# Chapter 9

# Density Matrices

In this chapter we want to introduce density matrices, also called density operators, which conceptually take the role of the state vectors discussed so far, as they encode all the (accessible) information about a quantum mechanical system. It turns out that the "pure" states, described by state vectors[1] $|\psi\rangle$ on Hilbert space, are idealized descriptions that cannot characterize statistical (incoherent) mixtures, which often occur in the experiment, i.e. in Nature. These objects are very important for the theory of quantum information and quantum communication. More detailed information about the density matrix formalism can be found in [17].

## 9.1 General Properties of Density Matrices

Consider an observable $A$ in the "pure" state $|\psi\rangle$ with the expectation value given by

$$\langle A \rangle_\psi = \langle \psi | A | \psi \rangle \,, \tag{9.1}$$

then the following definition is obvious:

**Definition 9.1**      *The **density matrix** $\rho$ for the pure state $|\psi\rangle$*
*is given by*

$$\rho := |\psi\rangle\langle\psi|$$

This density matrix has the following properties:

$$\text{I)} \quad \rho^2 = \rho \quad \text{projector} \tag{9.2}$$

$$\text{II)} \quad \rho^\dagger = \rho \quad \text{hermiticity} \tag{9.3}$$

$$\text{III)} \quad \text{Tr}\,\rho = 1 \quad \text{normalization} \tag{9.4}$$

$$\text{IV)} \quad \rho \geq 0 \quad \text{positivity} \tag{9.5}$$

---

[1]Remark for experts: It is possible to find a vector representation for every given quantum mechanical state, even those represented by a density matrix. This can be done via the so-called GNS (Gelfand-Neumark-Segal) construction. This vector representation need not, however, be of any practical form and the concept of the density matrix is therefore inevitable.

The first two properties follow immediately from Definition 9.1 and property $\mathrm{III}$) can be verified using the definition of the trace operation for an arbitrary operator $D$:

**Definition 9.2**        *The **trace** of an operator $D$ is given by*

$$\mathrm{Tr}\,D \; := \; \sum_n \langle\,n\,|\,D\,|\,n\,\rangle$$

*where $\{\,|\,n\,\rangle\,\}$ is an arbitrary CONS.*

Lets e.g. take the operator $D = |\,\psi\,\rangle\langle\,\phi\,|$ and calculate its trace

$$\mathrm{Tr}\,D \; = \; \sum_n \langle\,n\,|\,\psi\,\rangle\langle\,\phi\,|\,n\,\rangle \; = \; \sum_n \langle\,\phi\,\underbrace{|\,n\,\rangle\langle\,n\,|}_{\mathbb{1}}\,\psi\,\rangle \; = \; \langle\,\phi\,|\,\psi\,\rangle\;. \tag{9.6}$$

Property $\mathrm{IV}$) means that the eigenvalues of $\rho$ are greater or equal to zero, which can also be expressed as

$$\langle\,\varphi\,|\,\rho\,|\,\varphi\,\rangle \; = \; \langle\,\varphi\,|\,\psi\,\rangle\langle\,\psi\,|\,\varphi\,\rangle \; = \; |\langle\,\varphi\,|\,\psi\,\rangle|^2 \geq 0\;, \tag{9.7}$$

which is an important property because probabilities are always greater or equal to zero. What we still have to ensure is that the expectation value of an observable in the state $|\,\psi\,\rangle$ can be reproduced, which we will formulate in the following theorem:

**Theorem 9.1**        *The expectation value of an observable $A$ in a state, represented by a density matrix $\rho$, is given by*

$$\langle\,A\,\rangle_\rho \; = \; \mathrm{Tr}\,(\rho\,A)$$

**Proof:**

$$\mathrm{Tr}\,(\rho\,A) \;\; = \;\; \mathrm{Tr}\,(|\,\psi\,\rangle\langle\,\psi\,|\,A) \; = \; \sum_n \langle\,n\,|\,\psi\,\rangle\langle\,\psi\,|\,A\,|\,n\,\rangle \; =$$

$$= \;\; \sum_n \langle\,\psi\,|\,A\,\underbrace{|\,n\,\rangle\,\langle\,n\,|}_{\mathbb{1}}\,\psi\,\rangle \; = \; \langle\,\psi\,|\,A\,|\,\psi\,\rangle \; = \; \langle\,A\,\rangle\;. \quad \text{q.e.d.} \tag{9.8}$$

## 9.2   Pure and Mixed States

Now we can introduce a broader class of states represented by density matrices, the so-called **mixed states** in contrast to the states we have considered until now, the so-called **pure states**.

### 9.2.1 Pure States

Let's begin with the pure states. Consider an ensemble of given objects in the states $\{\,|\psi_i\,\rangle\,\}$. If all the objects are in the same state, the ensemble is represented by a **pure state**. To make probabilistic statements the whole ensemble of identically prepared systems must be considered.

