11 Density operators

Let
\[ S(\mathcal{H}) = \{ \psi \in \mathcal{H} : \|\psi\| = 1 \} \]  
(11.1)
denote the unit sphere in Hilbert space. It is common to write \( \langle \psi \rangle \) for the linear form \( \phi \mapsto \langle \psi | \phi \rangle \), and \( |\psi\rangle \) for \( \psi \). (The latter notation also allows us to write \( |1\rangle, |2\rangle, \ldots \) instead of \( \psi_1, \psi_2, \ldots \)). Then \( |\psi\rangle \langle \psi| \) is an operator, viz. \( \phi \mapsto \langle \psi| \phi \rangle \psi \); for \( \psi \in S(\mathcal{H}) \), this is the projection \( P_{C_\psi} \) to the 1d subspace spanned by \( \psi \). Note also that \( \langle \psi | \) applied to \( |\phi\rangle \) gives \( \langle \psi| \phi \rangle \), and \( \langle \psi|A|\phi \rangle = \langle \psi|A\phi \rangle \), so no ambiguity arises.

Suppose that (by whatever mechanism) we have generated a random wave function \( \Psi \in S(\mathcal{H}) \) with distribution given by the probability measure \( \mu \) on \( S(\mathcal{H}) \). Then for any experiment \( \mathcal{E} \) with POVM \( E(\cdot) \), the probability distribution of the outcome \( Z \) is

\[
\operatorname{Prob}(Z \in \Delta) = E\langle \Psi| E(\Delta)|\Psi \rangle = \int_{S(\mathcal{H})} \mu(d\psi) \langle \psi| E(\Delta)|\psi \rangle = \operatorname{tr}(\rho_{\mu} E(\Delta)),
\]  
(11.2)
where \( E \) means expectation,

\[
\rho_{\mu} = E|\Psi\rangle\langle \Psi| = \int_{S(\mathcal{H})} \mu(d\psi) |\psi\rangle\langle \psi| \]  
(11.3)
is called the density operator or density matrix (rarely: statistical operator) of the distribution \( \mu \), and \( \operatorname{tr} \) means the trace. Equation (11.2) is called the trace formula.

11.1 Trace of an operator

Let \( \mathcal{H} \) be separable. The trace of an operator \( T \) is defined to be the sum of the diagonal elements of its matrix representation \( T_{nm} = \langle n|T|m \rangle \) relative to an arbitrary orthonormal basis \( \{|n\} \),

\[
\operatorname{tr} T = \sum_{n=1}^{\infty} \langle n|T|n \rangle .
\]  
(11.4)
However, the series may not converge, or may converge for one orthonormal basis and not for another. That is why one splits the rigorous definition in two steps.

Step 1: If \( T \in \mathcal{B}(\mathcal{H}) \) is a positive operator then its trace is defined by (11.4), which is either a nonnegative real number or \( +\infty \).

Proposition 11.1. This value does not depend on the choice of orthonormal basis. The trace has the following properties:

(i) \( \operatorname{tr}(A + B) = \operatorname{tr} A + \operatorname{tr} B \)

(ii) \( \operatorname{tr}(\lambda A) = \lambda \operatorname{tr} A \) for all \( \lambda \geq 0 \)

(iii) \( \operatorname{tr}(UAU^{-1}) = \operatorname{tr} A \) for any unitary operator \( U \)
(iv) If \( 0 \leq A \leq B \) then \( \text{tr} A \leq \text{tr} B \).

Proof. Let \( \phi = \{\phi_n\} \) and \( \psi = \{\psi_m\} \) be two ONBs of \( \mathcal{H} \).

\[
\text{tr}_\phi(A) = \sum_{n=1}^{\infty} \langle \phi_n | A \phi_n \rangle = \sum_{n=1}^{\infty} \| A^{1/2} \phi_n \|^2
\]

(11.5)

\[
= \sum_{n=1}^{\infty} \left( \sum_{m=1}^{\infty} |\langle \psi_m | A^{1/2} \phi_n \rangle|^2 \right)
\]

(11.6)

\[
= \sum_{m=1}^{\infty} \left( \sum_{n=1}^{\infty} |\langle A^{1/2} \psi_m | \phi_n \rangle|^2 \right)
\]

(11.7)

\[
= \sum_{m=1}^{\infty} \| A^{1/2} \psi_m \|^2 = \sum_{m=1}^{\infty} \langle \psi_m | A \psi_m \rangle = \text{tr}_\psi A.
\]

(11.8)

Interchanging the sums is allowed because all terms are non-negative. For (iii), note that \( \{U \phi_n\} \) is an ONB, too; (i), (ii), (iv) are obvious.

\[ \square \]

**Example 11.2.** If \( P \) is the projection to the closed subspace \( X \subseteq \mathcal{H} \) then \( \text{tr} P = \text{dim} X \leq \infty \).

