# The Density Matrix

## Review

In Quantum Mechanics, a system is completely determined once its state at an initial time is known. The Schrödinger equation describes its *deterministic* evolution. In other words, knowledge of the state represents all the information that can be obtained about the system.

We briefly summarize some quantum mechanical concepts that will be useful in what follows:

1. The state dynamics is governed by the Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}\left|\psi\right\rangle = \hat{H}\left|\psi\right\rangle. \tag{1}$$

2. Given the initial state $|\psi(0)\rangle$, its time-evolved state is obtained by applying a unitary operator (*evolution operator*):

$$\left|\psi(t)\right\rangle = \hat{U}(t)\left|\psi(0)\right\rangle, \tag{2}$$

which is derived from (1). In particular, for a time-independent Hamiltonian $\hat{H}$:

$$\hat{U}(t) = e^{-i\frac{\hat{H}}{\hbar}t}. \tag{3}$$

3. States are assumed to be normalized to 1:

$$\left\langle\psi(t)|\psi(t)\right\rangle = 1. \tag{4}$$

Time evolution, as well as the application of any unitary transformation, preserves the norm:

$$\left\langle\psi(t)|\psi(t)\right\rangle = \left\langle\psi(0)\right|\underbrace{\hat{U}^{\dagger}(t)\hat{U}(t)}_{\mathbf{1}}\left|\psi(0)\right\rangle = \left\langle\psi(0)|\psi(0)\right\rangle = 1. \tag{5}$$

4. An observable $\hat{A}$ is a Hermitian operator ($\hat{A}^{\dagger} = \hat{A}$) acting on the Hilbert space of the system state. The eigenvalues $\{a_j\}$ of $\hat{A}$ represent the possible outcomes of a measurement. Note that these outcomes may not be known deterministically even when the state itself is fully known[1].

5. A *projector* is an operator acting on a vector in an $N$-dimensional Hilbert space $\mathcal{H}$, projecting it onto its component in an $M$-dimensional subspace $\bar{\mathcal{H}} \subset \mathcal{H}$. Let $\{|1\rangle, |2\rangle, \ldots, |N\rangle\}$ be an orthonormal basis of $\mathcal{H}$ and let $\bar{\mathcal{H}}$ be the subspace spanned by the vectors $\{|1\rangle, |2\rangle, \ldots, |M\rangle\}$; the projector onto this subspace is:

$$\hat{P} = \sum_{j=1}^{M}\left|j\right\rangle\left\langle j\right|. \tag{6}$$

[1] The *probabilistic* nature of quantum mechanics emerges only through the measurement process, not in terms of the quantum state and its deterministic evolution.

6. The eigenstates of an observable $\hat{A}$ form an orthonormal basis $\{|a_j\rangle\}$:

$$\hat{A}\,|a_j\rangle = a_j\,|a_j\rangle\,, \tag{7}$$

and the state of the system can be expanded in this basis as:

$$|\psi\rangle = \sum_j b_j\,|a_j\rangle\,, \tag{8}$$

with $b_j = \langle a_j|\psi\rangle$. The probability of obtaining the eigenvalue $a_j$ upon measuring $\hat{A}$ is $p_j = |b_j|^2$. Following the measurement, the state $|\psi\rangle$ is projected onto its component $|a_j\rangle$.

7. The expectation value of $\hat{A}$ is the average value of the outcomes obtained over a large number of measurements:

$$\left\langle \hat{A} \right\rangle = \sum_j a_j p_j = \langle\psi|\hat{A}|\psi\rangle\,. \tag{9}$$

# Density Matrix for a Pure State

It is possible to associate with the state of a quantum system the corresponding projector:

$$|\psi\rangle \to \hat{\rho} = |\psi\rangle\langle\psi|, \tag{10}$$

where $\hat{\rho}$ is called the *density matrix* of the pure state $|\psi\rangle$. Describing the system via $|\psi\rangle$ or $\hat{\rho}$ is entirely equivalent in this case; however, the latter formalism is more convenient in certain situations, such as in describing measurement processes. Given an observable $\hat{A}$ and its eigenstates $\{|a_j\rangle\}$, we can define the projectors onto these states as:

$$\hat{M}_j = |a_j\rangle\langle a_j|, \tag{11}$$

so the probability that measuring $\hat{A}$ on state $|\psi\rangle$ yields state $|a_j\rangle$ is given by:

$$p_j = \mathrm{tr}\left\{\hat{M}_j\hat{\rho}\right\}. \tag{12}$$

*Proof.*

$$\mathrm{tr}\left\{\hat{M}_j\hat{\rho}\right\} = \sum_k \langle a_k|\hat{M}_j\hat{\rho}|a_k\rangle = \sum_k \langle a_k|a_j\rangle\,\langle a_j|\psi\rangle\,\langle\psi|a_k\rangle = \langle a_j|\psi\rangle\,\langle\psi|a_j\rangle = p_j.$$

□

Similarly, we can express the quantum expectation value of $\hat{A}$ as:

$$\left\langle \hat{A} \right\rangle = \mathrm{tr}\left\{\hat{A}\hat{\rho}\right\}. \tag{13}$$

*Proof.*

$$\mathrm{tr}\left\{\hat{A}\hat{\rho}\right\} = \sum_k \langle\psi_k|\hat{A}|\psi\rangle\,\langle\psi|\psi_k\rangle\,,$$

where $\{|\psi_k\rangle\}$ is a basis chosen such that $|\psi_1\rangle = |\psi\rangle$, so that:

$$\mathrm{tr}\left\{\hat{A}\hat{\rho}\right\} = \langle\psi_1|\hat{A}|\psi\rangle\,\langle\psi|\psi_1\rangle = \langle\psi|\hat{A}|\psi\rangle\,.$$

□

# Density Matrix for Ensembles of Pure States

The state of a system is generally not known perfectly; for this reason, a statistical description must be introduced. The system is no longer described by a pure state, but by an ensemble of states (not necessarily orthogonal), each assigned a certain probability:

$$\left.\begin{array}{lcl} |\psi_1\rangle & \to & p_1 \\ |\psi_2\rangle & \to & p_2 \\ \vdots & & \end{array}\right\} \sum_j p_j = 1, \tag{14}$$

we denote this set by $\{|\psi_j\rangle, p_j\}$. In this case, we speak not of a pure state, but of a *mixed state* (or *statistical mixture*). It should be noted that for such states, classical ignorance about the system exists alongside quantum indefiniteness. Comparing with the pure state case:

**Pure state** :

- Perfectly known state (maximum knowledge of the system)
- Quantum uncertainty in measurement

**Mixed state** :

- State not fully known (an ensemble of states is introduced)
- Classical and quantum uncertainty in measurement

Expectation values of operators are now averages over both quantum states and the ensemble:

$$\left\langle \hat{A} \right\rangle = \sum_j p_j \langle\psi_j|\hat{A}|\psi_j\rangle, \tag{15}$$

that is, a statistical average must be performed over the quantum expectation values evaluated for each state in the ensemble.

A unified formalism can be adopted for quantum systems, whether in a pure state or a mixed state, by introducing the general definition of the density matrix. Given an ensemble $\{|\psi_j\rangle, p_j\}$, its density matrix is defined as:

$$\boxed{\hat{\rho} = \sum_j p_j |\psi_j\rangle \langle\psi_j|}. \tag{16}$$

Naturally, this definition coincides with (10) when all $p_j$ except one vanish (i.e., when the state becomes pure). It is easily verified that (15) is equivalent to writing:

$$\boxed{\left\langle \hat{A} \right\rangle = \mathrm{tr}\left\{\hat{\rho}\hat{A}\right\}}. \tag{17}$$

and similarly to (12):

$$p(a_k) = \mathrm{tr}\left\{\hat{\rho}\hat{M}_k\right\}. \tag{18}$$

The density matrix is therefore a more general concept than the state vector, enabling the description of both pure states and statistical ensembles within a single mathematical framework. The density matrix generalizes the classical concept of probability density:

$$\langle A \rangle = \int dx\, p(x) A(x). \tag{19}$$

From now on, following standard convention, we shall use the term *state* of a system to refer, depending on the context, to either its state vector or its density matrix.

