Chapter 22
The Density Operator

The density operator is the most general representation of states in quantum mechanics. It allows the description of those systems which are only partially known.

Up to now, we have characterized a quantum-mechanical system by a vector $|\psi\rangle$ of the Hilbert space. In the following, we will extend the concept of state, as we already promised in Chap. 14, Vol. 1. We will introduce the density operator or density matrix, the most general representation of states in quantum mechanics. This tool allows us to describe also states for which we do not have complete information, and which therefore cannot be represented by a vector in the Hilbert space. That such a description is useful or necessary may be surprising at first, but we will see that this formulation is quite handy, especially with regard to the discussion of the measurement process in quantum mechanics.

A remark on nomenclature: If a system can be represented by a vector in a Hilbert space $\mathcal{H}$, one speaks of a *pure state*. In this case, the maximum amount of information is available (one-dimensional subspace of $\mathcal{H}$). Otherwise, one speaks of a *mixed state*.

22.1 Pure States

We start by noting that we can characterize a quantum-mechanical system by the normalized state[1] $|\psi\rangle$, but just as well by a dyadic product called the *density operator* ρ or *statistical operator* [2]

$$\rho = |\psi\rangle \langle\psi|. \tag{22.1}$$

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[1] A dependence on time is not mentioned explicitly in the following.

[2] Actually, it would be better to say 'state operator', but the term 'density operator' has become established—and unfortunately also the use of ρ. Note: Previously, ρ was used exclusively for the probability density, i.e. $\rho = \langle\psi|\ \psi\rangle$. Which ρ is meant in a particular situation should follow unambiguously from the context.

J. Pade, *Quantum Mechanics for Pedestrians 2*, Undergraduate Lecture Notes in Physics, https://doi.org/10.1007/978-3-030-00467-5_22

The information content is the same whether we specify the state or the density operator. There is a small difference, however: We know that (normalized) states are determined up to an arbitrary global phase[3]:

$$|\psi\rangle \rightarrow e^{i\alpha} |\psi\rangle. \tag{22.2}$$

This phase disappears when we use the density operator

$$\rho = |\psi\rangle \langle\psi| \rightarrow e^{i\alpha} |\psi\rangle \langle\psi| e^{-i\alpha} = \rho, \tag{22.3}$$

and this may be seen at this point to represent a certain advantage of this formulation.

By the way, one is in good company if one does not immediately see the need to introduce the concept of the density operator which shows the following quote: "By introducing an operator ρ called the density matrix, expectation values can be written in a form that at first sight is opaque but which turns out to be very powerful".[4] In fact, it is only with the help of this operator that e.g. the extension of the term 'state' can be accomplished, as we shall see below.[5]

The density operator introduced in this way is obviously a projection operator (normalization of $|\psi\rangle$ presupposed):

$$\rho^2 = |\psi\rangle \langle\psi| \psi\rangle \langle\psi| = \rho; \rho^\dagger = \rho. \tag{22.4}$$

Just as with the state $|\psi\rangle$, one can formulate all those statements for a quantum-mechanical system which are accessible to measurements by using the density operator ρ. For example, we can calculate mean or expected values. Here, the term *trace* comes into play. We assume that there is a CONS $\{|n\rangle\}$. Then the trace tr of A is defined as[6]:

$$trA = tr(A) = \sum_n \langle n| A |n\rangle. \tag{22.5}$$

With this notation, the mean value of an operator A for the state $|\psi\rangle$ is given by

$$\begin{aligned} \langle A\rangle = \langle\psi| A |\psi\rangle &= \sum_{n,m} \langle\psi| n\rangle \langle n| A |m\rangle \langle m| \psi\rangle = \sum_{n,m} \langle m| \psi\rangle \langle\psi| n\rangle \langle n| A |m\rangle \\ &= \sum_{n,m} \langle m| \rho |n\rangle \langle n| A |m\rangle = \sum_m \langle m| \rho A |m\rangle = tr\left(\rho A\right). \end{aligned} \tag{22.6}$$

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[3] Indeed, states are strictly speaking not determined by vectors of $\mathcal{H}$, but instead by rays, see Chap. 14, Vol. 1.

[4] Gottfried and Yan, *Quantum Mechanics: Fundamentals*, p. 46.

[5] Another example for the quasi natural occurrence of the density operator is the theorem of Gleason, which deals with the question of how mean values (or probabilities) can be defined in quantum mechanics. It states in essence that in Hilbert spaces of dimension ≥3, the mean values of projection operators P can be described only by $\langle P\rangle = tr\left(\rho P\right)$ (see Appendix T, Vol. 2).

[6] See also Appendix F, Vol. 1.