Step 2: This definition is extended to non-positive operators as follows.

**Definition 11.3.** An operator \( T \in \mathcal{B}(\mathcal{H}) \) belongs to the trace class \( \mathcal{I}_1 \) iff the positive operator \( |T| = \sqrt{T^*T} \) has finite trace.

**Proposition 11.4.** \( \mathcal{I}_1 \) is a vector space. If \( A \in \mathcal{I}_1 \) and \( B \in \mathcal{B}(\mathcal{H}) \) then \( AB, BA \in \mathcal{I}_1 \) and \( A^* \in \mathcal{I}_1 \). If \( A \in \mathcal{I}_1 \) and \( \{|n\rangle\} \) is any ONB, then \( \text{tr} A := \sum_{n=1}^{\infty} \langle n | A | n \rangle \) converges absolutely and is independent of the ONB. \( \mathcal{I}_1(\mathcal{H}) \) is a Banach space with respect to the trace norm

\[
\|T\|_1 := \text{tr}\sqrt{T^*T}.
\]

(11.9)

(i) \( \text{tr} \) is linear

(ii) \( \text{tr}(A^*) = (\text{tr} A)^* \)

(iii) \( \text{tr}(AB) = \text{tr}(BA) \) for \( A \in \mathcal{I}_1 \) and \( B \in \mathcal{B}(\mathcal{H}) \).

Proof. Reed and Simon, Volume 1, pages 207–211.

\[ \square \]

**Remark 11.5.**

- If, for some ONB \( \{|n\rangle\} \), \( \sum_{n=1}^{\infty} |\langle n | A | n \rangle| < \infty \) then \( A \) does not have to be in the trace class.

- If \( T \in \mathcal{B}(\mathcal{H}) \) is positive then \( |T| = T \), and \( T \in \mathcal{I}_1 \) iff \( \text{tr} T < \infty \). The two definitions of trace (one for positive operators, one for trace class operators) obviously agree.
• By property (iii), the trace is invariant under cyclic permutation of any number of factors $A \in \mathcal{A}, B, \ldots, Z \in \mathcal{B}({\mathcal{H}})$:

$$\text{tr}(AB \cdots YZ) = \text{tr}(ZAB \cdots Y). \quad (11.10)$$

In particular $\text{tr}(ABC) = \text{tr}(CAB)$, which is, however, not always the same as $\text{tr}(CBA)$.

• If there exists an ONB of eigenvectors of $A$, then $\text{tr} A$ is the sum of the eigenvalues, counted with multiplicity (= degree of degeneracy).

• The trace of a self-adjoint operator $A \in \mathcal{A}$ is real. A self-adjoint operator lies in the trace class if and only its spectrum is discrete and bounded, all nonzero eigenvalues have finite multiplicity, and the sum of the eigenvalues (with multiplicity) is finite (i.e., converges absolutely).

11.2 The trace formula in quantum mechanics

In order to verify the trace formula (11.2), note first that

$$\text{tr}\left(\langle \psi|\psi| E(\Delta) \right) = \langle \psi|E(\Delta)|\psi\rangle \quad (11.11)$$

because, if we choose the basis $\{|n\rangle\}$ in (11.4) such that $|1\rangle = \psi$, then the summands in (11.4) are $\langle n|\psi\rangle\langle \psi|E(\Delta)|n\rangle$, which for $n = 1$ is $\langle \psi|E(\Delta)|\psi\rangle$ and for $n > 1$ is zero because $\langle n|1\rangle = 0$. By linearity, we also have that

$$\text{tr}\left(\sum_{i=1}^{M} p_i |\psi_i\rangle\langle \psi_i| E(\Delta) \right) = \sum_{i=1}^{M} p_i \langle \psi|E(\Delta)|\psi\rangle, \quad (11.12)$$

which yields (11.2) for any $\mu$ that is concentrated on finitely many points $\psi_i$ on $\mathcal{S}(\mathcal{H})$.

