

(μ) Global and Partial Trace

In this mathematical digression, we recall the notion of the **global trace** and introduce the **partial trace**, which is an important tool for approaching the general formulation of quantum theory (with noise).

The **trace** (or global trace) of a matrix representing an operator $M : \mathcal{H} \rightarrow \mathcal{H}$ (written in a given basis $|a\rangle$) is, by definition, the sum of its diagonal entries:

$$\text{Tr } M = \sum_{a \in A} \langle a | M | a \rangle$$

It is a linear functional of M .

The trace of a product of two linear maps $M : \mathcal{H}' \rightarrow \mathcal{H}$ and $N : \mathcal{H} \rightarrow \mathcal{H}'$ does not depend on the order of the factors, since

$$\begin{aligned} \text{Tr}(MN) &= \sum_a \sum_{a'} \langle a | M | a' \rangle \langle a' | N | a \rangle \\ &= \sum_{a'} \sum_a \langle a' | N | a \rangle \langle a | M | a' \rangle = \text{Tr}(NM), \end{aligned}$$

where the products $MN : \mathcal{H} \rightarrow \mathcal{H}$ and $NM : \mathcal{H}' \rightarrow \mathcal{H}'$ may have different sizes.

In particular, if one considers a new orthonormal basis of $\mathcal{H}$, it has the form $U|a\rangle$ where U is unitary. In this basis, the matrix of an operator $M : \mathcal{H} \rightarrow \mathcal{H}$ is equal to U^*MU , and $\text{Tr}(U^*MU) = \text{Tr}(MUU^*) = \text{Tr}(M\mathbb{1}) = \text{Tr } M$.

Theorem (Trace property). *For all linear maps $M : \mathcal{H}' \rightarrow \mathcal{H}$ and $N : \mathcal{H} \rightarrow \mathcal{H}'$,*

$$\text{Tr}(MN) = \text{Tr}(NM)$$

The trace does not depend on the chosen basis of $\mathcal{H}$.

This is therefore an **intrinsic** definition, independent of the choice of the basis of $\mathcal{H}$. These properties are also true for the determinant. In particular, when M is normal, its determinant $|M|$ and its trace $\text{Tr } M$ are respectively the product and the sum of its eigenvalues, counted with multiplicity.

Remark. It follows from the trace property $\text{Tr}(MN) = \text{Tr}(NM)$ that, more generally, if an operator is the product of several linear maps, its trace does not change if one performs a **cyclic permutation** of the factors of this product:

$$\text{Tr}(M_1 M_2 \cdots M_n) = \text{Tr}(M_2 \cdots M_n M_1) = \text{Tr}(M_n M_1 \cdots M_{n-1})$$

Example. The trace of an outer product $|\phi\rangle\langle\psi|$ is the inner product

$$\text{Tr}(|\phi\rangle\langle\psi|) = \text{Tr}(\langle\psi|\phi\rangle) = \langle\psi|\phi\rangle$$

since $\langle\psi|\phi\rangle$ is a scalar (a matrix of size 1). More generally, for any linear map M (of dimensions compatible with the vectors $|\psi\rangle$ and $|\phi\rangle$),

$$\langle\psi|M|\phi\rangle = \text{Tr}(M|\phi\rangle\langle\psi|).$$

Example. The trace of a tensor product $M \otimes N$ of two operators $M : \mathcal{H}_A \rightarrow \mathcal{H}_A$ and $N : \mathcal{H}_B \rightarrow \mathcal{H}_B$ is, by the formula $\langle ab|M \otimes N|ab\rangle = \langle a|M|a\rangle \langle b|N|b\rangle$ and by summing over a, b ,

$$\text{Tr}(M \otimes N) = (\text{Tr } M)(\text{Tr } N).$$

If M and N are normal, the same formula is recovered by summing the eigenvalues, $\sum_{ab} \lambda_a \mu_b = (\sum_a \lambda_a)(\sum_b \mu_b)$.