Knowledge of the density operator thus allows us to determine averages by taking the trace.[7] As a little exercise, we now calculate the trace of the density operator itself (which of course must be 1, since $tr\,(\rho \cdot 1) = \langle 1 \rangle$). We have:

$$tr\,(\rho) = \sum_n \langle n|\,\rho\,|n\rangle = \sum_n \langle n|\,\psi\rangle\,\langle\psi\,|n\rangle = \sum_n \langle\psi\,|n\rangle\,\langle n|\,\psi\rangle = \langle\psi\,|\psi\rangle = 1. \tag{22.7}$$

We can also start from

$$|\psi\rangle = \sum_n \langle n|\,\psi\rangle\,|n\rangle = \sum_n c_n\,|n\rangle \tag{22.8}$$

with $\sum\limits_n |c_n|^2 = 1$ due to $\langle\psi|\,\psi\rangle = 1$. It follows that:

$$tr\,(\rho) = \sum_n \langle n|\,\psi\rangle\,\langle\psi\,|n\rangle = \sum_n |c_n|^2 = 1. \tag{22.9}$$

A few remarks on the representation of the density operator as *density matrix*. With (22.8), we have:

$$\rho = |\psi\rangle\,\langle\psi| = \sum_{n,m} c_n c_m^*\,|n\rangle\,\langle m|. \tag{22.10}$$

Evidently we have the same information content whether we use the formulation (22.10) or the density matrix[8]:

$$\rho_{nm} = c_n c_m^* \;\text{ or }\; \rho \cong \begin{pmatrix} c_1 c_1^* & c_1 c_2^* \cdots \\ c_2 c_1^* & c_2 c_2^* \cdots \\ \cdots & \cdots \;\cdots \end{pmatrix}. \tag{22.11}$$

In fact, the two terms ‘density operator’ and ‘density matrix’ are quite often used synonymously (and one writes just $=$ instead of $\cong$; we have occasionally neglected this distinction, also), and depending on the context, ρ refers to the abstract operator or the matrix (22.11). A note on nomenclature: the diagonal elements are also called *populations* or *occupation numbers*, the off-diagonal elements *coherences* or *interference terms*. In addition, we see that the trace of the density matrix is given by $\sum |c_n|^2$, and thus by exactly the same term as in (22.9), as indeed it must be. We point out that the trace of a matrix is equal to the sum of its eigenvalues.[9] A comment and two examples using two-dimensional systems follow:

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[7] It holds that $tr\,(\rho A) = tr\,(A\rho)$; see the exercises.

[8] The density matrix is Hermitian, of course.

[9] Since the density matrix is Hermitian, its eigenvalues are real.

1. In the density matrix
$$\rho = \begin{pmatrix} c_1 c_1^* & c_1 c_2^* \\ c_2 c_1^* & c_2 c_2^* \end{pmatrix}, \tag{22.12}$$
we clearly cannot ensure that the interference terms vanish, while the two diagonal terms are nonzero. Either there are four non-zero entries or only one in this matrix; any other possibility is excluded.[10] (As always, we have discarded from the outset the trivial solution with $c_1 = c_2 = 0$). As is easily verified, we have $\rho^2 = \rho$ (see the exercises).
2. Two examples using polarization states:

   (a) Let $|\psi\rangle = |h\rangle$. Then it holds that:
$$\rho = |h\rangle\langle h| \text{ or } \rho = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \tag{22.13}$$

   (b) For $|\psi\rangle = \frac{|h\rangle - i|v\rangle}{\sqrt{2}}$, it follows that
$$\rho = \frac{|h\rangle\langle h| + i\,|h\rangle\langle v| - i\,|v\rangle\langle h| + |v\rangle\langle v|}{2} \text{ or } \rho = \frac{1}{2}\begin{pmatrix} 1 & i \\ -i & 1 \end{pmatrix}. \tag{22.14}$$

   The relation $\rho^2 = \rho$ of course holds also for these two examples.

22.2 Mixed States

We obtain the projection onto a pure state by means of the projection operator $|\psi\rangle\langle\psi|$. Here, it is assumed that we know the state exactly, e.g. by characterizing it using a complete system of commuting observables. But often, one has only incomplete information about a system or simply does not want to know everything—just think of the kinetic theory of gases, whose strength lies precisely in the fact that one does not have to take into account all 10^{23} particles explicitly. In statistical physics, one compensates ignorance of the precise state of a system by the introduction of *classical probabilities*.[11] That is what we do in quantum mechanics as well, if we do not have all the necessary information. One speaks of a *mixed state* or a *statistical mixture* as opposed to a pure state.