To allow arbitrary probability measures $\mu$ on $\mathcal{S}(\mathcal{H})$ (equipped with its Borel $\sigma$-algebra, which are the Borel sets in $\mathcal{H}$ that are subsets of $\mathcal{S}(\mathcal{H})$), we need the following.

**Proposition 11.6.**  
(i) The integral $\int \mu(d\psi)|\psi\rangle\langle \psi|$ is well defined as a weak integral, i.e., there is a unique $\rho \in \mathcal{B}(\mathcal{H})$ such that for all $\phi \in \mathcal{B}(\mathcal{H})$, $\langle \phi|\rho\phi\rangle = \int \mu(d\psi)\langle \phi|\psi\rangle\langle \psi|\phi\rangle$.

(ii) $\rho \geq 0$

(iii) $\rho \in \mathcal{A}$ and $\text{tr} \rho = 1$.

(iv) For any $E \in \mathcal{B}(\mathcal{H})$, $\text{tr}(\rho E) = \int \mu(d\psi)\langle \psi|E\psi\rangle$. This proves (11.2).
Proof. (i) The mapping $B(\phi, \chi) = \int \mu(d\psi) \langle \phi|\psi\rangle \langle \psi|\chi \rangle$ is well defined, is a sesqui-linear form $\mathcal{H} \times \mathcal{H} \to \mathbb{C}$, and is bounded, $|B(\phi, \chi)| \leq \|\phi\|\|\chi\|$. By the Riesz representation theorem, there is an operator $\rho \in \mathcal{B}(\mathcal{H})$ such that $B(\phi, \chi) = \langle \phi|\rho|\chi \rangle$. We have seen before that bounded operators are uniquely determined by their diagonal elements.

(ii) follows from $\langle \phi|\rho\phi \rangle = \int \mu(d\psi) \langle \phi|\psi\rangle \langle \psi|\phi \rangle = \int \mu(d\psi) |\langle \phi|\psi \rangle|^2 \geq 0$.

(iii) $\rho \in J_1$ follows when we have shown that $\text{tr} \rho < \infty$. By the Fubini–Tonelli theorem,

\[
\text{tr} \rho = \sum_{n=1}^{\infty} \langle n|\rho|n \rangle = \sum_{n=1}^{\infty} \int \mu(d\psi) |\langle n|\psi \rangle|^2 = \int \mu(d\psi) \sum_{n=1}^{\infty} |\langle n|\psi \rangle|^2 = \int \mu(d\psi) \|\psi\|^2 = 1. \tag{11.13}
\]

(iv) By the Fubini theorem,

\[
\text{tr}(\rho E) = \sum_{n=1}^{\infty} \langle n|\rho E|n \rangle = \sum_{n=1}^{\infty} \int \mu(d\psi) \langle n|\psi\rangle \langle \psi|E|n \rangle \tag{11.15}
\]

\[
= \int \mu(d\psi) \sum_{n=1}^{\infty} \langle n|\psi\rangle \langle \psi|E|n \rangle \tag{11.16}
\]

\[
= \int \mu(d\psi) \text{tr}(\psi\langle \psi|E \rangle) = \int \mu(d\psi) \langle \psi|E|\psi \rangle. \tag{11.17}
\]

To justify the interchange of summation and integration, we need that the integrand is in $L^1$, i.e.,

\[
\int \mu(d\psi) \sum_{n=1}^{\infty} |\langle n|\psi\rangle \langle \psi|E|n \rangle| \leq \int \mu(d\psi) \left( \sum_{n} |\langle n|\psi \rangle|^2 \right)^{1/2} \left( \sum_{n} |\langle E^*|\psi|n \rangle|^2 \right)^{1/2} \tag{11.18}
\]

\[
= \int \mu(d\psi) \|\psi\| \|E^*\psi\| \leq \|E\| < \infty. \tag{11.19}
\]

Now let us draw conclusions from the formula (11.2). It implies that the distribution of the outcome $Z$ depends on $\mu$ only through $\rho_\mu$. Different distributions $\mu_a, \mu_b$ can have the same $\rho = \rho_{\mu_a} = \rho_{\mu_b}$; for example, if $\mathcal{H} = \mathbb{C}^2$ then the uniform distribution over $S(\mathcal{H}) = S^3$ has $\rho = \frac{1}{2}I$, and for every orthonormal basis $|\phi_1\rangle, |\phi_2\rangle$ of $\mathbb{C}^2$ the probability distribution

\[
\frac{1}{2} \delta_{\phi_1} + \frac{1}{2} \delta_{\phi_2} \tag{11.20}
\]

also has $\rho = \frac{1}{2}I$. Such two distributions $\mu_a, \mu_b$ will lead to the same distribution of outcomes for any experiment, and are therefore empirically indistinguishable.