Let the system be, e.g., in the state $|\psi\rangle$ which we can expand with respect to the eigenstates of an (hermitian) operator $A$

$$|\psi\rangle = \sum_n c_n |n\rangle, \quad \text{where} \quad A|n\rangle = a_n |n\rangle. \tag{9.9}$$

The expectation value is then given by

$$\langle A\rangle_\psi = \sum_n |c_n|^2 a_n = \sum_n \frac{N_n}{N} a_n, \tag{9.10}$$

where $|c_n|^2$ is the probability to measure the eigenvalue $a_n$. It corresponds to the fraction $N_n/N$, the incidence the eigenvalue $a_n$ occurs, where $N_n$ is the number of times this eigenvalue has been measured out of an ensemble of $N$ objects.

The state is characterized by a density matrix of the form of Definition 9.1, with the properties I) - IV) (Eqs. (9.2) - (9.5)), where we can combine property I) and III) to conclude

$$\operatorname{Tr}\rho^2 = 1. \tag{9.11}$$

### 9.2.2 Mixed States

Let us next study the situation where not all of the $N$ systems (objects) of the ensemble are in the same state, i.e. $N_i$ systems are in the state $|\psi_i\rangle$ respectively, such that $\sum N_i = N$. The probability $p_i$ to find an individual system of the ensemble described by the state $|\psi_i\rangle$ is then given by

$$p_i = \frac{N_i}{N}, \quad \text{where} \quad \sum_i p_i = 1. \tag{9.12}$$

We can thus write down the **mixed state** as a convex sum, i.e. a weighted sum with $\sum_i p_i = 1$, of pure state density matrices

$$\rho_{\mathrm{mix}} = \sum_i p_i\, \rho_i^{\mathrm{pure}} = \sum_i p_i\, |\psi_i\rangle\langle\psi_i|. \tag{9.13}$$

The expectation value is again given by Theorem 9.1, i.e.

$$\langle A\rangle_{\rho_{\mathrm{mix}}} = \operatorname{Tr}(\rho_{\mathrm{mix}} A), \tag{9.14}$$

where we can express the expectation value of the mixed state as a convex sum of expectation values of its constituent pure states, i.e.

$$\langle A \rangle_{\rho_{\text{mix}}} = \sum_i p_i \langle \psi_i | A | \psi_i \rangle . \tag{9.15}$$

**Proof:**

$$
\begin{aligned}
\text{Tr} \left( \rho_{\text{mix}} A \right) &= \text{Tr} \left( \sum_i p_i | \psi_i \rangle \langle \psi_i | A \right) = \\
&= \sum_n \sum_i p_i \langle n | \psi_i \rangle \langle \psi_i | A | n \rangle = \\
&= \sum_i p_i \langle \psi_i | A \underbrace{\sum_n | n \rangle \langle n | }_{\mathbb{1}} \psi_i \rangle = \\
&= \sum_i p_i \langle \psi_i | A | \psi_i \rangle . \quad \text{q.e.d.} \tag{9.16}
\end{aligned}
$$

Properties II) - IV) (Eqs. (9.3) - (9.5)) are still valid for mixed states, but property I) does no longer hold

$$\rho_{\text{mix}}^2 = \sum_i \sum_j p_i p_j | \psi_i \rangle \underbrace{\langle \psi_i | \psi_j \rangle}_{\delta_{ij}} \langle \psi_j | = \sum_i p_i^2 | \psi_i \rangle \langle \psi_i | \neq \rho_{\text{mix}} , \tag{9.17}$$

where we, w.l.o.g., assumed that $| \psi_i \rangle$ and $| \psi_j \rangle$ are orthonormal. We can then calculate the trace of $\rho^2$, which, in contrast to pure states, is no longer equal to 1 but smaller

$$
\begin{aligned}
\text{Tr} \, \rho_{\text{mix}}^2 &= \sum_n \langle n | \sum_i \sum_j p_i p_j | \psi_i \rangle \langle \psi_i | \psi_j \rangle \langle \psi_j | n \rangle = \\
&= \sum_i \sum_j p_i p_j \langle \psi_i | \psi_j \rangle \langle \psi_j | \sum_n | n \rangle \langle n | \psi_i \rangle = \\
&= \sum_i \sum_j p_i p_j | \langle \psi_i | \psi_j \rangle |^2 = \\
&= \sum_i p_i^2 < \sum_i p_i = 1 . \tag{9.18}
\end{aligned}
$$

The last step in this calculation is obvious, since $0 \leq p_i \leq 1$ and therefore $p_i^2 \leq p_i$. We conclude that the trace of $\rho^2$ is a good measure for the mixedness of a density matrix, since it is equal to 1 for pure states and strictly smaller than 1 for mixed states. For a **_maximally mixed state_** we have for a given dimension $d$ of the system

$$\text{Tr} \, \rho_{\text{mix}}^2 = \tfrac{1}{d} > 0 . \tag{9.19}$$

## 9.3 Time Evolution of Density Matrices

We now want to find the equation of motion for the density matrix. We start from the time dependent Schrödinger equation and its hermitian conjugate

$$i\hbar \frac{\partial}{\partial t} \, |\psi\rangle \; = \; H \, |\psi\rangle \quad \overset{\dagger}{\to} \quad -i\hbar \frac{\partial}{\partial t} \, \langle\psi| \; = \; \langle\psi| \, H \; . \tag{9.20}$$