For a given mixture, we know only that the system is in the states $|\varphi_n\rangle$ with *classical probabilities* p_n ($0 \leq p_n \leq 1$ and $\sum_n p_n = 1$). The states $|\varphi_n\rangle$ are normalized, but

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[10] This does not change if we diagonalize the matrix (that is possible, since it is Hermitian). For the diagonal elements of the resulting diagonal matrix are the eigenvalues, and in this case they are 0 and 1 (because of $|c_1|^2 + |c_2|^2 = 1$); see the exercises.

[11] In contrast to the probabilities which are inevitable in quantum mechanics.

need not necessarily be mutually orthogonal. As the density operator for this system, we can choose the weighted superposition $\rho_{\text{stat}} = \sum\limits_n p_n \left|\varphi_n\right\rangle \left\langle\varphi_n\right|$. For clarity, we denote this density operator temporarily by ρ_{stat}.

To make life easier for us, we will not discuss the general case of non-orthogonal bases,[12] but instead refer to the CONS $\{|n\rangle\}$ introduced above:

$$\rho_{\text{stat}} = \sum_n p_n \left|n\right\rangle \left\langle n\right| \tag{22.15}$$

and

$$tr\left(\rho_{\text{stat}}\right) = \sum_m \left\langle m\right| \rho_{\text{stat}} \left|m\right\rangle = \sum_{mn} p_n \left\langle m \mid n\right\rangle \left\langle n \mid m\right\rangle = \sum_n p_n = 1. \tag{22.16}$$

We note that there are no interference terms (coherences) as in (22.10); the corresponding density matrix has only diagonal entries.

So we know with the classical probability p_n that the system is in state $|n\rangle$. It follows that

$$\rho_{\text{stat}}^2 = \sum_{n,m} p_n p_m \left|n\right\rangle \left\langle n \mid m\right\rangle \left\langle m\right| = \sum_n p_n^2 \left|n\right\rangle \left\langle n\right| \tag{22.17}$$

and

$$tr\left(\rho_{\text{stat}}^2\right) = \sum_{n,m} p_n^2 \left\langle m \mid n\right\rangle \left\langle n \mid m\right\rangle = \sum_n p_n^2. \tag{22.18}$$

The comparison of (22.15) and (22.17) shows immediately that $\rho_{\text{stat}}^2 = \rho_{\text{stat}}$ can apply only if all of the probabilities p_n vanish except for one,[13] $p_n = \delta_{nN}$. For a pure state, ρ_{stat} is a projection operator, but with mixtures, $\rho_{\text{stat}}^2 \neq \rho_{\text{stat}}$ applies—and this means that ρ_{stat} in this case is *not* a projection operator.

Considering the trace of the density operator, we see that for a mixture (i.e. two or more $p_n \neq 0$), it holds that $tr\left(\rho_{\text{stat}}^2\right) = \sum p_n^2 < 1$. All in all, we have[14]:

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[12] For the expansion in terms of not-necessarily-orthogonal states, see the exercises.

[13] The case that all the probabilities are zero is trivial.

[14] Note: For a change of basis to another CONS $\{|\varphi_m\rangle\}$ with

$$|n\rangle = \sum_m c_{nm} \left|\varphi_m\right\rangle,$$

off-diagonal terms can of course occur in the density matrix:

$$\rho_{\text{stat}} = \sum_{n,m,m'} p_n c_{nm} c_{n'm'}^* \left|\varphi_m\right\rangle \left\langle\varphi_{m'}\right| = \sum_{m,m'} \sum_n \left(p_n c_{nm} c_{n'm'}^*\right) \left|\varphi_m\right\rangle \left\langle\varphi_{m'}\right| = \sum_{m,m'} \alpha_{mm'} \left|\varphi_m\right\rangle \left\langle\varphi_{m'}\right|.$$

The occurrence of non-trivial off-diagonal terms is not crucial as a distinguishing feature between ρ and ρ_{stat}, but rather the criteria $\rho_{\text{stat}}^2 \neq \rho_{\text{stat}}$ and $tr\left(\rho_{\text{stat}}^2\right) < 1$ (thus the denotation of off-diagonal terms as 'coherences' or 'interference terms' is a bit unfortunate).

$$\rho_{\text{stat}}^2 \neq \rho_{\text{stat}};\, tr\left(\rho_{\text{stat}}^2\right) < 1 \quad \text{for a mixed state.} \tag{22.19}$$

In addition, we have the relation between the trace and the mean value:

$$\begin{aligned} tr\left(\rho_{\text{stat}} A\right) &= \sum_{n,m} p_n \langle m \,|n\rangle \langle n| \, A \, |m\rangle \\ &= \sum_{n,m} p_n \delta_{nm} \langle n| \, A \, |m\rangle = \sum_m p_m \langle m| \, A \, |m\rangle = \langle A \rangle \,. \end{aligned} \tag{22.20}$$

We point out that in the latter equation, there are two fundamentally different averaging processes, one being the *quantum-mechanical* mean, $\langle m| \, A \, |m\rangle$ of the operator A over the states $|m\rangle$, the other one being the *classical* mean value of this quantum-mechanical average, given by $\sum\limits_m p_m \langle m| \, A \, |m\rangle$.