We can turn this result into an argument showing that there must be facts we cannot find out by experiment: Suppose I choose $\mu$ to be either $\mu_a$ or $\mu_b$, then I choose $n = 10^4$
points $\psi_i$ on $S(\mathcal{H})$ at random independently with $\mu_i$, then I prepare $n$ systems with wave functions $\psi_i$, and then I hand these systems to you with the challenge to determine whether $\mu = \mu_a$ or $\mu = \mu_b$. As a consequence of (11.2), you cannot determine that by means of experiments on the $n$ systems. On the other hand, nature knows the right answer, as nature must remember the wave function of each system; after all, I might keep records of each $\psi_i$ and can predict that system $i$ will in a quantum measurement of $|\psi_i\rangle \langle \psi_i|$ yield the outcome $1$. Thus, there is a fact in nature (whether $\mu = \mu_a$ or $\mu = \mu_b$) that we cannot discover empirically. Nature can keep a secret.

If the random vector $\Psi$ evolves according to the Schrödinger equation, $\Psi_t = e^{-iHt/\hbar} \Psi$, the distribution changes into $\mu_t$ and the density matrix into

$$\rho_t = e^{-iHt/\hbar} \rho e^{iHt/\hbar}. \tag{11.21}$$

In analogy to the Schrödinger equation, this can be written as a differential equation,

$$\frac{d\rho_t}{dt} = -\frac{i}{\hbar} [H, \rho_t], \tag{11.22}$$

known as the von Neumann equation. $\rho_t$ is weakly differentiable, i.e., $t \mapsto \langle \psi | \rho_t | \psi \rangle$ is differentiable, for $\psi \in \mathcal{D}(\mathcal{H})$, and (11.22) is true in the weak sense for such $\psi$.

If $\rho = |\psi\rangle \langle \psi|$ with $\|\psi\| = 1$, then $\rho$ is usually called a pure quantum state, otherwise a mixed quantum state. A probability distribution $\mu$ has $\rho = |\psi\rangle \langle \psi|$ if and only if $\mu$ is concentrated on $\mathbb{C} \psi$, i.e., $\Psi = e^{i\Theta} \psi$ with a random global phase factor.

As we have seen, a density matrix $\rho$ is always a positive operator with $\text{tr} \rho = 1$. Conversely, every positive operator $\rho$ with $\text{tr} \rho = 1$ is a density matrix, i.e., $\rho = \rho_\mu$ for some probability distribution $\mu$ on $S(\mathcal{H})$. This is because any positive operator $A \in \mathcal{I}_1$ is bounded and thus self-adjoint; $A$ has a discrete spectrum, and thus there is an orthonormal basis $\{ |\phi_n\rangle : n \in \mathbb{N} \}$ of eigenvectors of $\rho$ with eigenvalues $p_n \in [0, \infty)$, and

$$\sum_n p_n = \text{tr} \rho = 1. \tag{11.23}$$

Now let $\mu$ be the distribution that gives probability $p_n$ to $\phi_n$; its density matrix is just the $\rho$ we started with.

### 11.3 Reduced density operators

There is another way in which density matrices arise, leading to what is called the reduced density matrix. Suppose that the system under consideration consists of two parts, system $a$ and system $b$, so that its Hilbert space is $\mathcal{H} = \mathcal{H}_a \otimes \mathcal{H}_b$, and that the experiment $\mathcal{E}$ has a POVM of the form

$$E(\Delta) = E_a(\Delta) \otimes I_b, \tag{11.24}$$

where $I_b$ is the identity on $\mathcal{H}_b$.