An important property of the trace concerns **positive** operators. If $M \geq 0$, then $\text{Tr } M = \sum_{a \in A} \langle a|M|a\rangle$ is a sum of nonnegative entries, so $\text{Tr } M \geq 0$. Applied to $M - N$ with the Löwner notation,

$$M \geq N \implies \text{Tr } M \geq \text{Tr } N.$$

More generally, if $M \geq 0$ and $N \geq 0$, the product operator MN is not always positive. However, this is the case for $\sqrt{M}N\sqrt{M} \geq 0$, so $\text{Tr}(MN) = \text{Tr}(\sqrt{M}\sqrt{M}N) = \text{Tr}(\sqrt{M}N\sqrt{M}) \geq 0$. Moreover, $\text{Tr}(MN) = 0$ implies $\sqrt{M}N\sqrt{M} = 0$, whence

$$\langle\psi|\sqrt{M}N\sqrt{M}|\psi\rangle = \|\sqrt{N}\sqrt{M}\psi\|^2 = 0$$

for every $|\psi\rangle$; that is, $\sqrt{N}\sqrt{M} = 0$, and therefore $NM = \sqrt{N}\sqrt{N}\sqrt{M}\sqrt{M} = 0$ (and similarly $MN = 0$, by symmetry or by taking the adjoint). We have obtained the following result.

Theorem (Trace positivity).

$$M, N \geq 0 \implies \text{Tr } MN \geq 0$$

with equality $\text{Tr } MN = 0$ if and only if $MN = NM = 0$.

The implication $M \geq 0 \implies \text{Tr } M \geq 0$ corresponds to the special case $N = \mathbb{1} \geq 0$. The condition $MN = NM = 0$ amounts to saying that, in a common diagonalizing basis, the product $\lambda_M \lambda_N$ of the eigenvalues is zero; in other words, the ranges of M and N are **orthogonal** subspaces. The property $M, N \geq 0 \implies \text{Tr } MN \geq 0$ does not extend to the product of three positive operators (or more).

The notion of trace generalizes to an operator $\mathbf{M} : \mathcal{H}_A \otimes \mathcal{H}_B \rightarrow \mathcal{H}_A \otimes \mathcal{H}_B$ defined on a tensor product of spaces with a given basis $|ab\rangle = |a\rangle \otimes |b\rangle$:

Definition (Partial trace). The *partial trace over A* is the linear map Tr_A that assigns to every operator $\mathbf{M}$ on $\mathcal{H}_A \otimes \mathcal{H}_B$ the operator $\text{Tr}_A \mathbf{M}$ on $\mathcal{H}_B$ defined by

$$\text{Tr}_A \mathbf{M} = \sum_{a \in A} (\langle a| \otimes \mathbb{1}_B) \mathbf{M} (|a\rangle \otimes \mathbb{1}_B),$$

that is, whose coefficients in the orthonormal basis $|b\rangle$ of $\mathcal{H}_B$ are

$$\langle b' | \text{Tr}_A \mathbf{M} | b \rangle = \sum_{a \in A} \langle ab' | \mathbf{M} | ab \rangle$$

for all $b, b' \in B$.

The partial trace over A makes it possible to pass from an operator on a compound system AB to an operator on B alone. We say that we have **traced out** A from the operator $\mathbf{M}$; in a sense, we have eliminated A (leaving this partial trace) in order to obtain only an operator on B .