For clarity, we emphasize again the differences between the two density operators:

1. If one can describe the system by a state in the Hilbert space with the basis $\{|n\rangle\}$ (pure state), e.g. by $|\psi\rangle = \sum_n c_n \, |n\rangle$, it is in a quantum-mechanical superposition of basis states (unless all c_n are zero except one). With respect to this basis, the system therefore has no defined state; that results only from a measurement. For the density operator ρ, $\rho^2 = \rho$ and $tr\left(\rho^2\right) = 1$ hold.
2. In a statistical mixture, the system is in a well-defined state; however, we do not know in which one. So this is a very different situation from that described in 1), in which it is simply not reasonable to ask about the status of the system—it is not defined in relation to the selected basis. For a statistical mixture, we have $\rho_{\text{stat}}^2 \neq \rho_{\text{stat}}$ and $tr\left(\rho_{\text{stat}}^2\right) < 1$.

We can now summarize the properties of the density operator ρ (we have derived some points only for the simpler case (22.15), but they hold true in general). In order to standardize the terminology, we dispense with the labelling ρ_{stat} and, following the usual practice, denote all density operators just by ρ.[15]

1. ρ is Hermitian, $\rho = \rho^\dagger$, and positive, $\langle \varphi| \, \rho \, |\varphi\rangle \geq 0$ for all $|\varphi\rangle$. The trace of ρ is 1, $tr\,(\rho) = 1$. Generally, an operator A with the three properties $A = A^\dagger$, A positive and $tr(A) = 1$ is called a density operator.
2. ρ is a projection operator if and only if the system is in a pure state ($p_n = \delta_{n,N}$). In this case, $\rho^2 = \rho$ and $tr(\rho^2) = 1$ applies, while a mixture is characterized by $\rho^2 \neq \rho$ and $tr(\rho^2) < 1$. This result does not depend on the choice of basis, because the trace is invariant under unitary transformations (see the exercises). The main criterion for a pure or mixed state is $tr(\rho^2) = 1$ or $tr(\rho^2) < 1$.
3. For the mean value of an observable A, we have $\langle A \rangle = tr\,(\rho A)$. By the way, from this it follows directly that $\langle \rho \rangle = tr\left(\rho^2\right)$.
4. The probability of finding the system in state $|m\rangle$ is given by $p_m = tr(\rho \, |m\rangle \langle m|)$ (see the exercises).

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[15] What is precisely meant must follow from the context, if necessary.

5. The time behavior of ρ is described by the *von Neumann equation*[16] (see the exercises):
$$i\hbar\partial_t\rho = [H, \rho]\,. \tag{22.21}$$
Due to
$$|\psi(t)\rangle = U(t)\,|\psi(0)\rangle\,, \tag{22.22}$$
the solution of this equation is
$$\rho(t) = U(t)\,\rho(0)\,U^\dagger(t)\,. \tag{22.23}$$
6. With the density operator, we have expanded upon the state concept, as promised in Chap. 14 of Vol. 1; we can now also describe systems whose state is not known in detail and which can therefore *not* be described by a state vector of $\mathcal{H}$.

22.3 Reduced Density Operator

For the next topic, we start from a system of two quantum objects. We have the product space $\mathcal{H}_1 \otimes \mathcal{H}_2$; $\{|n_1\rangle\}$ and $\{|m_2\rangle\}$ are CONS in $\mathcal{H}_1$ and $\mathcal{H}_2$. Using the notation $|n_1\rangle \otimes |m_2\rangle = |n_1 m_2\rangle$, it follows for an arbitrary state:

$$|\psi\rangle = \sum_{n,m} c_{nm}\,|n_1 m_2\rangle, \tag{22.24}$$

and thus for the density of a pure state:

$$\rho = \sum_{n,m,n',m'} c_{nm} c^*_{n'm'} |n_1 m_2\rangle\langle n'_1 m'_2|. \tag{22.25}$$

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[16] Compare this with the Liouville equation in classical mechanics:

$$\partial_t\rho = \{H, \rho\}_{\text{Poisson}}$$

where the Poisson bracket of two quantities A and B is defined by

$$\{F, G\}_{\text{Poisson}} = \sum_k \left(\frac{\partial F}{\partial q_k}\frac{\partial G}{\partial p_k} - \frac{\partial G}{\partial q_k}\frac{\partial F}{\partial p_k} \right).$$

This motivates once more the transition from classical mechanics to quantum mechanics by the substitution (keyword canonical quantization; see Appendix W, Vol. 2)

$$\{,\}_{\text{Poisson bracket}} \to \frac{1}{i\hbar}\,[,]_{\text{commutator}}$$

.

