22.2 The Density Matrix

We will now see how the information that defines a general ensemble can be used to construct an interesting operator ρ acting on the Hilbert space V of the theory. The operator $\rho \in \mathcal{L}(V)$ is called a density matrix. Our work begins with the general ensemble of equation (22.1.3):

$$E = \Big\{ (p_1, |\psi_1\rangle), \ \ldots, \ (p_n, |\psi_n\rangle) \Big\}, \quad p_1, \ldots, p_n > 0, \quad p_1 + \cdots + p_n = 1. \tag{22.2.1}$$

We recall that for this ensemble the expectation value of any observable $\hat{Q}$ is given by

$$\langle \hat{Q} \rangle_E = \sum_{a=1}^{n} p_a \langle \psi_a | \hat{Q} | \psi_a \rangle. \tag{22.2.2}$$

We now use the trace identity $\mathrm{tr}(.|u\rangle\langle w|). = \langle w|u\rangle$, derived in (14.9.27), to rewrite the above expectation value in terms of the trace of $\hat{Q}|\psi_a\rangle\langle\psi_a|$:

$$\langle \hat{Q} \rangle_E = \sum_{a=1}^{n} p_a \mathrm{tr}(\hat{Q}|\psi_a\rangle\langle\psi_a|). \tag{22.2.3}$$

For any constant p and any matrix A, we have $p\,\mathrm{tr}A = \mathrm{tr}(pA)$, and therefore

$$\langle \hat{Q} \rangle_E = \sum_{a=1}^{n} \mathrm{tr}(\hat{Q}\, p_a |\psi_a\rangle\langle\psi_a|) = \mathrm{tr}\left(\hat{Q} \sum_{a=1}^{n} p_a |\psi_a\rangle\langle\psi_a|\right), \tag{22.2.4}$$

where we also recalled the linearity property $\sum_i \mathrm{tr}(A_i) = \mathrm{tr}(\sum_i A_i)$. This result shows that *all* the relevant information about the ensemble E is encoded in the operator inside the trace, to the right of $\hat{Q}$. This operator will be called the density matrix operator $\rho_E \in \mathcal{L}(V)$ associated to the ensemble or mixed state E:

$$\boxed{\text{Density matrix for } E: \quad \rho_E \equiv \sum_{a=1}^{n} p_a |\psi_a\rangle\langle\psi_a|.} \tag{22.2.5}$$

Indeed, all the information about E is encoded in ρ_E because all we compute are expectation values of observables, and for them we now find that

$$\boxed{\langle \hat{Q} \rangle_E = \mathrm{tr}(\hat{Q}\rho_E).} \tag{22.2.6}$$

The expectation value of $\hat{Q}$ is obtained by multiplying $\hat{Q}$ by ρ_E and taking the trace.

The density matrix makes immediately clear some of the results we discussed before. For the E_z and E_x ensembles introduced in (22.1.2) and (22.1.7),

$$\rho_{E_z} = \tfrac{1}{2}|+\rangle\langle+| + \tfrac{1}{2}|-\rangle\langle-| = \tfrac{1}{2}\mathbb{1},$$
$$\rho_{E_x} = \tfrac{1}{2}|x;+\rangle\langle x;+| + \tfrac{1}{2}|x;-\rangle\langle x;-| = \tfrac{1}{2}\mathbb{1}, \tag{22.2.7}$$

where we simply used two different resolutions of the identity $\mathbb{1}$, one for the $|\pm\rangle$ basis states (*first line*) and one for the $|x; \pm\rangle$ basis states (*second line*). The two density matrices are identical, explaining why all observables in the two ensembles are the same. Recall that these ensembles represented unpolarized beams, which are, arguably, maximally random beams. We now see that for such a random state the density matrix is a multiple of the identity matrix. While a detailed computation would confirm it, the density matrix for the unpolarized ensemble E_{unp} is also $\mathbb{1}/2$. We know this is true because we showed that the expectation values in this ensemble are the same as in the E_z ensemble.

