

Chapter 5

Density matrix formalism

In chap 2 we formulated quantum mechanics for isolated systems. In practice systems interact with their environment and we need a description that takes this feature into account. Suppose the system of interest which has Hilbert space \mathcal{H} is coupled to some environment with space \mathcal{H}_E . The total system is isolated and is described by a state vector $|\Psi\rangle \in \mathcal{H} \otimes \mathcal{H}_E$. An observable for the system of interest is of the form $A \otimes I$ where A acts only in \mathcal{H} . We suppose that A has spectral decomposition $A = \sum_n a_n P_n$ so that

$$A \otimes I = \sum_n a_n P_n \otimes I$$

A measurement of the observable will leave the system in one of the states

$$\frac{P_n \otimes I |\Psi\rangle}{\langle \Psi | P_n \otimes I | \Psi \rangle^{1/2}}$$

with probability

$$\text{prob}(n) = \langle \Psi | P_n \otimes I | \Psi \rangle$$

and the average value of the observable is

$$\langle \Psi | A \otimes I | \Psi \rangle.$$

If we introduce the matrix¹

$$\rho = \text{Tr}_{\mathcal{H}_E} |\Psi\rangle\langle\Psi|$$

which acts on \mathcal{H} , we can rewrite all these formulas as follows,

$$\text{prob}(n) = \text{Tr} P_n \otimes I |\Psi\rangle\langle\Psi| = \text{Tr}_{\mathcal{H}} \text{Tr}_{\mathcal{H}_E} P_n \otimes I |\Psi\rangle\langle\Psi| = \text{Tr}_{\mathcal{H}} P_n \rho$$

¹here a partial trace is performed. This is formally defined in a later section. Readers who are not comfortable with this paragraph can skip to the next one.

and

$$\langle \Psi | A \otimes I | \Psi \rangle = \text{Tr} A \otimes I | \Psi \rangle \langle \Psi | = \text{Tr}_{\mathcal{H}} \text{Tr}_{\mathcal{E}} A \otimes I | \Psi \rangle \langle \Psi | = \text{Tr}_{\mathcal{H}} A \rho$$

Thus we see that the system of interest is described by the matrix ρ called “density matrix”. At the level of the reduced density matrix the collapse of the state vector becomes

$$\rho = \text{Tr}_{\mathcal{E}} | \Psi \rangle \langle \Psi | \rightarrow \rho_{after} = \text{Tr}_{\mathcal{E}} \frac{P_n \otimes I | \Psi \rangle \langle \Psi | P_n \otimes I}{\langle \Psi | P_n \otimes I | \Psi \rangle} = \frac{P_n \rho P_n}{\text{Tr} P_n \rho}$$

Thus a *density matrix can describe part of a system* (Landau).

There is also another kind of preparation of a quantum system for which density matrices are useful. Suppose a source emits with probability p_1 photons in state $|\Psi_1\rangle \in \mathcal{H}$ and with probability p_2 photons in state $|\Psi_2\rangle \in \mathcal{H}$ (with $p_1 + p_2 = 1$). Then the average value of an observable A acting in \mathcal{H} is

$$p_1 \langle \Psi_1 | A | \Psi_1 \rangle + p_2 \langle \Psi_2 | A | \Psi_2 \rangle = \text{Tr} \rho A$$

where

$$\rho = p_1 |\Psi_1\rangle \langle \Psi_1| + p_2 |\Psi_2\rangle \langle \Psi_2|$$

This *density matrix describes a system that is prepared in an ensemble of state vectors with a definite proportion for each state vector* (von Neumann). Of course this example can be generalized to an ensemble of more than two vectors.

These two examples are sufficient motivation for introducing a slightly more general formalism, that formulates the rules of QM in terms of the density matrix. This is the subject of this chapter.

5.1 Mixed states and density matrices

Let \mathcal{H} be the Hilbert space of a system of reference (isolated or not). From now on the vectors of the Hilbert space will be called *pure states*. As we remarked earlier a global phase is unobservable so that giving a pure state $|\Psi\rangle$ or its associated projector $|\Psi\rangle \langle \Psi|$ is equivalent. So a pure state can be thought of as a projector on a one dimensional subspace of \mathcal{H} .