**Homework problem.** Prove that in Bohmian mechanics, an experiment in which the apparatus interacts only with system $a$ but not with system $b$ has a POVM of the form
Theorem. To this end, adapt the proof of the main theorem of POVMs. Suppose the experiment $E$ begins at time $t_1$ and ends at time $t_2$, and suppose the wave function of the apparatus, system $a$, and system $b$ at time $t_1$ is $\Psi(t_1) = \phi \otimes \psi$ with $\psi \in \mathcal{H}_a \otimes \mathcal{H}_b$, so $\Psi(t_1) \in \mathcal{H}_{app} \otimes \mathcal{H}_a \otimes \mathcal{H}_b$. Assume further that the outcome $Z$ is a function $\zeta$ of the configuration $Q_{app}$ of the apparatus at time $t_2$.

In the case (11.24), the distribution of the outcome is

$$\text{Prob}(Z \in \Delta) = \langle \psi | E(\Delta) | \psi \rangle = \text{tr}(\rho_{\psi} E_a(\Delta))$$

(11.25)

with the reduced density matrix of system $a$

$$\rho_{\psi} = \text{tr}_b |\psi\rangle \langle \psi|,$$

(11.26)

where $\text{tr}_b$ means the partial trace over $\mathcal{H}_b$.

11.4 Partial trace

Homework problem 11.7. For $T_a \in \mathcal{B}(\mathcal{H}_a)$ and $T_b \in \mathcal{B}(\mathcal{H}_b)$, there is a unique operator $T_a \otimes T_b \in \mathcal{B}(\mathcal{H}_a \otimes \mathcal{H}_b)$ satisfying

$$(T_a \otimes T_b)(\psi_a \otimes \psi_b) = (T_a \psi_a) \otimes (T_b \psi_b)$$

(11.27)

for all $\psi_a \in \mathcal{H}_a$ and $\psi_b \in \mathcal{H}_b$. It has the following properties.

(i) $(T_a \otimes T_b)^* = T_a^* \otimes T_b^*$

(ii) $(T_a \otimes T_b)(S_a \otimes S_b) = (T_a S_a) \otimes (T_b S_b)$

(iii) If $T_a \geq 0$ and $T_b \geq 0$ then $T_a \otimes T_b \geq 0$. In that case, $\text{tr}(T_a \otimes T_b) = (\text{tr} T_a)(\text{tr} T_b)$.

(iv) If $T_a \in \mathcal{I}_{1,a} := \mathcal{I}_1(\mathcal{H}_a)$ and $T_b \in \mathcal{I}_{1,b}$ then $T_a \otimes T_b \in \mathcal{I}_{1,a \otimes b} := \mathcal{I}_1(\mathcal{H}_a \otimes \mathcal{H}_b)$. In that case, $\text{tr}(T_a \otimes T_b) = (\text{tr} T_a)(\text{tr} T_b)$ and $\|T_a \otimes T_b\|_{1,a \otimes b} = \|T_a\|_{1,a}\|T_b\|_{1,b}$.

(v) $\mathcal{I}_{1,a \otimes b} = \overline{\text{span}}\{T_a \otimes T_b : T_a \in \mathcal{I}_{1,a}, T_b \in \mathcal{I}_{1,b}\}$ (closure in the trace norm).

Example 11.8. When (and only when) the systems $a$, $b$ do not interact, the Hamiltonian is of the form

$$H = H_a \otimes I_b + I_a \otimes H_b,$$

(11.28)

and the propagator $U_t = e^{-iHt/\hbar}$ is of the form

$$U_t = U_{a,t} \otimes U_{b,t},$$

(11.29)

with $U_{a/b,t} = e^{-iH_{a/b}t/\hbar}$.
Definition 11.9. \( \text{tr}_b \) is the unique linear mapping \( \mathcal{I}_{1,a \otimes b} \rightarrow \mathcal{I}_{1,a} \) such that
\[
\| \text{tr}_b T \|_{1,a} \leq \| T \|_{1,a \otimes b}
\]
for all \( T \in \mathcal{I}_{1,a \otimes b} \), and
\[
\text{tr}_b(T_a \otimes T_b) = \text{tr}(T_b) T_a.
\]
for all \( T_a \in \mathcal{I}_{1,a} \) and \( T_b \in \mathcal{I}_{1,b} \).