Due to

$$\sum_{n,m} |c_{nm}|^2 = 1, \tag{22.26}$$

we have $\rho^2 = \rho$. So far there is nothing new. But we know that in the case of two quantum objects, entangled states can occur which *cannot* be represented as product states. This leads to a new question, namely: What is the density operator $\rho^{(1)}$ for the quantum object 1? This question *must* lead to something new, because the individual quantum objects in an entangled state do not have well-defined properties; this fact must have some impact on the density operator.

We consider an operator A_1 which acts only in the space $\mathcal{H}_1$; I_2 denotes the identity in $\mathcal{H}_2$. The total operator is $A_1 \otimes I_2$, and its average is given by

$$\begin{aligned} \langle A_1 \otimes I_2 \rangle &= tr\left(\rho\left[A_1 \otimes I_2\right]\right) = \sum_{n_1,m_2} \langle n_1 m_2| \rho\left[A_1 \otimes I_2\right] |n_1 m_2\rangle \\ &= \sum_{n_1,m_2} \langle n_1| \langle m_2| \rho |m_2\rangle A_1 |n_1\rangle = \sum_{n_1} \langle n_1| \left(\sum_{m_2} \langle m_2| \rho |m_2\rangle \right) A_1 |n_1\rangle. \end{aligned} \tag{22.27}$$

We have used a) $\langle m_2| \rho\left[A_1 \otimes I_2\right] |m_2\rangle = \langle m_2| \rho I_2 |m_2\rangle A_1$ (since the operator A_1 acts in $\mathcal{H}_1$only),[17] and b) $\langle m_2| \rho I_2 |m_2\rangle = \langle m_2| \rho |m_2\rangle$, because of $I_2 |m_2\rangle = |m_2\rangle$. The expression in parentheses means that we take the average of the density operator ρ (which acts in $\mathcal{H}_1$ *and* $\mathcal{H}_2$) *only in* $\mathcal{H}_2$, not in both spaces. Such a partial averaging is called a *partial trace* $tr_k(\rho)$, where the index k indicates the space in which the averaging is performed. The result of this partial averaging is an operator that acts only in $\mathcal{H}_1$, namely the *reduced density operator* $\rho^{(1)}$. We have therefore[18]:

$$\rho^{(1)} = \sum_{m_2} \langle m_2| \rho |m_2\rangle = tr_2(\rho). \tag{22.28}$$

We note that $\rho^{(1)}$ is a 'proper' density operator (Hermitian, positive, trace 1). For the mean value of $A_1 \otimes I_2$, we obtain

$$\langle A_1 \otimes I_2 \rangle = \sum_{n_1} \langle n_1| \rho^{(1)} A_1 |n_1\rangle = tr_1\left(\rho^{(1)} A_1\right). \tag{22.29}$$

The salient point is that the reduced density operator $\rho^{(1)}$ can have properties which are very different from those of the density operator ρ. For example, in a 2×2 matrix (as in (22.12)), it is not necessarily true that either one or all entries exist; it may happen that only the off-diagonal elements are equal to zero, which is impossible for a density operator with $tr\left(\rho^2\right) = 1$. In the reduced density operator,

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[17] We note that $\langle m_2| \rho |m_2\rangle$ is an operator in $\mathcal{H}_1$, and therefore, it generally holds that $\sum\limits_{m_2} \langle m_2| \rho |m_2\rangle A_1 \neq A_1 \sum\limits_{m_2} \langle m_2| \rho |m_2\rangle$.

[18] Other notations are $\hat{\rho}$, ρ_{red}, ρ_1 or similar forms.

we describe in general not a pure state, but a mixed state or a statistical mixture. This manifests itself in the fact that it applies in general that $\left(\rho^{(1)}\right)^2 \neq \rho^{(1)}$.

Before we continue with our general considerations, we illustrate these findings by an example.