Remarks:

1. The density matrix is a Hermitian operator.

This is manifest because the p_i are real, and $(|\chi\rangle\langle\eta|)^\dagger = |\eta\rangle\langle\chi|$, implying that $(|\psi\rangle\langle\psi|)^\dagger = |\psi\rangle\langle\psi|$. It follows that ρ can always be diagonalized and has real eigenvalues.

2. The density matrix is a positive semidefinite operator. All its eigenvalues are nonnegative.

In a complex vector space with inner product $\langle\cdot, \cdot\rangle$, an operator M is said to be positive semidefinite if for any vector v we have $\langle v, Mv\rangle \geq 0$. Using bra-ket notation, the condition that the density matrix ρ be positive semidefinite is

$$\langle\psi|\rho|\psi\rangle \geq 0 \quad \text{for all } |\psi\rangle. \tag{22.2.8}$$

Using the expression for ρ, we have

$$\langle\psi|\rho|\psi\rangle = \sum_{a=1}^{n} p_a\langle\psi|\psi_a\rangle\langle\psi_a|\psi\rangle = \sum_{a=1}^{n} p_a|\langle\psi_a|\psi\rangle|^2 \geq 0, \tag{22.2.9}$$

since we are adding the products of nonnegative numbers. It now follows that the eigenvalues of ρ cannot be negative. Indeed, a matrix M with a negative eigenvalue cannot be positive semidefinite because $\langle v, Mv\rangle < 0$ when v is the corresponding eigenvector.

3. The trace of ρ is equal to one:

$$\text{tr}\,\rho = 1. \tag{22.2.10}$$

This property also follows from direct computation:

$$\text{tr}\,\rho = \text{tr}\left(\sum_{a=1}^{n} p_a |\psi_a\rangle\langle\psi_a|\right) = \sum_{a=1}^{n} p_a \text{tr}(|\psi_a\rangle\langle\psi_a|), \tag{22.2.11}$$

by linearity of the trace. It then follows that

$$\text{tr}\,\rho = \sum_{a=1}^{n} p_a \langle\psi_a|\psi_a\rangle = \sum_{a=1}^{n} p_a = 1. \tag{22.2.12}$$

4. The density matrix removes redundancies from the ensemble description of mixed states.

We have seen that different ensembles E and E' sometimes give the same density matrices: $\rho_E = \rho'_E$. Since ρ is a Hermitian operator, we can use an orthonormal basis of V to write it as

$$\rho = \sum_{i,j=1}^{N} \rho_{ij} |i\rangle\langle j|, \tag{22.2.13}$$

where the ρ_{ij} are the entries of a Hermitian $N \times N$ matrix, with N the dimension of the vector space V of the theory. Such a matrix is specified by N^2 real numbers. Since the trace of this matrix is one, ρ is specified by $N^2 - 1$ real numbers if there are no additional constraints (in fact there are none!). On the other hand, ensembles can require arbitrarily large amounts of data, especially when the number of entries $(p_a, |\psi_a\rangle)$ is large. Thus, the density matrix removes redundant data in the ensemble description of the mixed state.

5. The phases in the states $|\psi_a\rangle$ of the ensemble are irrelevant to the density matrix.

Since the states $|\psi_a\rangle$ entering the description of the ensemble are normalized, they are only ambiguous up to a phase. That phase cancels out in the density matrix, so they have no physical import. Indeed, if $\rho_E = \rho'_E$, we have

$$|\psi'_a\rangle\langle\psi'_a| = e^{i\theta_a}|\psi_a\rangle\,\langle\psi_a|e^{-i\theta_a} = |\psi_a\rangle\langle\psi_a|. \tag{22.2.14}$$

6. With a little abuse of terminology, physicists sometimes speak of the density matrix as the "state" or the "state operator" of the quantum system. The density matrix can describe pure states and mixed states.