In particular, if $\mathbf{M} = M \otimes N$ is a Kronecker product of two operators $M : \mathcal{H}_A \rightarrow \mathcal{H}_A$ and $N : \mathcal{H}_B \rightarrow \mathcal{H}_B$, then

$$\text{Tr}_A(M \otimes N) = \sum_{a \in A} \langle a | M | a \rangle (\mathbb{1}_B N \mathbb{1}_B) = \text{Tr}(M) \cdot N,$$

an expression that does not depend on the choices of bases $|a\rangle$ and $|b\rangle$. This formula uniquely characterizes the linear map Tr_A for every operator $\mathbf{M} : \mathcal{H}_A \otimes \mathcal{H}_B \rightarrow \mathcal{H}_A \otimes \mathcal{H}_B$, because such an operator can always be written as a linear combination of Kronecker products of the form $|a'b'\rangle\langle ab| = |a'\rangle\langle a| \otimes |b'\rangle\langle b|$, for any choice of orthonormal bases $|a\rangle$ and $|b\rangle$. Consequently, the partial trace does not depend on the chosen bases: it is an **intrinsic** definition, independent of the choice of bases of $\mathcal{H}_A$ and $\mathcal{H}_B$.

If the matrix of an arbitrary operator $\mathbf{M} : \mathcal{H}_A \otimes \mathcal{H}_B \rightarrow \mathcal{H}_A \otimes \mathcal{H}_B$ (a square matrix of size $d_A d_B$) is written as a block matrix with blocks of size d_B ,

$$\mathbf{M} = \begin{pmatrix} \mathbf{M}_{1,1} & \cdots & \mathbf{M}_{1,d_A} \\ \vdots & \ddots & \vdots \\ \mathbf{M}_{d_A,1} & \cdots & \mathbf{M}_{d_A,d_A} \end{pmatrix}$$

then one observes that **the partial trace over A is the sum of the diagonal blocks**:

$$\text{Tr}_A(\mathbf{M}) = \sum_a \mathbf{M}_{a,a} = \mathbf{M}_{1,1} + \mathbf{M}_{2,2} + \cdots + \mathbf{M}_{d_A,d_A},$$

which is a matrix of size d_B . In the trivial case $d_B = 1$, one may identify $\mathcal{H}_A \otimes \mathcal{H}_B = \mathcal{H}_A$ and recover the usual definition of the trace.

The **partial trace over B** is defined analogously:

$$\text{Tr}_B \mathbf{M} = \sum_{b \in B} (\mathbb{1}_A \otimes \langle b |) \mathbf{M} (\mathbb{1}_A \otimes | b \rangle),$$

with coefficients

$$\langle a' | \text{Tr}_B \mathbf{M} | a \rangle = \sum_{b \in B} \langle a'b | \mathbf{M} | ab \rangle,$$

and in particular, for $\mathbf{M} = M \otimes N$,

$$\text{Tr}_B(M \otimes N) = M \cdot \text{Tr}(N) = \text{Tr}(N) \cdot M.$$

As for Tr_A , this formula uniquely characterizes the linear map Tr_B for every operator $\mathbf{M}$ on $\mathcal{H}_A \otimes \mathcal{H}_B$.

The partial trace over B is independent of the chosen bases. Here again, the partial trace over B makes it possible to pass from an operator on a compound system AB to an operator on A alone: we have **traced out** B from the operator $\mathbf{M}$; in a sense, we have eliminated B (leaving this partial trace) in order to obtain only an operator on A .

Writing the matrix of an arbitrary operator $\mathbf{M} : \mathcal{H}_A \otimes \mathcal{H}_B \rightarrow \mathcal{H}_A \otimes \mathcal{H}_B$ (a square matrix of size $d_A d_B$) as a block matrix with blocks of size d_B , as above, one observes that **the partial trace over B is the matrix of the traces of the blocks**:

$$\mathrm{Tr}_B(\mathbf{M}) = \begin{pmatrix} \mathrm{Tr} \mathbf{M}_{1,1} & \cdots & \mathrm{Tr} \mathbf{M}_{1,d_A} \\ \vdots & \ddots & \vdots \\ \mathrm{Tr} \mathbf{M}_{d_A,1} & \cdots & \mathrm{Tr} \mathbf{M}_{d_A,d_A} \end{pmatrix},$$

which is a matrix of size d_A . This visualization differs from the preceding one for Tr_A because of the chosen lexicographic order for the indices a, b . By the block-composition formula, it can be written as

$$\mathrm{Tr}_B(\mathbf{M}) = \sum_{a',a} \mathrm{Tr}(\mathbf{M}_{a',a}) |a'\rangle\langle a|.$$

