Chapter 9

Mixed States: the density matrix

Up to now, we have always treated a single particle, with spatial and spin (or polarization) properties. We have mostly discussed just one of these properties and ignored the other. This can safely be done when the particle is in a so-called **product state**, e.g.

$$|\text{total state}\rangle = |\text{state in coordinate space}\rangle \otimes |\text{state in spin space}\rangle.$$

(See also ch. 9.5.2). Often we have only considered the x-direction and implicitly assumed that

$$|\psi\rangle = |\psi_x\rangle\,|\psi_y\rangle\,|\psi_z\rangle\,|\psi_{spin}\rangle \quad \Leftrightarrow \quad \psi(\vec{x},\sigma) = \psi_1(x)\,\psi_2(y)\,\psi_3(z)\,\psi_{spin}(\sigma) \ ,$$

i.e. that the state is also a product state with respect to x,y, and z coordinates. However, in general a quantum mechanical states will contain a *linear combination of product states* which cannot be factorized. In that case, one cannot simply treat coordinate space and spin (or polarization) separately. Such a non-factorizable linear combination is called an **entangled state** (see also ch. 10). It appears, for example, in the Stern-Gerlach experiment. Before the screen, the total state consists of an upper beam with spin-up particles and a lower beam with spin-down particles. This can be written as

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|\text{top},\uparrow\rangle + |\text{bottom},\downarrow\rangle\right).$$

To what extent can location and spin then still be treated separately ?

More generally on needs to ask in how far one can *describe a subsystem (e.g. a single particle) separately from the rest of the world*, even though it interacts with the world quantum mechanically.

It turns out that the question of how to describe an *unpolarized* beam of particles (e.g. photons) is closely related. This would be an ensemble of particles whose polarization has not been fixed (prepared, measured). A measurement of polarization on this ensemble should produce results $|e_x\rangle$ and $|e_y\rangle$ with equal probability, with respect to any basis $|e_x\rangle$, $|e_y\rangle$ of polarizations. One might be tempted to try a state like

$$|\psi\rangle \;=\; \frac{1}{\sqrt{2}}\left(\,|e_x\rangle + |e_y\rangle\,\right). \qquad \textbf{?}$$

However, this linear combination does *not* describe an unpolarized state, but instead a state with a different polarization, rotated by 45 degrees with respect to $|e_x\rangle$. Indeed, a state which is represented by any *vector* in Hilbert space (a so-called *pure state*) is not able to describe an unpolarized state.

The solution to these question requires an extension (re-writing) of the formalism of quantum mechanics, from pure states to so-called **mixed states**. We shall see that mixed states occur naturally when one studies a subsystem of a total system[1], which may itself be in a pure state $|\psi\rangle$, whenever the subsystem is *entangled* with the rest of the system. This is true for an arbitrary subset, e.g. the separate consideration of spins, or of a subset of particles. Mixed states are the most general quantum mechanical states. In a special case, they are equivalent to pure states.

Mixed states typically also contain parts which cannot interfere with each other (see below). Then the corresponding *probabilities* (instead of the probability *amplitudes*) are added, for example the probablities of finding some polarization $|e_x\rangle$ or $|e_y\rangle$.

Mixed states can also be used to describe a quantum mechanical system for which one does not know all properties. It turns out that mixed states have to be described by an *operator*, the so-called *density operator* (or by some matrix representation of this operator, the so-called density matrix), instead of by a vector in Hilbert space.
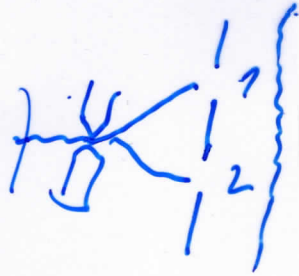
---

[1]e.g. the whole universe (?)