22.3.1 Example

We consider a two-state system whose single components have the basis $\{|a\rangle, |b\rangle\}$. The total state is

$$|\psi\rangle = c_{11}\,|a_1a_2\rangle + c_{12}\,|a_1b_2\rangle + c_{21}\,|b_1a_2\rangle + c_{22}\,|b_2b_2\rangle \quad \text{with} \quad \sum \left|c_{ij}\right|^2 = 1. \tag{22.30}$$

The density matrix is correspondingly a 4 × 4 matrix; we will not write it explicitly here (but see the exercises). The reduced density operator is constructed via

$$\rho^{(1)} = \langle a_2|\ \psi\rangle\,\langle\psi\ |a_2\rangle + \langle b_2|\ \psi\rangle\,\langle\psi\ |b_2\rangle, \tag{22.31}$$

and obviously corresponds to a 2 × 2 matrix (see exercises). With

$$\begin{aligned} \langle a_2\ |\psi\rangle &= c_{11}\,|a_1\rangle + c_{21}\,|b_1\rangle \\ \langle b_2\ |\psi\rangle &= c_{12}\,|a_1\rangle + c_{22}\,|b_1\rangle, \end{aligned} \tag{22.32}$$

it follows that

$$\begin{aligned} \rho^{(1)} = &\left[c_{11}^*c_{11}\,|a_1\rangle + c_{21}\,|b_1\rangle\right]\left[c_{11}^*\,\langle a_1| + c_{21}^*\,\langle b_1|\right] \\ &+ \left[c_{11}^*c_{12}\,|a_1\rangle + c_{22}\,|b_1\rangle\right]\left[c_{12}^*\,\langle a_1| + c_{22}^*\,\langle b_1|\right]. \end{aligned} \tag{22.33}$$

Multiplying and collecting similar terms leads to the density matrix

$$\rho^{(1)} = \begin{pmatrix} |c_{11}|^2 + |c_{12}|^2 & c_{11}c_{21}^* + c_{12}c_{22}^* \\ c_{21}c_{11}^* + c_{22}c_{12}^* & |c_{21}|^2 + |c_{22}|^2 \end{pmatrix}. \tag{22.34}$$

It is clear that $tr\left(\rho^{(1)}\right) = 1$. For the determination of $tr\left(\rho^{(1)2}\right)$, we notice that we can represent the reduced density matrix as[19]:

$$\rho^{(1)} = CC^\dagger;\ C = \begin{pmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \end{pmatrix}. \tag{22.35}$$

One can show (see exercises) that it then holds that

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[19] In this representation, we can see directly that $\rho^{(1)}$ is Hermitian and positive.

$$tr\left(\rho^{(1)2}\right) = 1 - 2\left|\det C\right|^2. \tag{22.36}$$

We therefore have $tr\left(\rho^{(1)2}\right) = 1$, if and only if $|\det C| = 0$, i.e. for $c_{11}c_{22} = c_{12}c_{21}$. But this is just the way we defined a product state in Chap. 20. In other words, for entangled states, $(c_{11}c_{22} \neq c_{12}c_{21})$ is always $tr\left(\rho^{(1)2}\right) < 1$; thus, the reduced density matrix describes a statistical mixture in this case.

22.3.2 Comparison

We want to compare again the various density matrices of our standard example:

We first consider a single quantum object. For a pure state of the form $|\psi\rangle = c_1|a\rangle + c_2|b\rangle$, the density matrix is

$$\rho = \begin{pmatrix} |c_1|^2 & c_1c_2^* \\ c_2c_1^* & |c_2|^2 \end{pmatrix}; \quad |c_1|^2 + |c_2|^2 = 1. \tag{22.37}$$

As stated above, either one entry or four entries are nonzero.

For a statistical mixture, there is a basis in which it holds that:

$$\rho = \begin{pmatrix} p_1 & 0 \\ 0 & p_2 \end{pmatrix}; \quad p_1 + p_2 = 1. \tag{22.38}$$

Here, we have that either one entry or two entries are nonzero (in another basis, four entries could also be nonzero). If there is only one nontrivial entry, we have a pure state.

Next, we consider two quantum objects. For the reduced density matrix we start from the state $|\psi\rangle = c_{11}|a_1a_2\rangle + c_{12}|a_1b_2\rangle + c_{21}|b_1a_2\rangle + c_{22}|b_2b_2\rangle$. It follows that

$$\rho^{(1)} = \begin{pmatrix} |c_{11}|^2 + |c_{12}|^2 & c_{11}c_{21}^* + c_{12}c_{22}^* \\ c_{21}c_{11}^* + c_{22}c_{12}^* & |c_{21}|^2 + |c_{22}|^2 \end{pmatrix}; \sum \left|c_{ij}\right|^2 = 1. \tag{22.39}$$

In this case, there are choices for the coefficients (or unitary transformations of $\rho^{(1)}$), such that the coherences vanish, but not the two populations, which is impossible for the density matrix of a pure state. We choose, for example, $c_{22} = -c_{21}c_{11}^*/c_{12}^*$ and obtain in this special case

$$\rho^{(1)}_{\text{special}} = \left(|c_{11}|^2 + |c_{12}|^2\right)\begin{pmatrix} 1 & 0 \\ 0 & \frac{|c_{21}|^2}{|c_{12}|^2} \end{pmatrix}. \tag{22.40}$$

Especially for $|c_{21}|^2 = |c_{12}|^2$, we have equidistribution.