**Exercise 0.0.1.** Consider a spin-1/2 system described by the usual Pauli matrices. In one scenario, let the state be:

$$|\psi\rangle = \frac{\sqrt{3}}{2}|0\rangle + \frac{1}{2}|1\rangle, \tag{20}$$

and in another scenario consider the ensemble $\left\{|0\rangle, p_0 = \frac{3}{4}; |1\rangle, p_1 = \frac{1}{4}\right\}$:

1. Write the density matrix in both cases.
2. Calculate $\langle\hat{\sigma}_z\rangle$ in both cases.
3. Calculate $\langle\hat{\sigma}_x\rangle$ in both cases.

# Properties of the Density Matrix

We list below the fundamental properties that any density matrix must satisfy:

1. Hermiticity:
$$\hat{\rho}^\dagger = \hat{\rho}. \tag{21}$$
2. Unit trace:
$$\mathrm{tr}\{\hat{\rho}\} = 1. \tag{22}$$

   *Proof.* Choose an orthonormal basis $\{|n\rangle\}$:

$$\begin{aligned}\mathrm{tr}\{\hat{\rho}\} &= \sum_n \langle n|\hat{\rho}|n\rangle = \\ &= \sum_{n,k} p_k \langle n|\psi_k\rangle\langle\psi_k|n\rangle = \sum_k p_k \langle\psi_k|\left[\sum_n |n\rangle\langle n|\right]|\psi_k\rangle = \\ &= \sum_k p_k \langle\psi_k|\psi_k\rangle = \sum_k p_k = 1.\end{aligned} \tag{23}$$

   □

3. $\hat{\rho}$ is *positive semi-definite*, meaning that for any state $|\chi\rangle$:
$$\langle\chi|\hat{\rho}|\chi\rangle \geq 0. \tag{24}$$

   This is equivalent to stating that all eigenvalues are non-negative and, due to condition (22), lie between 0 and 1.

   *Proof.*

$$\begin{aligned}\langle\chi|\hat{\rho}|\chi\rangle &= \sum_k p_k \langle\chi|\psi_k\rangle\langle\psi_k|\chi\rangle = \\ &= \sum_k p_k |\langle\chi|\psi_k\rangle|^2 \geq 0.\end{aligned} \tag{25}$$

   Furthermore, to show that the eigenvalues are bounded between 0 and 1, consider the unitary transformation $\hat{V}$ that diagonalizes $\hat{\rho}$. From the above inequality, we have:

$$\langle\chi|\hat{V}\hat{V}^\dagger\hat{\rho}\hat{V}\hat{V}^\dagger|\chi\rangle = \langle\chi|\hat{V}\hat{\rho}_D\hat{V}^\dagger|\chi\rangle = \langle\bar{\chi}|\hat{\rho}_D|\bar{\chi}\rangle \geq 0, \tag{26}$$

where $\hat{\rho}_D$ is the diagonal matrix:

$$\hat{\rho}_D = \sum_j \lambda_j \left|j\right\rangle \left\langle j\right|, \tag{27}$$

with eigenvalues $\lambda_j$ and eigenvectors $|j\rangle$:

$$\langle\bar{\chi}|\hat{\rho}_D|\bar{\chi}\rangle = \sum_j \lambda_j |\left\langle\bar{\chi}|j\right\rangle|^2 \geq 0 \; \forall \left|\bar{\chi}\right\rangle, \tag{28}$$

which implies $\lambda_j \geq 0$. Thus, since $\mathrm{tr}\left\{\hat{\rho}\right\} = \sum_j \lambda_j = 1$, it follows that $\lambda_j \leq 1$. □

The listed properties constitute *necessary and sufficient* conditions: every density matrix satisfies them, and any operator satisfying them can be interpreted as a density matrix.

## Purity

We define the quantity:

$$\boxed{P = \mathrm{tr}\left\{\hat{\rho}^2\right\}}$$

called *purity*. It satisfies the property:

$$0 < P \leq 1, \tag{29}$$

where $P = 1$ holds if and only if $\hat{\rho}$ represents a pure state.