A very general notion of state is as follows (Von Neumann)

General definition of a state. Given a Hilbert space \mathcal{H} , consider $\mathcal{B}(\mathcal{H})$ the space of bounded linear self-adjoint operators from $\mathcal{H} \rightarrow \mathcal{H}$. A state is a *positive linear functional*

$$Av : \mathcal{B}(\mathcal{H}) \rightarrow C, A \rightarrow Av(A) \tag{5.1}$$

such that $Av(A) = 1$ (normalization condition).

A general theorem (that we do not prove here) then shows that it is always possible to represent this functional by a positive selfadjoint operator ρ with $Tr\rho = 1$. That is

$$Av(A) = Tr\rho A, \quad \rho^\dagger = \rho, \quad \rho \geq 0, \quad Tr\rho = 1$$

This operator is called a density matrix.

If ρ is a one dimensional projector² it is said to be a *pure state*, while if it is not a projector, i.e. $\rho^2 \neq \rho$ it is said to be a *mixed state*.

Examples.

- A pure state $\rho = |\Psi\rangle\langle\Psi|$.
- A mixture of pure states - *not necessarily orthogonal* - $\rho = \sum_n \lambda_n |\phi_n\rangle\langle\phi_n|$, $\lambda_n \geq 0$, $\sum_n \lambda_n = 1$.

There are two kind of physical interpretations of ρ that we have already given in the introduction. In fact these correspond also to two mathematical facts.

First we will see at the end of the chapter that a system that is in a mixed state can always be “purified”. By this we mean that one can always construct (mathematically) a bigger Hilbert space and find a pure state $|\Psi\rangle$ such that $\rho = Tr|\Psi\rangle\langle\Psi|$. Thus we may always *interpret* ρ as describing part of a bigger system (Landau).

Second, given ρ , since it is selfadjoint, positive and its trace is normalized it always has a spectral decomposition

$$\rho = \sum_i \rho_i |i\rangle\langle i|, \quad \rho_i \geq 0, \quad \sum_i \rho_i = 1$$

Thus we can always *interpret* ρ as describing a mixture of pure states $|i\rangle$ each state occurring in the proportion ρ_i (von Neumann). In quantum statistical mechanics for example we have $\rho_i = \frac{e^{-\beta E_i}}{Z}$, $Z = \sum_i e^{-\beta E_i}$, β the inverse temperature. Of course there are other ways (not corresponding to the spectral decomposition) of rewriting ρ as a convex combination of one dimensional projectors so there is an ambiguity in this interpretation. In quantum information theory it is important to have in mind that, given ρ , if we do not

²to check this it enough to have $\rho^2 = \rho$ because then it is a projector so its eigenvalues are 1 and 0; so if we already know that $Tr\rho = 1$ the multiplicity of 1 is one so its a one-dimensional projector

know the state preparation of the system - that is the set $\{\lambda_n, |\phi_n\rangle\}$ - there is an ambiguity in the interpretation as a mixture. We can access part of the information about the preparation by making measurements, and as we will see in the next chapter the Holevo quantity gives a bound on the mutual information between the preparation and the measurement outcomes.

Lemma 1. *The set of states of a quantum system is convex. The extremal points are pure states, in other words they are one dimensional projectors $|\Psi\rangle\langle\Psi|$. Conversely the pure states are extremal points of this set.*

Proof. Let ρ_1 and ρ_2 be two density matrices. Then evidently any convex combination $\rho = \lambda\rho_1 + (1 - \lambda)\rho_2$ for $\lambda \in [0, 1]$ satisfies $\rho^\dagger = \rho$, $\rho \geq 0$ and $\text{Tr}\rho = 1$. Hence the set of density matrices is convex.

If ρ is an extremal point then it cannot be written as a non trivial linear combination of other density matrices. But all ρ have a spectral decomposition $\rho = \sum_i \rho_i |i\rangle\langle i|$ with $0 \leq \rho_i$ and $\sum_i \rho_i = 1$. Since this is a convex combination it must be trivial so only one of the ρ_i equals 1 and the other vanish: thus $\rho = |i\rangle\langle i|$ for some i .