9.1 Expectation values for subsystems of an entangled pure state

We shall look at two examples. First we consider a double slit experiment with particles that all have spin $|\uparrow\rangle$. The state of the particles immediately after the screen is something like

$$|\psi_\uparrow\rangle = \frac{1}{\sqrt{2}} \Big(|\text{slit } 1,\uparrow\rangle + |\text{slit } 2,\uparrow\rangle \Big) \tag{9.1}$$

$$\equiv \frac{1}{\sqrt{2}} \Big(|\text{slit } 1\rangle + |\text{slit } 2\rangle \Big) \otimes |\uparrow\rangle, \tag{9.2}$$

where we have used the notation $|\text{slit } 1,\uparrow\rangle \equiv |\text{slit } 1\rangle \otimes |\uparrow\rangle$. The state $|\psi_\uparrow\rangle$ is a **product state** consisting of spatial and spin degrees of freedom. We calculate the probability $|\langle\psi_\uparrow|x\rangle|^2 = \langle\psi_\uparrow|x\rangle\langle x|\psi_\uparrow\rangle$ of finding the particles at a location x at the screen. It is equal to the expectation value of the operator $\hat{O}_x := |x\rangle\langle x|$:

$$\langle\psi_\uparrow|\hat{O}_x|\psi_\uparrow\rangle = \frac{1}{2} \langle\uparrow| \Big(\langle\text{slit } 1| + \langle\text{slit } 2| \Big) \hat{O}_x \Big(|\text{slit } 1\rangle + |\text{slit } 2\rangle \Big) |\uparrow\rangle$$

$$= \frac{1}{2} \Big(\langle\text{slit } 1| + \langle\text{slit } 2| \Big) \hat{O}_x \Big(|\text{slit } 1\rangle + |\text{slit } 2\rangle \Big)$$

because of $\langle\uparrow|\uparrow\rangle = 1$. The result does not contain the spin degree of freedom any more, that is we obtain the same result as when we ignore the spin from the start !

For the location, we will typically find quantum mechanical *interference* between the two beams, because of the terms $\langle\text{slit } 1| \hat{O}_x |\text{slit } 2\rangle$ and $\langle\text{slit } 2| \hat{O}_x |\text{slit } 1\rangle$.

As a second example we consider a Gedanken-experiment, in which the two beams of a Stern-Gerlach experiment hit the double-slit setup. The state at the screen is now

$$|\psi_{\uparrow\downarrow}\rangle = \frac{1}{\sqrt{2}} \Big(|\text{slit } 1,\uparrow\rangle + |\text{slit } 2,\downarrow\rangle \Big). \tag{9.3}$$

This is an **entangled state**, between the spatial degree of freedom and the spin, which cannot be written as a product state $|\psi_{\text{space}}\rangle \otimes |\psi_{\text{spin}}\rangle$.

The above spatial probability now becomes

$$
\begin{aligned}
\langle \psi_{\uparrow\downarrow} | \hat{O}_x | \psi_{\uparrow\downarrow} \rangle &= \frac{1}{2} \Big(\langle \text{slit } 1, \uparrow | + \langle \text{slit } 2, \downarrow | \Big) \hat{O}_x \Big(|\text{slit } 1, \uparrow\rangle + |\text{slit } 2, \downarrow\rangle \Big) \\
&= \frac{1}{2} \ \langle \text{slit } 1| \hat{O}_x |\text{slit } 1\rangle + \langle \text{slit } 2| \hat{O}_x |\text{slit } 2\rangle
\end{aligned}
$$

since $\langle \uparrow | \uparrow \rangle = 1$ and $\langle \uparrow | \downarrow \rangle = 0$. The mixed terms and thus the interference have *vanished* with this entangled state ! We obtain the two *classical indivi-dual probablities* for particles which have travelled through either the first or the second slit. This happens since particles at slit 1 (with spin $|\uparrow\rangle$) can-not interfere with those at slit 2 (with spin $|\downarrow\rangle$) because of the orthogonality $\langle \uparrow | \downarrow \rangle = 0$.

We see that for the description of subsystems *by themselves* we need a formalism which allows both interference as well as classical probabilities. We will come back to this example in ch. 9.5.4.

9.2 Density operator, mixed state

In order to motivate a suitable formalism, we first rewrite the usual quantum mechanical probabilites for a system in a pure state $|\psi\rangle$.