22.3.3 General Formulation

In this section, we consider the reduced density operator for general dimensionality. We have two quantum systems $|n_1\rangle$ and $|m_2\rangle$ in the superposition state

$$|\psi\rangle = \sum_{n,m} c_{nm} \, |n_1 m_2\rangle, \tag{22.41}$$

or the density operator:

$$\rho = \sum_{n,m,n',m'} c_{nm} c^*_{n'm'} |n_1 m_2\rangle \langle n'_1 m'_2| \quad \text{with} \quad \sum_{n,m} |c_{nm}|^2 = 1. \tag{22.42}$$

For the reduced density operator $\rho^{(1)}$, it follows[20] that:

$$\begin{aligned} \rho^{(1)} &= \sum_M \langle M_2| \, \rho \, |M_2\rangle = \sum_M \langle M_2| \sum_{n,m,n',m'} c_{nm} c^*_{n'm'} \, |n_1 m_2\rangle \, \langle n'_1 m'_2| \, M_2\rangle \\ &= \sum_{n,n'} \left(\sum_M c_{nM} \cdot c^*_{n'M} \right) |n_1\rangle \, \langle n'_1| = \sum_{n,n'} \rho^{(1)}_{n,n'} |n_1\rangle \langle n'_1|. \end{aligned} \tag{22.43}$$

To keep the notation transparent, we use the matrix representation. With $\rho^{(1)}_{n,n'} = \sum\limits_M c_{nM} \cdot c^*_{n'M}$, it follows that

$$\rho^{(1)} = CC^\dagger; C = (c_{nm}) = \begin{pmatrix} c_{11} & c_{12} & c_{13} & \ldots \\ c_{21} & c_{22} & \ldots & \cdots \\ c_{31} & \vdots & \ddots & \ldots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \tag{22.44}$$

In this reduced density operator, off-diagonal terms also occur, but the fact that it nevertheless describes a statistical mixture is shown by considering $\left[\rho^{(1)}\right]^2$. We examine under which conditions it holds that

$$\left[\rho^{(1)}\right]^2 = \rho^{(1)}. \tag{22.45}$$

Since $\rho^{(1)}$ is a projection operator in this case, it can be written as

$$\rho^{(1)} = |A\rangle \, \langle A| = |A\rangle \, \langle B| \, B\rangle \, \langle A| \, , \tag{22.46}$$

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[20] In the following chapters, we will consider three or more quantum objects. The reduced density operator for quantum object 1 is then given by taking the trace over all other quantum objects (colloquially, 'tracing out' these degrees of freedom).

where $|A\rangle$ and $|B\rangle$ are suitable normalized vectors,

$$|A\rangle \cong \begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix} \text{ and } |B\rangle \cong \begin{pmatrix} b_1 \\ b_2 \\ \vdots \end{pmatrix}. \tag{22.47}$$

Thus, we can identify by comparison with (22.44) (only the structure matters here):

$$C = |A\rangle \langle B| \text{ or } c_{nm} = a_n b_m. \tag{22.48}$$

We insert this condition into (22.41) and obtain

$$|\psi\rangle = \sum_{n,m} c_{nm} |n_1 m_2\rangle = \sum_{n,m} a_n b_m |n_1 m_2\rangle = \sum_n a_n |n_1\rangle \sum_m b_m |m_2\rangle, \tag{22.49}$$

i.e. a factorized state. This means that the reduced density operator for entangled states always describes a statistical mixture; for factorized states, however, it is a projection operator onto the state in space 1.

22.4 Exercises

1. Write the density operator

$$\rho = \sum_n |\varphi_n\rangle \, p_n \, \langle\varphi_n| \tag{22.50}$$

   with normalized, but not necessarily orthogonal states $|\varphi_n\rangle$ when it is transformed unitarily.
2. Show that $tr\,(AB) = tr\,(BA)$.
3. Show that the trace is cyclically invariant, i.e.

$$tr\,(ABC) = tr\,(BCA) = tr\,(CAB). \tag{22.51}$$

4. Prove that the trace is invariant under unitary transformations.
5. Show that the trace is independent of the basis. (This *must* apply, since a basis transformation is unitary.)
6. Given a CONS $\{|n\rangle\}$ and a state $|\psi\rangle = \sum_n c_n |n\rangle$ with $\sum_n |c_n|^2 = 1$, show that the probability of finding the system in the state m is given by $p_m = tr(\rho\,|m\rangle\,\langle m|) = tr(\rho P_m)$.
7. Show that for the reduced density operator $\rho^{(1)}$, it holds in general that $tr\left(\left[\rho^{(1)}\right]^2\right) \leq 1$; hence, we have a mixture if the strict inequality applies.