Now let ρ be a pure state: there exists a $|\Psi\rangle$ st $\rho = |\Psi\rangle\langle\Psi|$. We want to show that it is impossible to find $\rho_1 \neq \rho_2$ and $0 < \lambda < 1$ st $\rho = \lambda\rho_1 + (1 - \lambda)\rho_2$. If P_\perp is the projector on the orthogonal complement of $|\Psi\rangle$,

$$0 = \text{Tr}P_\perp\rho P_\perp = \lambda\text{Tr}P_\perp\rho_1 P_\perp + (1 - \lambda)\text{Tr}P_\perp\rho_2 P_\perp$$

The positivity of ρ_1, ρ_2 and the strict positivity of λ and $1 - \lambda$ imply that

$$\text{Tr}P_\perp\rho_1 P_\perp = \text{Tr}P_\perp\rho_2 P_\perp = 0$$

and by the positivity again we deduce

$$P_\perp\rho_1 P_\perp = P_\perp\rho_2 P_\perp = 0$$

(because $P\rho P = P\rho^{1/2}\rho^{1/2}P = (\rho^{1/2}P)^\dagger(\rho P)$ and $\text{Tr}A^\dagger B$ is an inner product in the space $\mathcal{B}(\mathcal{H})$) Thus we have

$$\rho_1 = (P_\perp + |\Psi\rangle\langle\Psi|)\rho_1(P_\perp + |\Psi\rangle\langle\Psi|) = (|\Psi\rangle\langle\Psi|)\langle\Psi|\rho_1|\Psi\rangle$$

But $\text{Tr}\rho_1 = 1$ so $\langle\Psi|\rho_1|\Psi\rangle = 1$ and $\rho_1 = |\Psi\rangle\langle\Psi|$. The same argument applies to ρ_2 and thus $\rho_1 = \rho_2$. \square

The density matrix of a single Qbit. The set of states of a single Qbit can easily be described in terms of 2×2 density matrices as we now show. A basis for all matrices is given by the Pauli matrices $\{I, X, Y, Z\}$,

$$\rho = a_0 I + a_1 X + a_2 Y + a_3 Z$$

We have $\text{Tr}\rho = 2a_0$ so we require that $a_0 = \frac{1}{2}$. We rewrite the density matrix as

$$\rho = \frac{1}{2}(I + \mathbf{a} \cdot \Sigma) = \frac{1}{2} \begin{pmatrix} 1 + a_3 & a_1 - ia_2 \\ a_1 + ia_2 & 1 - a_3 \end{pmatrix}$$

where $\mathbf{a} = (a_1, a_2, a_3)$ and $\Sigma = (X, Y, Z)$ is the vector with the three Pauli matrices as components. We need $\rho^\dagger = \rho$ so the vector \mathbf{a} has real components (Pauli matrices are hermitian). In order to have also $\rho \geq 0$ we necessarily need $\det\rho \geq 0$. This is also sufficient because we already have $\text{Tr}\rho = 1$ so that both eigenvalues cannot be negative and hence they are both positive. The positivity of the determinant is equivalent to

$$\det\rho = 1 - |\mathbf{a}|^2 \geq 0$$

Therefore the space of 2×2 density matrices is

$$\{\rho = \frac{1}{2}(I + \mathbf{a} \cdot \Sigma) \mid |\mathbf{a}| \leq 1\}$$

Evidently we can identify it to the unit ball $|\mathbf{a}| \leq 1$ and is commonly called the ‘‘Bloch sphere’’. Of course it is convex and the extremal states are those which cannot be written as a non-trivial linear combination, that is the states with $|\mathbf{a}| = 1$. Let us check that the later are pure states. We compute

$$\begin{aligned} \rho^2 &= \frac{1}{4}(I + \mathbf{a} \cdot \Sigma)^2 \\ &= \frac{1}{4}(1 + a_1^2 X^2 + a_2^2 Y^2 + a_3^2 Z^2) \\ &\quad + \frac{1}{4}a_x a_y (XY + YX) + a_x a_z (XZ + ZX) + a_y a_z (YZ + ZY) \\ &\quad + \frac{1}{4}2\mathbf{a} \cdot \Sigma \end{aligned}$$

The squares of Pauli matrices equal the unit matrix and they anticommute, so

$$\rho^2 = \frac{1}{4}(1 + |\mathbf{a}|^2) + \frac{1}{2}\mathbf{a} \cdot \Sigma$$

which equal ρ iff $|\mathbf{a}|^2 = 1$.