Exercise 22.2. *Show that an operator M that is positive semidefinite must be Hermitian.*

If the system is described by a pure state $|\psi\rangle$, the ensemble collapses to one entry, $E = \{(1, |\psi\rangle)\}$, and the associated density matrix is the

$$\text{pure state:} \quad \rho = |\psi\rangle\langle\psi|. \tag{22.2.15}$$

In this case ρ is in fact a *rank-one orthogonal projector* to the subspace of V generated by $|\psi\rangle$. It is an orthogonal projector because ρ is Hermitian and satisfies

$$\rho^2 = |\psi\rangle\langle\psi|\psi\rangle\langle\psi| = |\psi\rangle\langle\psi| = \rho. \tag{22.2.16}$$

It is rank one because it has unit trace or, equivalently, because it projects to a one-dimensional subspace of V. Note that given the density matrix ρ of a pure state we can easily recover the state $|\psi\rangle$: we simply let ρ act on any vector in V that is not in the kernel of ρ, the result being a vector along $|\psi\rangle$. Because of the projector property and the trace property of ρ, we see that

$$\text{tr}\,\rho^2 = \text{tr}\rho = 1, \quad \text{for a pure state.} \tag{22.2.17}$$

Interestingly, the value of trρ^2 allows us to decide if we have a pure state or a mixed state:

Theorem 22.2.1. *tr $\rho^2 \leq 1$, with the inequality saturated only for pure states.*

Proof. We begin by computing the object of interest, the trace of ρ^2:

$$\text{tr}\rho^2 = \text{tr}\left(\sum_{a=1}^{n} p_a|\psi_a\rangle\langle\psi_a|\sum_{b=1}^{n} p_b|\psi_b\rangle\langle\psi_b|\right) = \text{tr}\left(\sum_{a,b=1}^{n} p_a p_b|\psi_a\rangle\langle\psi_a|\psi_b\rangle\langle\psi_b|\right)$$

$$= \sum_{a,b=1}^{n} p_a p_b \langle\psi_a|\psi_b\rangle \text{tr}|\psi_a\rangle\langle\psi_b| = \sum_{a,b=1}^{n} p_a p_b |\langle\psi_a|\psi_b\rangle|^2. \tag{22.2.18}$$

Adding and subtracting "one" we have

$$\text{tr}\rho^2 = \sum_{a,b=1}^{n} p_a p_b \left(1 - \left(1 - |\langle \psi_a | \psi_b \rangle|^2\right)\right) = \sum_{a,b=1}^{n} p_a p_b - \sum_{a,b=1}^{n} p_a p_b \left(1 - |\langle \psi_a | \psi_b \rangle|^2\right). \quad (22.2.19)$$

The first term on the right-hand side is $\sum_{a,b=1}^{n} p_a p_b = \sum_{a=1}^{n} p_a \sum_{b=1}^{n} p_b = 1 \cdot 1 = 1$. Therefore,

$$\text{tr}\rho^2 = 1 - \sum_{a \neq b} p_a p_b \left(1 - |\langle \psi_a | \psi_b \rangle|^2\right). \quad (22.2.20)$$

The sum over unrestricted $a,\ b$ running from 1 to n was changed to include only $a \neq b$ terms since the terms with $a = b$ vanish. The Schwarz inequality tells us that the expression in parentheses is always nonnegative because

$$|\langle \psi_a | \psi_b \rangle|^2 \leq \langle \psi_a | \psi_a \rangle \cdot \langle \psi_b | \psi_b \rangle = 1. \quad (22.2.21)$$

Since, additionally, all $p_a > 0$, equation (22.2.20) implies that

$$\text{tr}\,\rho^2 \leq 1. \quad (22.2.22)$$

This inequality is saturated only if $|\langle \psi_a | \psi_b \rangle|^2 = 1$ for all $a \neq b$ in the ensemble. This saturation of Schwarz's inequality requires $|\psi_a\rangle$ to be parallel to $|\psi_b\rangle$ for all $a \neq b$. Given that the states are normalized, it means *all* the states in the ensemble are the same up to phases. Since phases are immaterial to the density matrix, the ensemble involves only one state, and it describes a pure state. This is what we wanted to prove.