*Proof.* Recalling that the trace is invariant under unitary transformations, we work in the basis where $\hat{\rho}$ is diagonal. In this basis, it is immediately clear that:

$$P = \sum_j \lambda_j^2, \tag{30}$$

where $\lambda_j$ are the eigenvalues of $\hat{\rho}$. As noted earlier, these eigenvalues are non-negative numbers less than or equal to 1, and their sum is 1. Thus:

$$\sum_j \lambda_j^2 \leq 1, \tag{31}$$

unless only one eigenvalue $\lambda$ is non-zero (and thus equal to 1), in which case the state is pure and $P = 1$. □

Furthermore, it is straightforward to see that $P$ is minimized when all eigenvalues of $\hat{\rho}$ are equal, $\lambda_j = 1/N$ (where $N$ is the dimension of the Hilbert space of the system), yielding $P = 1/N$. This case corresponds to the maximally mixed state, in which our knowledge of the system is minimal. We shall see later that maximally mixed states correspond to maximum entropy. We can thus state tighter bounds for $P$:

$$\boxed{\frac{1}{N} \leq P \leq 1}.$$

Purity provides a measure of the degree of purity of a state. The closer $P$ is to 1, the closer the state is to being pure (and thus the greater our knowledge of the state).

**Exercise 0.0.2.** Calculate the purity of the density matrix:

$$\hat{\rho} = \begin{pmatrix} a & b \\ b^* & 1-a \end{pmatrix} \tag{32}$$

## Time Evolution of the Density Matrix in a Closed System

Just as the density matrix is defined from projectors onto quantum state vectors, its time evolution directly derives from the evolution of these vectors:

$$\hat{\rho}(t) = \sum_k p_k \left|\psi_k(t)\right\rangle \left\langle\psi_k(t)\right| . \tag{33}$$

In the Schrödinger picture, time evolution gives:

$$\left|\psi_k(t)\right\rangle = \hat{U}(t) \left|\psi_k(0)\right\rangle , \tag{34}$$

$$i\hbar \frac{d}{dt}\hat{U}(t) \left|\psi_k(0)\right\rangle = \hat{H}\hat{U}(t) \left|\psi_k(0)\right\rangle , \tag{35}$$

from which follows the equation of motion for the time-evolution operator:

$$i\hbar \frac{d}{dt}\hat{U}(t) = \hat{H}\hat{U}(t). \tag{36}$$

Similarly, for the density matrix:

$$\hat{\rho}(t) = \hat{U}(t)\hat{\rho}(0)\hat{U}^\dagger(t), \tag{37}$$

$$\frac{d}{dt}\hat{\rho}(t) = \frac{d}{dt}\hat{U}(t)\hat{\rho}(0)\hat{U}^\dagger(t) + \hat{U}(t)\hat{\rho}(0)\frac{d}{dt}\hat{U}^\dagger(t) = -\frac{i}{\hbar}\left[\hat{H}, \hat{\rho}(t)\right] , \tag{38}$$

yielding the equation of motion[2]:

$$\boxed{\frac{d}{dt}\hat{\rho}\,(t) = -\frac{i}{\hbar}\left[\hat{H}, \hat{\rho}\right]}.$$

In particular, if the Hamiltonian is time-independent, the evolution is given by:

$$\hat{\rho}(t) = e^{-i\frac{\hat{H}}{\hbar}t}\hat{\rho}(0)e^{i\frac{\hat{H}}{\hbar}t}. \tag{40}$$

Note that the density matrix evolves with a time sign opposite to that of operators in the Heisenberg picture: unlike observables, it is time-dependent in the Schrödinger picture and time-independent in the Heisenberg picture. For example, expectation values of an operator in the two pictures are given by:

$$\left\langle \hat{A} \right\rangle = \mathrm{tr}\left\{\hat{\rho}_S(t)\hat{A}_S\right\} = \mathrm{tr}\left\{\hat{\rho}_H\hat{A}_H(t)\right\} , \tag{41}$$

with:

$$\hat{\rho}_S(t) = \hat{U}(t)\hat{\rho}\hat{U}^\dagger(t), \tag{42}$$

$$\hat{A}_H(t) = \hat{U}^\dagger(t)\hat{A}\hat{U}(t). \tag{43}$$

We have seen that quantum mechanics also features another type of evolution, contrasting with the deterministic dynamics of the Schrödinger equation: measurement. During measurement, the wave packet collapses into an eigenstate of the observable with a certain probability. In terms of the density matrix, this implies a transition from a pure state to a statistical mixture. Thus, given an observable $\hat{A}$ with eigenstates $\{|\psi_k\rangle\}$, the density matrix of a pure state prior to measurement is:

$$\hat{\rho}_{\mathrm{pre}} = \left|\psi\right\rangle \left\langle\psi\right| , \tag{44}$$