Figure 1 shows the pure states of the three basis X, Y, Z on the Bloch sphere. General pure states can be parametrized by two angles while for mixed states one also needs the length of the vector inside the ball.

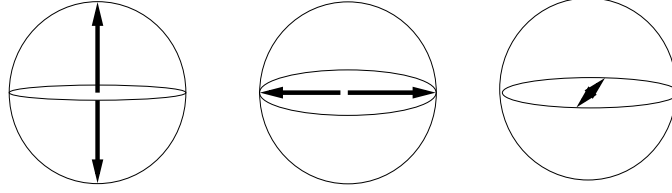


Figure 5.1: Z basis $\{|0\rangle, |1\rangle\}$, Y basis $\{\frac{1}{\sqrt{2}}(|0\rangle \pm |1\rangle)\}$, X basis $\{\frac{1}{\sqrt{2}}(|0\rangle \pm i|1\rangle)\}$

5.2 Postulates of QM revisited

We briefly give the postulates of QM in the density matrix formalism.

1. States. A quantum system is described by a Hilbert space \mathcal{H} . The state of the system is a density matrix ρ satisfying $\rho = \rho^\dagger$, $\rho \geq 0$ and $\text{Tr}\rho = 1$. One may also think of the state as a positive linear functional $A \in \mathcal{B}(\mathcal{H}) \rightarrow \text{Tr}A\rho \in \mathbb{C}$. These form a convex set. The extremal points are one dimensional projectors and are called pure states. Other states that are non-trivial linear combinations of one dimensional projectors are called mixed states. Any density matrix is of the form

$$\rho = \sum_n \lambda_n |\phi_n\rangle\langle\phi_n|$$

with $0 \leq \lambda_n \leq 1$ and $\sum_n \lambda_n = 1$.

2. Evolution. The dynamics of the system is given by a unitary matrix acting on the states as

$$\rho(t) = U_t \rho(0) U_t^\dagger$$

Indeed let the initial condition be $\rho(0) = \sum_n \lambda_n |\phi_n\rangle\langle\phi_n|$. At time t each state of the mixture is $U_t |\phi_n\rangle$ thus $\rho(t) = \sum_n \lambda_n U_t |\phi_n\rangle\langle\phi_n| U_t^\dagger = U_t \rho(0) U_t^\dagger$.

3. Observables. They are described by linear selfadjoint operators $A = A^\dagger$. they have a spectral decomposition $A = \sum_n \alpha_n P_n$ with real eigenvalues α_n and an orthonormal set of projectors P_n satisfying the closure or completeness relation $\sum_n P_n = 1$.

4. Measurements. The measurement of an observable A is described by the measurement basis formed by the eigenprojectors of A . When the system is prepared in state ρ the possible outcomes of the measurement are

$$\rho_{after} = \frac{P_n \rho P_n}{\text{Tr} P_n \rho P_n}$$

with probability

$$\text{Prob}(n) = \text{Tr} P_n \rho P_n$$

As we will see one can always purify the system, which means constructing a bigger system whose reduced density matrix is ρ . Applying the usual measurement postulate to the purified system leads to the above formulas (we showed this at the very beginning of the chapter).

5. Composite systems. A system composed of two (or more) parts $\mathcal{A} \cup \mathcal{B}$ has a tensor product Hilbert space $\mathcal{H}_{\mathcal{A}} \otimes \mathcal{H}_{\mathcal{B}}$. A density matrix for this system is of the general form

$$\rho = \sum_n \lambda_n |\phi_n\rangle\langle\phi_n|$$

with $|\phi_n\rangle \in \mathcal{H}_{\mathcal{A}} \otimes \mathcal{H}_{\mathcal{B}}$, $0 \leq \lambda_n \leq 1$ and $\sum_n \lambda_n = 1$. Note that $\rho = \rho_{\mathcal{A}} \otimes \rho_{\mathcal{B}}$ only if there are no correlations between the parts.