$\square$

In summary, the various traces of the density matrix satisfy

$$\boxed{\text{tr}\rho^2 \leq \text{tr}\,\rho = 1.} \quad (22.2.23)$$

The value of $\text{tr}\rho^2$ can be used to characterize quantum states. We define the **purity** $\zeta(\rho)$ of a density matrix ρ using this value:

$$\zeta(\rho) \equiv \text{tr}\,\rho^2. \quad (22.2.24)$$

When $\zeta = 1$, the state is pure. As the value of the purity ζ goes below one, the state becomes mixed. We declare that the lower the value of ζ, the less pure or more mixed the state. Thus, a *maximally mixed* state is a state with the lowest possible value of ζ. We will now show that for a maximally

mixed state the density matrix is actually a multiple of the identity matrix. This fixes the density matrix, as the trace must be equal to one. The unpolarized spin density matrix discussed in (22.2.7) is in fact maximally mixed.

Since the density matrix is diagonalizable, we can search for the lowest-purity one by restricting ourselves to diagonal matrices. Writing $N = \dim V$, we write

$$\rho = \text{diag} (p_1, \ldots, p_N) \quad \Rightarrow \quad \text{tr}\rho^2 = \sum_{i=1}^{N} p_i^2. \tag{22.2.25}$$

The p_i can be viewed as probabilities in an ensemble $E = \{(p_1, |e_1\rangle), \ldots, (p_N, |e_N\rangle)\}$ for which $\rho = p_1|e_1\rangle\langle e_1| + \cdots + p_N|e_N\rangle\langle e_N|$, with $|e_i\rangle$ orthonormal basis vectors that make ρ diagonal. We want to minimize the sum of squares of probabilities, subject to the trace condition $\sum_{i=1}^{N} p_i = 1$ and the positivity condition $p_i \geq 0$, for all i. The trace condition can be implemented with a Lagrange multiplier λ. We need not worry about the positivity condition because, as it will turn out, the only critical point we find has nonnegative p_i's. We must therefore find the stationary point of the following function L of the p_i's and λ:

$$L(p_1, \ldots, p_N; \lambda) = \sum_{i=1}^{N} p_i^2 - \lambda\left(-1 + \sum_{i=1}^{N} p_i\right). \tag{22.2.26}$$

The stationarity conditions are

$$0 = \frac{\partial L}{\partial p_i} = 2p_i - \lambda, \quad i = 1, \ldots, N, \qquad 0 = \frac{\partial L}{\partial \lambda} = 1 - \sum_{i=1}^{N} p_i. \tag{22.2.27}$$

The first condition sets $p_i = \lambda/2$ for all i, setting all probabilities equal. The second condition fixes λ as it sets the sum of the N probabilities equal to one: $N\lambda/2 = 1$. All in all,

$$p_i = \tfrac{\lambda}{2}, \quad N\tfrac{\lambda}{2} = 1 \quad \Rightarrow \quad p_i = \tfrac{1}{N}, \text{ for all } i. \tag{22.2.28}$$

As claimed, the lowest-purity density matrix, which we call $\bar{\rho}$, is a multiple of the identity matrix:

$$\text{Maximally mixed state:} \qquad \bar{\rho} = \frac{1}{N} \mathbb{1}. \tag{22.2.29}$$

Here $\mathbb{1}$ is the $N \times N$ identity matrix, with N the dimensionality of the state space. It follows also that the purity of the maximally mixed state is $1/N$:

$$\zeta(\bar{\rho}) = \operatorname{tr}\bar{\rho}^2 = \frac{1}{N^2}\operatorname{tr}\mathbb{1} = \frac{1}{N}. \tag{22.2.30}$$

This is the minimum possible value of the purity. The concept of purity is natural because the purity of a system is conserved under unitary time evolution, as we will see in section 22.3.

