I) \rho^{\text{C}}] = \text{Tr}_A [\rho^{\text{C}}], \end{aligned} \quad (\text{A.35})$$

and so it is independent of the measurement as required. Here we have used the (very useful!) cyclic property of the trace:  $\text{Tr}[ABC] = \text{Tr}[CAB] = \text{Tr}[BCA]$ . Note, however, that because we are taking the *partial* trace over A, we can only cycle operators that act purely on A inside the trace - operators that act on the subspace for system B cannot be cycled in this way.

### Two examples of correlated systems

There are two fundamentally different ways that two quantum systems can be correlated. The first is the same way in which classical systems can be correlated. An example for two qubits is the mixed state

$$\rho^{\text{C}} = \frac{1}{2} |0\rangle\langle 0| \otimes |0\rangle\langle 0| + \frac{1}{2} |1\rangle\langle 1| \otimes |1\rangle\langle 1|. \quad (\text{A.36})$$

In this case if we measure system B and get  $|0\rangle$ , then if we measure system A in the basis  $\{|0\rangle, |1\rangle\}$ , we will always get the result  $|0\rangle$ . Thus in the basis  $\{|0\rangle, |1\rangle\}$ , the two systems are perfectly correlated. Classical systems can also be correlated in precisely this way, since the origin of the correlation is merely the classical probability to be in the joint state  $|0\rangle\langle 0| \otimes |0\rangle\langle 0|$ , or the joint state  $|1\rangle\langle 1| \otimes |1\rangle\langle 1|$ .

The other way in which two quantum systems can be correlated is when the correlation is due to the joint system being in a *superposition* of various joint states of the two subsystems. For example, if the joint system is in the state

$$\rho^{\text{C}} = \frac{1}{\sqrt{2}} |0\rangle \otimes |0\rangle + \frac{1}{\sqrt{2}} |1\rangle \otimes |1\rangle, \quad (\text{A.37})$$

then the two systems are again perfectly correlated in the basis  $\{|0\rangle, |1\rangle\}$ . This time there is an entirely new feature to the correlation, however: if we transform both systems in the same way to a new basis, then we find that they are perfectly correlated in the new basis! This means that they are perfectly correlated in *all bases*. This uniquely quantum mechanical type of correlation also has other remarkable properties that cannot be replicated by classical systems. It is the subject of Bell's inequalities [231–237] and entanglement [25, 228–230].

**The origin of the term “tensor product”**

As a final note, the reason that the product operation “ $\otimes$ ” is called the “tensor product” is due to its relationship with tensors. From a mathematical point of view, a tensor is defined as a linear functional on one or more vector spaces. A functional is something that maps elements in its domain (in this case a set of vectors from a set of vector spaces) to a scalar. Without going into the details, the representation of a vector that acts on two vector spaces is a matrix. When representing tensors as matrices, the natural product of two tensors is given by taking the “tensor product” of their respective matrices.