A remark about the Schroedinger and Heisenberg pictures. In the Schroedinger picture of QM the states evolve as in postulate 2 above and observables stay fixed. The average value of A at time t is given by $\text{Tr} A \rho(t)$ where $\rho(t) = U_t \rho U_t^\dagger$. The Heisenberg picture is a mathematically equivalent description where the states ρ stay fixed and the observables evolve according to $A(t) = U_t^\dagger A U_t$. In the Heisenberg picture the average is $\text{Tr} A(t) \rho$. Both pictures are equivalent because of the cyclicity of the trace.

5.3 Partial trace and Reduced density matrix

Suppose we have a composite system with Hilbert space $\mathcal{H}_{\mathcal{A}} \otimes \mathcal{H}_{\mathcal{B}}$ and let it be described by a density matrix ρ . The *reduced density matrix* of \mathcal{A} (resp. \mathcal{B}) is

$$\rho_{\mathcal{A}} = \text{Tr}_{\mathcal{H}_{\mathcal{B}}} \rho \quad \rho_{\mathcal{B}} = \text{Tr}_{\mathcal{H}_{\mathcal{A}}} \rho$$

Here the trace is performed over $\mathcal{H}_{\mathcal{B}}$ only (resp. $\mathcal{H}_{\mathcal{A}}$ only). This is known as a partial trace and can be defined as follows

$$\text{Tr}_{\mathcal{B}} \underbrace{(|a_1\rangle\langle a_2| \otimes |b_1\rangle\langle b_2|)}_{\text{operator in } \mathcal{H}_{\mathcal{A}} \otimes \mathcal{H}_{\mathcal{B}}} = |a_1\rangle\langle a_2| (\text{Tr} |b_1\rangle\langle b_2|) = \underbrace{(|a_1\rangle\langle a_2|)}_{\text{operator in } \mathcal{H}_{\mathcal{A}}} \underbrace{\langle b_2|b_1\rangle}_{\in \mathbb{C}}$$

This rule combined with linearity enables one to compute all partial traces in practice. You can translate this rule for computing a partial trace in the usual matrix language but you will see that the Dirac notation is much more powerful at this point. In general if $\rho = \sum_n \lambda_n |\phi_n\rangle\langle\phi_n|$ and $|\phi_n\rangle =$

$\sum_{i,j} a_{ij}^n |\phi_i\rangle_{\mathcal{A}} \otimes |\chi_j\rangle_{\mathcal{B}}$, we have

$$\rho = \sum_{n,i,j,k,l} \lambda_n a_{ij}^n (|\phi_i\rangle_{\mathcal{A}} \otimes |\chi_j\rangle_{\mathcal{B}}) (\langle\phi_k|_{\mathcal{A}} \otimes \langle\chi_l|_{\mathcal{B}}) \quad (5.2)$$

$$= \sum_{n,i,j,k,l} \lambda_n a_{ij}^n (|\phi_i\rangle_{\mathcal{A}} \langle\phi_k|_{\mathcal{A}}) \otimes (|\chi_j\rangle_{\mathcal{B}} \langle\chi_l|_{\mathcal{B}}) \quad (5.3)$$

The partial traces are

$$\rho_{\mathcal{A}} = \text{Tr}_{\mathcal{H}_{\mathcal{B}}} \rho = \sum_{i,k} \left(\sum_{n,j,l} \lambda_n a_{ij}^n \langle\chi_l|\chi_j\rangle_{\mathcal{B}} \right) (|\phi_i\rangle_{\mathcal{A}} \langle\phi_k|_{\mathcal{A}})$$

and

$$\rho_{\mathcal{B}} = \text{Tr}_{\mathcal{H}_{\mathcal{A}}} \rho = \sum_{j,l} \left(\sum_{n,i,k} \lambda_n a_{ij}^n \langle\phi_k|\phi_i\rangle_{\mathcal{A}} \right) (|\chi_j\rangle_{\mathcal{B}} \langle\chi_l|_{\mathcal{B}})$$

Examples.