[2]This equation represents the quantum analogue of Liouville's theorem in classical mechanics:

$$\frac{d}{dt}\rho_{\mathrm{cl}}(t) = -\left\{H, \rho_{\mathrm{cl}}\right\}_{\mathrm{cl}} \tag{39}$$

where $\{\cdots\}_{\mathrm{cl}}$ denotes the Poisson bracket.

with:

$$|\psi\rangle = \sum_k b_k |\psi_k\rangle . \tag{45}$$

After measurement, it evolves into:

$$\hat{\rho}_{\text{post}} = \sum_k |b_k|^2 |\psi_k\rangle \langle\psi_k| . \tag{46}$$

**Exercise 0.0.3.** A beam of particles, all with spin $|\uparrow\rangle$, characterized by a density matrix $\hat{\rho}_0$, is sent into a Stern-Gerlach apparatus oriented along the $x$-axis. After the interaction, the density matrix changes to $\hat{\rho}_1$. Next, one of the two emerging beams (for example, the beam with spin $|+\rangle$) is sent into a second Stern-Gerlach apparatus, this time oriented along the $z$-axis, after which the density matrix becomes $\hat{\rho}_2$. Determine $\hat{\rho}_0$, $\hat{\rho}_1$, and $\hat{\rho}_2$.

## Non-Uniqueness of Ensemble Representations

It should be noted that the same density matrix can correspond to different state ensembles.

**Example 0.0.4.** Consider a two-level system with orthonormal basis $|\uparrow\rangle, |\downarrow\rangle$. Consider two state ensembles: $\{|\uparrow\rangle , p_\uparrow = 3/4; |\downarrow\rangle , p_\downarrow = 1/4\}$ and $\{|\alpha_+\rangle , p_+ = 1/2; |\alpha_-\rangle , p_- = 1/2\}$, where:

$$|\alpha_\pm\rangle = \sqrt{\frac{3}{4}} |\uparrow\rangle \pm \sqrt{\frac{1}{4}} |\downarrow\rangle . \tag{47}$$

Note that the states $|\alpha_\pm\rangle$ are not orthogonal. We construct the density matrices corresponding to both ensembles:

$$\begin{aligned} \hat{\rho}_1 &= \frac{3}{4} |\uparrow\rangle \langle\uparrow| + \frac{1}{4} |\downarrow\rangle \langle\downarrow| , \\ \hat{\rho}_2 &= \frac{1}{2} |\alpha_+\rangle \langle\alpha_+| + \frac{1}{2} |\alpha_-\rangle \langle\alpha_-| . \end{aligned}$$

With straightforward algebra, one easily verifies that $\hat{\rho}_1 = \hat{\rho}_2$; that is, two distinct ensembles yield the exact same density matrix.

Which classes of ensembles generate the same density matrix? Consider an ensemble of $N$ states $\{p_j, |\psi_j\rangle\}$ (where $N$ can be arbitrarily large and is not constrained by the dimension of the Hilbert space), corresponding to the density matrix:

$$\hat{\rho} = \sum_{j=1}^{N} p_j |\psi_j\rangle \langle\psi_j| , \tag{48}$$

What other ensembles correspond to the same $\hat{\rho}$? We use the following trick to index the ensemble states:

1. Switch from normalized states $|\psi_j\rangle$ to unnormalized states $|\tilde{\psi}_j\rangle$:

$$|\psi_j\rangle \to |\tilde{\psi}_j\rangle = \sqrt{p_j} |\psi_j\rangle \tag{49}$$

2. Extend the index $j$ up to infinity and define the states as:

$$|\tilde{\psi}_j\rangle = \begin{cases} \sqrt{p_j} |\psi_j\rangle & j \leq N \\ 0 & j > N \end{cases} \tag{50}$$