Here is an explicit construction of \( \text{tr}_b \). Let \( \{ \phi_n^a \} \) be an ONB of \( \mathcal{H}_a \) and \( \{ \phi_m^b \} \) an ONB of \( \mathcal{H}_b \). Then \( \{ \phi_n^a \otimes \phi_m^b \} \) is an ONB of \( \mathcal{H}_a \otimes \mathcal{H}_b \). If \( T \in \mathcal{I}_{1,a \otimes b} \) then
\[
\text{tr}_b T = \sum_{m=1}^{\infty} \langle \phi_m^b | T | \phi_m^b \rangle ,
\]
where the inner product is a partial inner product, so that each term in the sum is an operator in \( \mathcal{I}_{1,a} \),
\[
\langle \phi_m^b | T | \phi_m^b \rangle \psi_a = L_{\phi_m} T \psi_a \otimes \phi_m^b ,
\]
and the series converges in the trace norm. Equivalently, we can characterize the operator \( S = \text{tr}_b T \) by its matrix elements \( \langle \phi_n^a | S | \phi_k^b \rangle \):
\[
\langle \phi_n^a | \text{tr}_b T | \phi_k^b \rangle = \sum_{m=1}^{\infty} \langle \phi_n^a \otimes \phi_m^b | T | \phi_k^b \otimes \phi_m^b \rangle ,
\]
where the inner products on the right hand side are inner products in \( \mathcal{H}_a \otimes \mathcal{H}_b \).

The partial trace has the following properties:

(i) \( \text{tr}(\text{tr}_b(T)) = \text{tr}(T) \). Here, the first \( \text{tr} \) symbol means the trace in \( \mathcal{H}_a \), the second one the partial trace, and the last one the trace in \( \mathcal{H}_a \otimes \mathcal{H}_b \). This property follows from (11.34) by setting \( k = n \) and summing over \( n \).

(ii) \( \text{tr}_b(T^*) = (\text{tr}_b T)^* \).

(iii) If \( T \geq 0 \) then \( \text{tr}_b T \geq 0 \).

(iv) \( \text{tr}_b[ S(T_a \otimes I_b) ] = (\text{tr}_b S)T_a \).

From properties (iv) and (i) we obtain that
\[
\text{tr}[ S(T_a \otimes I_b) ] = \text{tr}[ (\text{tr}_b S)T_a ] .
\]
Setting \( S = | \psi \rangle \langle \psi | \) and \( T_a = E_a(\Delta) \), we find that \( \text{tr}_b S = \rho_\psi \) and
\[
\langle \psi | E_a(\Delta) \otimes I_b | \psi \rangle = \text{tr}[ | \psi \rangle \langle \psi | (E_a(\Delta) \otimes I_b) ] = \text{tr}[ \rho_\psi E_a(\Delta) ] ,
\]
which proves (11.25).
From properties (i) and (iii) it follows also that $\rho_\psi$ is a positive operator with trace 1. Conversely, every positive operator $\rho$ on $\mathcal{H}_a$ with $\text{tr} \rho = 1$ arises as a reduced density matrix. To see this, we use that $\rho$ must have an orthonormal basis $\{\phi^n_a\}$ of eigenvectors with eigenvalues $p_n \in [0, \infty)$ such that $\sum p_n = 1$. Let $\{\phi^n_b\}$ be an arbitrary orthonormal basis of $\mathcal{H}_b$ and set

$$\psi = \sum_n \sqrt{p_n} \phi^n_a \otimes \phi^n_b .$$

Then

$$\rho_\psi = \text{tr}_b |\psi\rangle \langle \psi|$$

$$= \sum_{n,n',m} \langle \phi^b_m | \phi^n_a \otimes \phi^n_b \rangle \sqrt{p_n p_{n'}} \langle \phi^a_{n'} \otimes \phi^b_{n'} | \phi^b_m \rangle$$

$$= \sum_{n,n',m} \delta_{nm} |\phi^n_a \rangle \sqrt{p_n p_{n'}} \langle \phi^a_{n'} | \delta_{n'm}$$

$$= \sum_m |\phi^a_m \rangle p_m |\phi^a_m \rangle = \rho .$$

Statistical density matrices as in (11.3) and reduced density matrices can be combined: If $\Psi \in \mathcal{H}_a \otimes \mathcal{H}_b$ is random then set

$$\rho = \mathbb{E} \text{tr}_b |\Psi\rangle \langle \Psi| = \text{tr}_b \mathbb{E} |\Psi\rangle \langle \Psi| .$$