Exercise 22.3. *Examine the following two density matrices and determine if the states are pure or mixed. If pure, write the density matrix in the form $|\psi\rangle\langle\psi|$ that makes this manifest.*

$$\rho_1 = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}, \quad \rho_2 = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix}. \tag{22.2.31}$$

Example 22.3. *Density matrix for spin one-half pure states.*
Here the density matrix is very simple: $|\mathbf{n}\rangle\langle{-}n$ for a pure state $|\mathbf{n}\rangle$ pointing along the direction of the unit vector $\mathbf{n}$. Since the density matrix is a Hermitian operator and the set of 2×2 Hermitian matrices is spanned by the identity and the Pauli matrices, we should be able to write

$$|\mathbf{n}\rangle\langle\mathbf{n}| = \tfrac{1}{2}a_0\,\mathbb{1} + \tfrac{1}{2}\sum_{i=1}^{3}a_i\sigma_i, \tag{22.2.32}$$

where the factors of $\frac{1}{2}$ have been included for convenience, and a_0 as well as a_1, a_2, a_3 are real constants. But we have solved this problem before! We did so when constructing the projector $P_{\mathbf{n}} = |\mathbf{n}\rangle\langle\mathbf{n}|$ to the spin state $|\mathbf{n}\rangle$. The answer was given in (14.9.33), which we copy here:

$$\boxed{|\mathbf{n}\rangle\langle\mathbf{n}| = \tfrac{1}{2}(\mathbb{1} + \mathbf{n}\cdot\boldsymbol{\sigma}).} \tag{22.2.33}$$

We will discuss the density matrix for mixed spin one-half states below.

$\square$

We have shown that starting from an ensemble, the associated density matrix is a positive semidefinite matrix with unit trace (the condition of Hermiticity follows from positivity, as you showed in exercise 22.2).

There are no extra conditions on the density matrix. Indeed, we claim the following:

Theorem 22.2.2. *To any unit trace, positive semidefinite matrix M $\in \mathcal{L}(V)$, we can associate an ensemble for which M is the density matrix.*

Proof. The matrix M, being Hermitian and positive semidefinite, can be diagonalized and will have nonnegative eigenvalues $\lambda_i \geq 0$ with $i = 1, \ldots, N$, with $N = \dim V$. Let us call $|e_i\rangle$ the eigenvector associated with λ_i. We then have

$$M = \sum_{i=1}^{N} \lambda_i |e_i\rangle\langle e_i|, \qquad \sum_{i=1}^{N} \lambda_i = 1. \tag{22.2.34}$$

The second equality arises from the unit trace condition on M. Now consider the ensemble E_M defined by

$$E_M \equiv \{(\lambda_1, |e_1\rangle), \ldots, (\lambda_N, |e_N\rangle)\}, \tag{22.2.35}$$

which is consistent because the λ_i are all nonnegative and add up to one. Note that in this ensemble we allow the value zero for some of the λ_i's; this, of course, means the corresponding terms do not contribute to the density matrix. The density matrix ρ_{E_M} associated with the ensemble E_M is constructed as usual:

$$\rho_{E_M} = \sum_{i=1}^{N} \lambda_i |e_i\rangle\langle e_i| = M, \tag{22.2.36}$$

using (22.2.34) and confirming the claim of the theorem.

$\square$

Example 22.4. *Density matrix for general spin one-half states.*
We again begin by writing the density matrix ρ as a general 2×2 Hermitian matrix:

$$\rho = \tfrac{1}{2} a_0 \mathbb{1} + \tfrac{1}{2} \mathbf{a} \cdot \boldsymbol{\sigma}, \quad a_0, a_1, a_2, a_3 \in \mathbb{R}. \tag{22.2.37}$$

As before, $\operatorname{tr} \rho = 1$ fixes $a_0 = 1$. On account of the above theorem, the only remaining condition on ρ is that of positivity: none of its eigenvalues can

be negative. The eigenvalues of $\mathbf{a} \cdot \boldsymbol{\sigma}$ are $\pm |\mathbf{a}|$, and therefore the eigenvalues of ρ are

$$\tfrac{1}{2}(1 \pm |\mathbf{a}|) \geq 0. \tag{22.2.38}$$

Positivity requires $1 - |\mathbf{a}| \geq 0$ or, equivalently, $|\mathbf{a}| \leq 1$. All in all, the density matrix for a general mixed or pure state is as follows:

$$\boxed{\text{Spin one-half density matrix:} \quad \rho = \tfrac{1}{2}(\mathbb{1} + \mathbf{a} \cdot \boldsymbol{\sigma}), \quad |\mathbf{a}| \leq 1.} \tag{22.2.39}$$