Example. For two qubits AB , let us compute the two partial traces of

$$\mathbf{M} = |0\rangle\langle 0| \otimes |0\rangle\langle 0| + |1\rangle\langle 1| \otimes |+\rangle\langle +|$$

where $|0\rangle\langle 0| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$, $|1\rangle\langle 1| = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$, and $|+\rangle\langle +| = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$. We find the matrix

$$\mathbf{M} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1/2 & 1/2 \\ 0 & 0 & 1/2 & 1/2 \end{pmatrix}.$$

The trace over A is the sum of the diagonal 2×2 blocks:

$$\mathrm{Tr}_A \mathbf{M} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix} = \begin{pmatrix} 3/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix},$$

and the trace over B is the matrix of the 2×2 block traces:

$$\mathrm{Tr}_B \mathbf{M} = \begin{pmatrix} \mathrm{Tr} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} & \mathrm{Tr} \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \\ \mathrm{Tr} \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} & \mathrm{Tr} \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \mathbb{1}_A.$$

Remark. In general calculations, it is often more convenient to use the linearity of the trace by decomposing the operator $\mathbf{M}$ into Kronecker products of the form $M \otimes N$. Indeed, every operator is a linear combination of such products, such as $|a'b'\rangle\langle ab| = |a'\rangle\langle a| \otimes |b'\rangle\langle b|$.

Another possibility is to return to the definitions of the partial traces:

$$\mathrm{Tr}_A \mathbf{M} = \sum_{a \in A} (\langle a| \otimes \mathbb{1}_B) \mathbf{M} (|a\rangle \otimes \mathbb{1}_B) \quad \text{or} \quad \mathrm{Tr}_B \mathbf{M} = \sum_{b \in B} (\mathbb{1}_A \otimes \langle b|) \mathbf{M} (\mathbb{1}_A \otimes |b\rangle).$$

Example. Let us compute the expression $\text{Tr}_B((M_1 \otimes \mathbb{1}_B) \cdot \mathbf{M} \cdot (M_2 \otimes \mathbb{1}_B))$. When $\mathbf{M} = M \otimes N$, we have

$$\begin{aligned} & \text{Tr}_B((M_1 \otimes \mathbb{1}_B) \cdot (M \otimes N) \cdot (M_2 \otimes \mathbb{1}_B)) \\ &= \text{Tr}_B(M_1 M M_2 \otimes N) = M_1 M M_2 \text{Tr}(N) = M_1 \cdot \text{Tr}_B(M \otimes N) \cdot M_2 \end{aligned}$$

by the product formula and by the formula $\text{Tr}_B(M \otimes N) = M \cdot \text{Tr}(N)$. By linearity, from the identity

$$\text{Tr}_B((M_1 \otimes \mathbb{1}_B) \cdot (M \otimes N) \cdot (M_2 \otimes \mathbb{1}_B)) = M_1 \cdot \text{Tr}_B(M \otimes N) \cdot M_2$$

obtained for $M \otimes N$, it follows that

$$\text{Tr}_B((M_1 \otimes \mathbb{1}_B) \cdot \mathbf{M} \cdot (M_2 \otimes \mathbb{1}_B)) = M_1 \cdot \text{Tr}_B(\mathbf{M}) \cdot M_2.$$

Another possible calculation is to go back to the definition:

$$\text{Tr}_B((M_1 \otimes \mathbb{1}_B) \cdot \mathbf{M} \cdot (M_2 \otimes \mathbb{1}_B)) = \sum_{b \in B} (\mathbb{1}_A \otimes \langle b |) (M_1 \otimes \mathbb{1}_B) \mathbf{M} (M_2 \otimes \mathbb{1}_B) (\mathbb{1}_A \otimes |b\rangle).$$