Statistical and reduced density matrices sometimes get confused; here is an example. Consider again the wave function of the measurement problem,

$$\Psi = \sum_\alpha \Psi_\alpha ,$$

the wave function of an object and an apparatus after a “quantum measurement” of the “observable” $A = \sum \alpha P_\alpha$. (In (11.43), $\Psi$ is capitalized not because it is random—it isn’t—but because it is the wave function of the “big” system including the apparatus.) Suppose that $\Psi_\alpha$, the contribution corresponding to the outcome $\alpha$, is of the form

$$\Psi_\alpha = c_\alpha \psi_\alpha \otimes \phi_\alpha ,$$

where $c_\alpha = \| P_\alpha \psi \|$, $\psi$ is the initial object wave function $\psi$, $\psi_\alpha = P_\alpha \psi / \| P_\alpha \psi \|$, and $\phi_\alpha$ with $\| \phi_\alpha \| = 1$ is a wave function of the apparatus after having “measured” $\alpha$. Since the $\phi_\alpha$ have disjoint supports in configuration space, they are mutually orthogonal; thus, they are a subset of some orthonormal basis $\{\phi_n\}$. The reduced density matrix of the object is

$$\rho_\Psi = \text{tr}_b |\Psi\rangle \langle \Psi| = \sum_n \langle \phi_n |\Psi\rangle \langle \Psi| \phi_n \rangle = \sum_\alpha |c_\alpha|^2 |\psi_\alpha\rangle \langle \psi_\alpha| .$$
This is the same density matrix as the statistical density matrix associated with the probability distribution

\[ \mu = \sum_{\alpha} |c_{\alpha}|^2 \delta_{\psi_\alpha}, \]  

(11.46)

since

\[ \rho_{\mu} = \sum_{\alpha} |c_{\alpha}|^2 |\psi_\alpha\rangle \langle \psi_\alpha|. \]  

(11.47)

It is sometimes claimed that this fact solves the measurement problem. The argument is: From (11.43) follows (11.45), which is the same as (11.47), which means that the system’s wave function has distribution (11.46), so we have a random outcome \( \alpha \). This argument is incorrect, as the mere fact that two situations—one with \( \Psi \) as in (11.43), the other with random \( \psi' \)—define the same density matrix for the object does not mean the two situations are physically equivalent. And obviously from (11.43), the situation after a quantum measurement involves neither a random outcome nor a random wave function. As John Bell once put it, “and is not or.”

It is often taken as the definition of decoherence that the reduced density matrix is (approximately) diagonal in the eigenbasis of the relevant operator \( A \).

It is common to call a density matrix that is a 1-dimensional projection a pure state and otherwise a mixed state, even if it is a reduced density matrix and thus does not arise from a mixture (i.e., from a probability distribution \( \mu \)).

PROPOSITION 11.10. A reduced density matrix \( \rho_\psi \) is pure if and only if \( \psi \) is a tensor product, i.e., there are \( \chi^a \in \mathcal{H}_a \) and \( \chi^b \in \mathcal{H}_b \) such that \( \psi = \chi^a \otimes \chi^b \).

Proof. The “if” part is clear; to prove the “only if” part, suppose that \( \rho_\psi = |\phi\rangle \langle \phi| \), set \( \phi^a = \chi \), choose an orthonormal basis \( \{\phi^a_n\} \) of \( \mathcal{H}_a \) such that \( \phi^a_1 = \chi \), choose an orthonormal basis \( \{\phi^b_n\} \) of \( \mathcal{H}_b \), and expand \( \psi \) in the product basis:

\[ \psi = \sum_{n,m} c_{nm} \phi^a_n \otimes \phi^b_m. \]  

(11.48)

Then

\[ \rho_\psi = \sum_{n,n'} \left( \sum_m c_{nm} c^*_m \right) \phi^a_n \langle \phi^a_{n'} \rangle, \]  

(11.49)

and since we know \( \rho_\psi = |\phi^a_1\rangle \langle \phi^a_1| \), we can read off that

\[ \sum_m c_{nm} c^*_m = \delta_{n1} \delta_{n'1}. \]  

(11.50)

By considering \( n = n' \neq 1 \) we obtain that \( c_{nm} = 0 \) for all \( m \) and all \( n \neq 1 \). Thus,

\[ \psi = \phi^a_1 \otimes \sum_m c_{1m} \phi^b_m, \]  

(11.51)

which is what we wanted to show.

\[ \square \]