- The partial trace of a tensor product state is a pure state. Indeed let $|\Psi\rangle = |\phi\rangle_{\mathcal{A}} \otimes |\chi\rangle_{\mathcal{B}}$. Then one finds

$$\rho_{\mathcal{A}} = |\phi\rangle_{\mathcal{A}} \langle\phi|_{\mathcal{A}}, \quad \rho_{\mathcal{B}} = |\chi\rangle_{\mathcal{B}} \langle\chi|_{\mathcal{B}}$$

- The partial trace of an entangled pure state is a mixed state (we prove this in full generality later). The reader should check that if $\rho = |B_{00}\rangle$ then

$$\rho_{\mathcal{A}} = \frac{1}{2} I_{\mathcal{A}}, \quad \rho_{\mathcal{B}} = \frac{1}{2} I_{\mathcal{B}}$$

- Another instructive calculation is for $\rho = \frac{1}{2} |B_{00}\rangle \langle B_{00}| + \frac{1}{2} |01\rangle \langle 01|$,

$$\rho_{\mathcal{A}} = \frac{3}{4} |0\rangle_{\mathcal{A}} \langle 0|_{\mathcal{A}} + \frac{1}{4} |1\rangle_{\mathcal{A}} \langle 1|_{\mathcal{A}}, \quad \rho_{\mathcal{B}} = \frac{1}{4} |0\rangle_{\mathcal{B}} \langle 0|_{\mathcal{B}} + \frac{3}{4} |1\rangle_{\mathcal{B}} \langle 1|_{\mathcal{B}}$$

The eigenvalues of the two reduced density matrices are the same. Do you think this is a coincidence?

Physical interpretation. Basically the interpretation of the reduced density matrix is the same as the one discussed in the introduction to this chapter. For a composite system \mathcal{AB} is the state ρ , the RDM $\rho_{\mathcal{A}}$ describes everything that is accessible by local operations in the part \mathcal{A} .

In particular if we measure a local observable $A \otimes I = \sum_n \alpha_n P_n \otimes I$ according to postulate 4) the measured value of the observable is α_n , and the total state collapses to

$$\rho_{after} = \frac{(P_n \otimes I)\rho}{Tr(P_n \otimes I)\rho}$$

with probability

$$prob(n) = Tr(P_n \otimes I)\rho$$

Thus the average value of the observable is $\sum_n \alpha_n prob(n) = Tr(A \otimes I)\rho$. This is also equal to $Tr A \rho$. Since this is true for *any* local observable, from the point of view of a local observer in \mathcal{A} , before the measurement the system is in state $\rho_{\mathcal{A}}$ and after it is found in the state

$$\rho_{\mathcal{A}, after} = Tr_{\mathcal{H}_B} \rho_{after} = \frac{P_n \rho_{\mathcal{H}_A}}{Tr P_n \rho_{\mathcal{A}}}$$

with probability

$$prob(n) = Tr A \rho_{\mathcal{A}}$$

As an example consider the composite system formed of an EPR pair in the state state $|B_{00}\rangle$. Imagine Alice does measurements on her photons and does not communicate with Bob. From the discussions of chapter 4 we know that for any measurement basis $\{|\alpha\rangle, |\alpha_{\perp}\rangle\}$ (this means she measures any observable $A = \lambda_1 |\alpha\rangle\langle\alpha| + \lambda_2 |\alpha_{\perp}\rangle\langle\alpha_{\perp}|$) she will find outcomes α or α_{\perp} each with probability $\frac{1}{2}$. Since this is true for *any* choice of α some thought will show that the only compatible state with the outcomes is the mixed state $\rho_{\mathcal{A}} = \frac{1}{2}I$. Within the density matrix formalism we can arrive at this result in an immediate manner. Indeed the reduced density matrix of the Bell state is indeed $\rho_{\mathcal{A}} = \frac{1}{2}I$. The physical interpretation is that if Alice and Bob share an EPR pair the result of local measurements of Alice cannot distinguish between the entangled state and the mixed state $\frac{1}{2}I$. We will see that this has an interesting consequence for the notion of quantum mechanical entropy: the entropy of the composite system is zero (it is in a well defined pure state) but at the same time the entropy of its parts is maximal (it is $\ln 2$). Thus in the quantum world the entropy³ of a system can be lower than the entropy of its parts. This is one of the effects of entanglement which violates classical inequalities such as Shannon's $H(X, Y) \geq H(X)$.

³we will introduce in the next chapter the von Neumann entropy which is a direct generalization of Shannon's entropy

5.4 Schmidt decomposition and purification

The Schmidt decomposition and purifications are two useful that we will use extensively later on.