By the product formula,

$$(\mathbb{1}_A \otimes \langle b |) (M_1 \otimes \mathbb{1}_B) = M_1 \otimes \langle b | = (M_1 \otimes 1) (\mathbb{1}_A \otimes \langle b |) = M_1 (\mathbb{1}_A \otimes \langle b |),$$

and similarly

$$(M_2 \otimes \mathbb{1}_B) (\mathbb{1}_A \otimes |b\rangle) = M_2 \otimes |b\rangle = (\mathbb{1}_A \otimes |b\rangle) (M_2 \otimes 1) = (\mathbb{1}_A \otimes |b\rangle) M_2.$$

Here we identify $M_i \otimes 1$ with M_i , because 1 is a scalar operator (on a one-dimensional space). Substituting this gives the formula directly.

Theorem (Formula for tracing out identity operators).

$$\text{Tr}_B((M_1 \otimes \mathbb{1}_B) \cdot \mathbf{M} \cdot (M_2 \otimes \mathbb{1}_B)) = M_1 \cdot \text{Tr}_B(\mathbf{M}) \cdot M_2,$$

in particular

$$\text{Tr}_B((M \otimes \mathbb{1}_B) \cdot \mathbf{M}) = M \cdot \text{Tr}_B(\mathbf{M}) \quad \text{and} \quad \text{Tr}_B(\mathbf{M} \cdot (M \otimes \mathbb{1}_B)) = \text{Tr}_B(\mathbf{M}) \cdot M.$$

Exchanging the roles of A and B , we similarly have

$$\text{Tr}_A((\mathbb{1}_A \otimes N_1) \cdot \mathbf{M} \cdot (\mathbb{1}_A \otimes N_2)) = N_1 \cdot \text{Tr}_A(\mathbf{M}) \cdot N_2.$$

These formulas will be very useful in what follows. They show that, in a partial trace, one can eliminate, in the tensor products (on the left and on the right), all identity operators for the system that is traced out.

Remark. Unlike the global trace property $\text{Tr}(MN) = \text{Tr}(NM)$,

$$\text{Tr}_B((M \otimes \mathbb{1}_B) \cdot \mathbf{M})$$

is not equal to $\text{Tr}_B(\mathbf{M} \cdot (M \otimes \mathbb{1}_B))$ in general.

On the other hand, this is true for the same product but for the other partial trace. Indeed, for $\mathbf{M} = M' \otimes N'$ we have

$$\begin{aligned}\mathrm{Tr}_A((M \otimes \mathbb{1}_B) \cdot \mathbf{M}) &= \mathrm{Tr}_A((M \otimes \mathbb{1}_B)(M' \otimes N')) \\ &= \mathrm{Tr}_A(MM' \otimes N') = \mathrm{Tr}(MM')N' \\ &= \mathrm{Tr}(M'M)N' = \mathrm{Tr}_A(M'M \otimes N') \\ &= \mathrm{Tr}_A((M' \otimes N')(M \otimes \mathbb{1}_B)) \\ &= \mathrm{Tr}_A(\mathbf{M} \cdot (M \otimes \mathbb{1}_B)),\end{aligned}$$

whence, by linearity, the following property.

Theorem (Commutativity under the partial trace).

$$\mathrm{Tr}_A((M \otimes \mathbb{1}_B) \cdot \mathbf{M}) = \mathrm{Tr}_A(\mathbf{M} \cdot (M \otimes \mathbb{1}_B)).$$

We similarly have

$$\mathrm{Tr}_B((\mathbb{1}_A \otimes N) \cdot \mathbf{M}) = \mathrm{Tr}_B(\mathbf{M} \cdot (\mathbb{1}_A \otimes N)).$$