8. Write the density operator in the position representation (cf. Chaps. 12 and 13, Vol. 1).
9. Show explicitly for

$$\rho = \begin{pmatrix} c_1 c_1^* & c_1 c_2^* \\ c_2 c_1^* & c_2 c_2^* \end{pmatrix} \tag{22.52}$$

that

$$\rho^2 = \rho \tag{22.53}$$

applies; using this matrix, show explicitly that $\rho^2 = \rho$. Here, it must hold that $|c_1|^2 + |c_2|^2 = 1$.

10. Show that the eigenvalues $\lambda_{1/2}$ of the matrix

$$\rho = \begin{pmatrix} c_1 c_1^* & c_1 c_2^* \\ c_2 c_1^* & c_2 c_2^* \end{pmatrix} \tag{22.54}$$

are 0 and 1.

11. Given the density matrix for a statistical mixture in the form $\rho = p_h \left|h\right\rangle \left\langle h\right| + p_v \left|v\right\rangle \left\langle v\right|$ or

$$\rho = \begin{pmatrix} p_h & 0 \\ 0 & p_v \end{pmatrix}; \tag{22.55}$$

How does this read in the circularly-polarized basis?

12. Given two quantum objects Q1 and Q2 with the respective N-dimensional CONS $\{\left|\varphi_i\right\rangle\}$ for Q1 and $\{\left|\psi_i\right\rangle\}$ for Q2 (by the choice of notation, we can omit the index for the number of the quantum object). The initial state is

$$\left|\chi\right\rangle = \sum_{ij} c_{ij} \left|\varphi_i\right\rangle \left|\psi_j\right\rangle. \tag{22.56}$$

Calculate the probability $w(\lambda)$ of measuring the quantum object 1 in a state $\left|\lambda\right\rangle$, and formulate it in terms of the reduced density operator $\rho^{(1)}$.

13. Given the density operator $\rho = \sum_n p_n \left|\varphi_n\right\rangle \left\langle \varphi_n\right|$, where it holds that $i\hbar\partial_t \left|\varphi_n\right\rangle = H\left|\varphi_n\right\rangle$. Show that the time behavior of ρ is described by the von-Neumann equation:

$$i\hbar\partial_t \rho = [H, \rho]. \tag{22.57}$$

14. Using the example of a polarized photon, show explicitly that a given density matrix does not allow a unique decomposition.

   (a) First formulate the projection operators for the states $\left|h\right\rangle$, $\left|v\right\rangle$, $\left|r\right\rangle$ and $\left|l\right\rangle$.

   (b) Given the density matrix $\rho = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$; now formulate the decomposition of ρ in terms of linearly- and circularly-polarized states.

15. The spin state of an electron is represented (in the basis of eigenstates of the spin matrix $s_z = \frac{\hbar}{2}\sigma_z$) by the density matrix $\rho = \begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix}$, with $a + b = 1$; $a \geq 0, b \geq 0$.

    (a) What is the probability of obtaining $\pm\frac{\hbar}{2}$, if one measures s_x?
    (b) Calculate the expectation value of s_x and compare it with the trace formalism.

16 Given a system of two quantum objects; the basis states are in each case $|1\rangle$ and $|2\rangle$.[21]

    (a) How is the general total state $|\psi\rangle$ formulated?
    (b) Give explicitly the density matrix for this system.
    (c) Starting from this matrix, calculate the reduced density matrix $\rho^{(1)}$.
    (d) Show that $tr\left(\rho^{(1)}\right) = 1$ holds.
    (e) Show that $\rho^{(1)} = CC^\dagger$ with $C = \begin{pmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \end{pmatrix}$ holds.
    (f) Calculate $\rho^{(1)2}$.
    (g) Show that $tr\left(\rho^{(1)2}\right) = 1 - 2\left|\det C\right|^2$ is true.

17. $\{|\varphi_i\rangle, i = 1, \ldots, N\}$ are normalized, but not necessarily orthogonal states. Show that the density matrix $\rho = \frac{1}{N}\sum_{i=1}^{N} |\varphi_i\rangle\langle\varphi_i|$ describes a pure state, iff these N states are equal up to a phase.

    (a) Let $|\varphi_n\rangle = e^{i\delta_n}|\varphi\rangle$. Show that $\rho^2 = \rho$.
    (b) Let $\rho^2 = \rho$; show that the N states $|\varphi_i\rangle$ are equal up to a phase.

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[21] One can imagine e.g. two photons, and by $|1\rangle$ and $|2\rangle$ e.g. $|h\rangle$ and $|v\rangle$ or $|r\rangle$ and $|l\rangle$.