Theorem 2. *Let $|\Psi\rangle$ be a pure state for a bipartite system with Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$. then*

a) $\rho_A = \text{Tr}_B |\Psi\rangle\langle\Psi|$ and $\rho_B = \text{Tr}_A |\Psi\rangle\langle\Psi|$ have the same non-zero eigenvalues with the same multiplicities. The multiplicity of the zero eigenvalue (if present) may or may not be different. Thus the spectral decompositions of the two reduced density matrices are

$$\rho_A = \sum_i \rho_i |i\rangle_A \langle i|_A, \quad \rho_B = \sum_i \rho_i |i\rangle_B \langle i|_B$$

with $\lambda_i > 0$ and $\sum_i \lambda_i = 1$. Note that we do not write explicitly the contribution of the zero eigenvalues since they contribute a vanishing term. Here $|i\rangle_A$ are orthonormal states of \mathcal{H}_A and $|i\rangle_B$ are other orthonormal states of \mathcal{H}_B . Note that they do not form a complete basis unless we include also the eigenstates of the 0 eigenvalues. If the non-zero eigenvalues are not degenerate the vectors $|i\rangle_A$ and $|i\rangle_B$ are unique (up to a phase). Otherwise there is freedom in their choice (rotations in the ρ_i subspaces).

b) The pure state $|\Psi\rangle$ has the Schmidt decomposition

$$|\Psi\rangle = \sum_i \sqrt{\rho_i} |i\rangle_A \otimes |i\rangle_B$$

This expansion (with positive coefficients) is unique up to rotations in the span of ρ_i .

An immediate consequence is

Corollary 3. *For any $|\Psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$ we can form $\rho = |\Psi\rangle\langle\Psi|$ and ρ_A, ρ_B . We have*

$$\text{Tr} F(\rho_A) = \sum_i F(\rho_i) + g_A F(0), \quad \text{Tr} F(\rho_B) = \sum_i F(\rho_i) + g_B F(0)$$

and

$$\text{Tr} F(\rho_A) - \text{Tr} F(\rho_B) = (g_A - g_B) F(0)$$

where g_A and g_B are the degeneracies of the zero eigenvalues of ρ_A and ρ_B .

Proof. Let us prove the Schmidt theorem. Let $\{|\mu\rangle_{\mathcal{A}}\}$ be an orthonormal basis of \mathcal{A} and $\{|\mu'\rangle_{\mathcal{B}}\}$ an orthonormal basis of \mathcal{B} . We can expand any pure state in the tensor product basis,

$$|\Psi\rangle = \sum_{\mu, \mu'} a_{\mu\mu'} |\mu\rangle_{\mathcal{A}} \otimes |\mu'\rangle_{\mathcal{B}}$$

For each $|\mu\rangle_{\mathcal{A}}$ set

$$|\tilde{\mu}\rangle_{\mathcal{B}} = \sum_{\mu'} a_{\mu\mu'} |\mu'\rangle_{\mathcal{B}}$$

so that

$$|\Psi\rangle = \sum_{\mu} |\mu\rangle_{\mathcal{A}} \otimes |\tilde{\mu}\rangle_{\mathcal{B}}$$

Note that $\{|\tilde{\mu}\rangle_{\mathcal{B}}\}$ is not necessarily an orthonormal basis so this is not yet a Schmidt decomposition. For the reduced density matrix of the \mathcal{A} part we get

$$\rho_{\mathcal{A}} = \sum_{\mu_1, \mu_2} \langle \tilde{\mu}_2 | \tilde{\mu}_1 \rangle_{\mathcal{B}} |\mu_1\rangle_{\mathcal{A}} \langle \mu_2|_{\mathcal{A}}$$

Suppose now that

$$\rho_{\mathcal{A}} |i\rangle_{\mathcal{A}} = \rho_i |i\rangle_{\mathcal{A}}$$

For the basis $\{|\mu\rangle_{\mathcal{A}}\}$ we take $\{|i\rangle_{\mathcal{A}}\}$, so

$$\rho_{\mathcal{A}} = \sum_{i_1, i_2} \langle \tilde{i}_2 | \tilde{i}_1 \rangle_{\mathcal{B}} |i_1\rangle_{\mathcal{A}} \langle i_2|_{\mathcal{A}}$$