The usual (global) trace is a special partial trace. Indeed, if $\mathbf{M} : \mathcal{H}_A \otimes \mathcal{H}_B \rightarrow \mathcal{H}_A \otimes \mathcal{H}_B$, the usual trace $\mathrm{Tr} \mathbf{M}$ can be interpreted as the **global trace** over AB , as opposed to the partial traces over A or over B :

$$\mathrm{Tr} \mathbf{M} = \mathrm{Tr}_{AB} \mathbf{M} = \sum_{a,b} \langle ab | \mathbf{M} | ab \rangle.$$

By first tracing out B and then A , this can be written in the form

$$\mathrm{Tr} \mathbf{M} = \sum_a \langle a | \left(\sum_b (\mathbb{1}_A \otimes \langle b |) \mathbf{M} (\mathbb{1}_A \otimes | b \rangle) \right) | a \rangle,$$

and similarly after exchanging the roles of A and B . We therefore have the following result.

Theorem (Decomposition of the global trace into partial traces).

$$\mathrm{Tr}_{AB} \mathbf{M} = \mathrm{Tr}_A(\mathrm{Tr}_B \mathbf{M}) = \mathrm{Tr}_B(\mathrm{Tr}_A \mathbf{M}).$$

In particular, we recover the formula

$$\mathrm{Tr}(M \otimes N) = \mathrm{Tr}_B(\mathrm{Tr}_A(M \otimes N)) = \mathrm{Tr}_B((\mathrm{Tr} M) \cdot N) = (\mathrm{Tr} M)(\mathrm{Tr} N).$$

The notion of partial trace naturally generalizes to the case of several systems, for instance ABC . For a tensor product of three spaces $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$, the linear map Tr_B is defined by

$$\mathrm{Tr}_B \mathbf{M} = \sum_{b \in B} (\mathbb{1}_A \otimes \langle b | \otimes \mathbb{1}_C) \mathbf{M} (\mathbb{1}_A \otimes | b \rangle \otimes \mathbb{1}_C),$$

which is an operator on $\mathcal{H}_A \otimes \mathcal{H}_C$, whereas the partial trace over AB ,

$$\text{Tr}_{AB} \mathbf{M} = \sum_{a \in A, b \in B} (\langle a| \otimes \langle b| \otimes \mathbb{1}_C) \mathbf{M} (|a\rangle \otimes |b\rangle \otimes \mathbb{1}_C) = \sum_{a,b} (\langle ab| \otimes \mathbb{1}_C) \mathbf{M} (|ab\rangle \otimes \mathbb{1}_C),$$

is an operator on $\mathcal{H}_C$. By fixing the order of the systems (for example, by considering ACB or BAC rather than ABC), one can always reduce to the case of the first definition of the partial trace above. By associativity, one can generalize to tensor products of any finite number of spaces.

For a partial trace, for example Tr_B , of an operator $\mathbf{M} \geq 0$, we compute, for every $|\psi\rangle \in \mathcal{H}_A$,

$$\begin{aligned} \langle \psi | \text{Tr}_B \mathbf{M} | \psi \rangle &= \sum_{b \in B} (\langle \psi | \otimes \langle b |) \mathbf{M} (| \psi \rangle \otimes | b \rangle) \\ &= \sum_{b \in B} \langle \psi \otimes b | \mathbf{M} | \psi \otimes b \rangle \geq 0. \end{aligned}$$

As for the global trace, we therefore have the following result.

Theorem (Partial trace positivity). *The partial trace of a positive operator is a positive operator:*

$$\mathbf{M} \geq 0 \implies \text{Tr}_B \mathbf{M} \geq 0.$$

On the other hand, unlike the case of the (global) trace, $\mathbf{M}, \mathbf{N} \geq 0$ does not imply $\text{Tr}_B(\mathbf{MN}) \geq 0$ in general. This already occurs when $d_B = 1$ and $\text{Tr}_B(\mathbf{MN}) = \mathbf{MN}$, which is not necessarily positive, or even Hermitian, if the two operators $\mathbf{M}, \mathbf{N} \geq 0$ do not commute.