The set of allowed pure and mixed states above is called the *Bloch ball*, a unit ball in the euclidean three-dimensional space $\{a_1, a_2, a_3\}$. When $\mathbf{a}$ is a unit vector, ρ is of the type (22.2.33) and represents a pure state. Thus, the boundary $|\mathbf{a}| = 1$ of the Bloch ball is a two-sphere's worth of pure states. The interior of the Bloch ball represents mixed states. The center $\mathbf{a} = 0$ of the Bloch ball represents the unpolarized state; it is the maximally mixed state.

$\square$

Measurement along an orthonormal basis Recall that we can measure a pure state $|\psi\rangle$ along an orthonormal basis $|1\rangle$, ..., $|N\rangle$ of a dimension N vector space V, and the probability $p(i)$ of being in the state $|i\rangle$ is $|\langle i|\psi\rangle|^2$ (see (16.6.9)). After measurement, the state will be in one of the states $|i\rangle$.

This is readily extended to cases in which the measurement is conducted on a mixed-state ensemble (22.1.3). This time the probability $p(i)$ of finding $|i\rangle$ is obtained by weighting, with probability p_a, the probability $|\langle i|\psi_a\rangle|^2$ of finding the state $|\psi_a\rangle$ in $|i\rangle$:

$$p(i) = \sum_{a=1}^{n} p_a |\langle i|\psi_a\rangle|^2 = \sum_{a=1}^{n} p_a \langle i|\psi_a\rangle \langle \psi_a|i\rangle = \langle i| \sum_{a=1}^{n} p_a |\psi_a\rangle \langle \psi_a|i\rangle. \tag{22.2.40}$$

From this we get the simple expression

$$p(i) = \langle i|\rho|i\rangle. \tag{22.2.41}$$

As it should, this probability depends only on ρ and not on the ensemble that defines ρ. After this measurement the system will be in one of the

basis states. If we obtain $|i\rangle$, the density matrix ρ becomes $|i\rangle\langle i|$. This state is in fact the orthogonal projector $M_i \equiv |i\rangle\langle i|$ where

$$M_i^\dagger = M_i, \quad M_i M_i = M_i, \quad \sum_i M_i = \mathbb{1}. \tag{22.2.42}$$

The collection $\{M_i\}$ forms a complete set of orthogonal projectors.

Assume that a measurement along the basis has been performed, but the result is not available to us. What becomes of the density matrix? We know that after measurement we have, for each i, the probability $p(i)$ for the system to be in the state $|i\rangle$. The new ensemble $\tilde{E}$ is therefore

$$\tilde{E} = \left\{ (p(1), |1\rangle), \ldots, (p(N), |N\rangle) \right\}. \tag{22.2.43}$$

The new, after-measurement density matrix $\tilde{\rho}$ is now easily constructed:

$$\tilde{\rho} = \sum_i p(i)|i\rangle\langle i| = \sum_i |i\rangle \langle i|\rho|i\rangle \langle i|, \tag{22.2.44}$$

where we used our result for $p(i)$. This can now be rewritten in a suggestive way:

$$\boxed{\tilde{\rho} = \sum_i M_i \rho M_i.} \tag{22.2.45}$$

This passage from ρ to $\tilde{\rho}$ gives us the effect of measurement along a basis on a quantum system when the result is not available. We quickly check that, as required, the trace of the new density matrix remains equal to one:

$$\mathrm{tr}\,\tilde{\rho} = \sum_i \mathrm{tr}(M_i\,\rho\,M_i) = \sum_i \mathrm{tr}(\rho\,M_i M_i) = \sum_i \mathrm{tr}(\rho\,M_i) = \mathrm{tr}\,(\rho\sum_i M_i) = \mathrm{tr}\rho = 1. \tag{22.2.46}$$

In the various steps, we used the cyclicity of the trace as well as the second and third properties in (22.2.42).