But we also have

$$\rho_{\mathcal{A}} = \sum_{i_1} \rho_{i_1} |i_1\rangle_{\mathcal{A}} \langle i_1|_{\mathcal{A}}$$

So for all non zero terms, $\rho_{i_1} \neq 0$, we must have $\langle \tilde{i}_2 | \tilde{i}_1 \rangle_{\mathcal{B}} = \lambda_{i_1} \delta_{i_1 i_2}$. Thus the states $|\tilde{i}\rangle_{\mathcal{B}}$ are orthogonal and we can make them orthonormal by defining

$$|i\rangle_{\mathcal{B}} = \lambda_i^{-1/2} |\tilde{i}\rangle_{\mathcal{B}}$$

In this way we obtain the expansion

$$|\Psi\rangle = \sum_i |i\rangle_{\mathcal{A}} \otimes |\tilde{i}\rangle_{\mathcal{B}} = \sum_i \sqrt{\rho_i} |i\rangle_{\mathcal{A}} \otimes |i\rangle_{\mathcal{B}}$$

which is the Schmidt decomposition (statement b)). To obtain statement a) we simply compute the partial traces from this expansion which leads to

$$\rho_{\mathcal{A}} = \sum_i \rho_i |i\rangle_{\mathcal{A}} \langle i|_{\mathcal{A}}, \quad \rho_{\mathcal{B}} = \sum_i \rho_i |i\rangle_{\mathcal{B}} \langle i|_{\mathcal{B}}$$

These expressions show that $\rho_{\mathcal{A}}$ and $\rho_{\mathcal{B}}$ have the same non zero eigenvalues with the same multiplicities. Now suppose we have a second Schmidt decomposition. This will lead to a second spectral decomposition for $\rho_{\mathcal{A}}$ and $\rho_{\mathcal{B}}$. Thus the unicity of the Schmidt decomposition up to rotations in the span of each ρ_i follows from the same fact for the spectral decomposition. \square

Notion of Schmidt number. The number of non-zero coefficients (including multiplicity) in the Schmidt decomposition of $|\Psi\rangle$ is called the *Schmidt number* of the state. It is invariant under unitary evolutions that do not couple \mathcal{A} and \mathcal{B} . Indeed if $U = U_{\mathcal{A}} \otimes U_{\mathcal{B}}$ then

$$U|\Psi\rangle = \sum_i \sqrt{\rho_i} U_{\mathcal{A}}|i\rangle_{\mathcal{A}} \otimes U_{\mathcal{B}}|i\rangle_{\mathcal{B}}$$

which has the same number of non zero coefficients. This number is also the number of non-zero eigenvalues of the reduced density matrices $Tr_{\mathcal{B}}|\Psi\rangle\langle\Psi|$ and $Tr_{\mathcal{A}}|\Psi\rangle\langle\Psi|$. This number can change only if \mathcal{A} and \mathcal{B} interact in some way.

Obviously a tensor product state has Schmidt number equal to 1. Since an entangled state is one which cannot be written as a tensor product state its Schmidt number is necessarily ≥ 2 . The Schmidt number is our first attempt to quantify the degree of entanglement.

Purification. This turns out to be a powerful mathematical tool. Given a system S with Hilbert space \mathcal{H}_S and density matrix ρ_S one can view it a part of a bigger system $S \cup R$ with Hilbert space $\mathcal{H}_S \otimes \mathcal{H}_R$ in a *pure* state $|\Psi\rangle_{SR}$ such that

$$\rho_S = Tr_R|\Psi\rangle_{SR}\langle\Psi|_{SR}$$

The Schmidt decomposition can be used to explicitly construct the pure state $|\Psi\rangle_{SR}$. We remark however that the purification is *not unique*. One uses the spectral decomposition

$$\rho_S = \sum \rho_i |i\rangle_{\mathcal{A}}\langle i|_{\mathcal{A}}$$

and takes a copy of the space \mathcal{H}_S - call it \mathcal{H}_R . Each vector $|i\rangle_S$ has a copy which we call $|i\rangle_R$. Then form

$$|\Psi\rangle_{SR} = \sum_i \sqrt{\rho_i} |i\rangle_S \otimes |i\rangle_R$$

The reader can easily check that $\rho_S = Tr_R|\Psi\rangle_{SR}\langle\Psi|_{SR}$.