Then we differentiate the density matrix of a mixed state (Eq. (9.13)) with respect to time, we multiply it by $i\hbar$ and combine this with Eq. (9.20)

$$
\begin{aligned}
i\hbar \frac{\partial}{\partial t} \rho \; &= \; i\hbar \sum_i p_i \, ( \; \underbrace{|\dot{\psi}_i\rangle}_{-\frac{i}{\hbar} H |\psi_i\rangle} \, \langle\psi_i| \; + \; |\psi_i\rangle \, \underbrace{\langle\dot{\psi}_i|}_{\frac{i}{\hbar} \langle\psi_i| H} \; ) \; = \\
&= \; \sum_i p_i \, ( \, H \, \rho_i^{\text{pure}} \; - \; \rho_i^{\text{pure}} \, H \, ) \; = \\
&= \; [\, H \, , \rho \,] \; . \tag{9.21}
\end{aligned}
$$

---

**Theorem 9.2**  *Density matrices satisfy the **von Neumann Equation***

$$i\hbar \tfrac{\partial}{\partial t} \rho \; = \; [\, H \, , \rho \,]$$

---

The von Neumann equation is the quantum mechanical analogue to the classical Liouville equation, recall the substitution (2.85).

The time evolution of the density matrix we can also describe by applying an unitary operator, the ***time shift operator*** $U(t, t_0)$, also called ***propagator***

$$U(t, t_0) \; = \; e^{-\frac{i}{\hbar} H \, (t - t_0)} \; . \tag{9.22}$$

It allows us to relate the density matrix at a later time $t$ to the density matrix at some earlier time $t_0$

$$\rho(t) \; = \; U(t, t_0) \, \rho(t_0) \, U^\dagger(t, t_0) \; . \tag{9.23}$$

Furthermore, it helps us to prove, for instance, that the *mixedness* $\text{Tr} \, \rho^2$ *of a density matrix is time independent*

$$\text{Tr} \, \rho^2(t) \; = \; \text{Tr} \, (U \, \rho(t_0) \, \underbrace{U^\dagger U}_{\mathbb{1}} \, \rho(t_0) \, U^\dagger) \; = \; \text{Tr} \, (\rho(t_0) \, \rho(t_0) \, \underbrace{U^\dagger U}_{\mathbb{1}}) \; = \; \text{Tr} \, \rho^2(t_0) \; , \tag{9.24}$$

where we used the cyclicity of the trace operation.

**Example: Density matrix for spin $\frac{1}{2}$**

Generally, this will be a $2 \times 2$ matrix that can be written as linear combination of the identity $\mathbb{1}$ and the Pauli matrices $\sigma_x, \sigma_y$ and $\sigma_z$, as

$$\rho = \tfrac{1}{2} \left( \mathbb{1} + \vec{a}\,\vec{\sigma} \right) . \tag{9.25}$$

The coefficient $\vec{a}$ is named the **Bloch vector** and can be calculated as the expectation value of the Pauli matrices

$$\vec{a} = \mathrm{Tr}\,(\rho\,\vec{\sigma}) = \langle\,\vec{\sigma}\,\rangle . \tag{9.26}$$

All spin $\frac{1}{2}$ density matrices lie on or within the so-called **Bloch sphere** (with radius $\vec{a} = 1$) and are determined by the Bloch vector $\vec{a}$. The length of the Bloch vector thus tells us something about the mixedness, the polarization of an ensemble, i.e. of a beam of spin $\frac{1}{2}$ particles, e.g. electrons or neutrons. We say the beam is polarized if $a_i = 1$ and completely unpolarized if $a_i = 0$, for all $i$. This means that pure and mixed states can be characterized via the Bloch vector in the following way

$$\text{pure state} \quad \rho^2 = \rho \quad \Rightarrow \quad |\vec{a}| = 1 \tag{9.27}$$

$$\text{mixed state} \quad \rho^2 \neq \rho \quad \Rightarrow \quad |\vec{a}| < 1 . \tag{9.28}$$

A totally mixed state ($a_i = 0$ for all $i$) can then be written as

$$\rho_{\mathrm{mix}} = \frac{1}{2} \left( |\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow| \right) = \frac{1}{2}\,\mathbb{1} , \tag{9.29}$$

such that

$$\mathrm{Tr}\,\rho_{\mathrm{mix}} = 1 \quad \text{and} \quad \mathrm{Tr}\,\rho_{\mathrm{mix}}^2 = \frac{1}{2} . \tag{9.30}$$

**Remark:** Note, the decomposition (9.29) into up $|\uparrow\rangle\langle\uparrow|$ and down $|\downarrow\rangle\langle\downarrow|$ states is by no means unique, we can achieve the totally mixed state $\rho_{\mathrm{mix}} = \frac{1}{2}\,\mathbb{1}$ in many different ways.