When measuring a state $|\psi\rangle$ with a hermitian operator $\hat{A} = \sum_i a_i |a_i\rangle\langle a_i|$, the probability to obtain a final state $|a_i\rangle$, and thus a measured value a_i, is according to postulate (2.15)

$$
W(a_i) = |\langle a_i | \psi \rangle|^2 = \langle a_i | \underbrace{|\psi\rangle\langle\psi|}_{\hat{\rho}_\psi} a_i \rangle . \tag{9.4}
$$

We see that this probability can be expressed with an operator $\hat{\rho}_\psi = |\psi\rangle\langle\psi|$. Different parts of $|\psi\rangle$ can interfere here.

In a mixed state such *probabilities* (9.4) will add up for several contributing pure states, instead of the probability *amplitudes*. The proper description for such mixed states is then a linear combination of operators like $\hat{\rho}_\psi$, namely the so-called

---

DENSITY OPERATOR (IN ITS SPECTRAL REPRESENTATION)

$$\hat{\rho} = \sum_{\nu} p_{\nu} |\varphi_{\nu}\rangle\langle\varphi_{\nu}| \quad \text{with} \quad \sum_{\nu} p_{\nu} = 1. \tag{9.5}$$

Here, $|\varphi_{\nu}\rangle$ are orthonormal vectors, namely the eigenvectors[2] of the hermitian operator $\hat{\rho}$, and the eigenvalues $p_{\nu} \in [0, 1]$ are weights for the contributing pure states $|\varphi_{\nu}\rangle$. This operator is also called **statistical operator** or **state operator** or **mixed state**.[3]

In another basis, $\{\tilde{\varphi}_{\nu}\}$, the operator $\hat{\rho}$ will have the generic form

$$\hat{\rho} = \sum_{\nu\nu'} \rho_{\nu\nu'} |\tilde{\varphi}_{\nu}\rangle\langle\tilde{\varphi}_{\nu'}| \tag{9.6}$$

with a hermitian matrix $\rho_{\nu\nu'}$. The density operator $\hat{\rho}$ contains the complete probability information of a quantum system. Its representation in some basis is the corresponding **density *matrix*** $\rho_{\nu\nu'}$, which becomes a diagonal matrix with entries p_{ν} in the eigenbasis.

For a system that was prepared in the mixed state $\hat{\rho}$, we now have the

---

PROBABILITY FOR OBTAINING THE RESULT a_j IN STATE $\hat{\rho}$

$$W(a_j) = \langle a_j| \hat{\rho} |a_j\rangle \equiv \sum_{\nu} p_{\nu} |\langle a_j|\varphi_{\nu}\rangle|^2. \tag{9.7}$$

---

when measuring with the operator $\hat{A}$. Calculation for the 2nd part:

$$\langle a_j|\hat{\rho}|a_j\rangle = \langle a_j| \sum_{\nu} p_{\nu} |\varphi_{\nu}\rangle\langle\varphi_{\nu}| |a_j\rangle = \sum_{\nu} p_{\nu} \langle a_j| |\varphi_{\nu}\rangle\langle\varphi_{\nu}| |a_j\rangle = \sum_{\nu} p_{\nu} |\langle a_j|\varphi_{\nu}\rangle|^2.$$

This is inded the weighted sum of probabilites for the individual contributing pures states $|\varphi_{\nu}\rangle$, with weights p_{ν}. The $\mathbf{p_{\nu}}$ **can therefore be interpreted as *probabilities*** for finding the state $|\varphi_{\nu}\rangle$ upon examining the mixed state $\hat{\rho}$, and the state $\hat{\rho}$ itself can be interpreted as a *statistical mixture*.

We can now use eq.A.25:

---

[2]The vectors of a spectral representation are non-unique within subspaces of constant eigenvalues. Within such a subspace they can be transformed by any unitary transformation.

[3]Note that the vector $|\psi\rangle$ for any pure state is determined only up to an overall phase factor which cancels in expectation values. Such a phase factor also cancels for $\hat{\rho}$, so that the density operator does not have a phase ambiguity.

$$\mathrm{tr}\,\hat{O}\,|\varphi\rangle\langle\psi| \;=\; \sum_n \langle n|\hat{O}|\varphi\rangle\langle\psi|n\rangle \;=\; \sum_n \langle\psi|n\rangle\langle n|\hat{O}|\varphi\rangle \;=\; \langle\psi|\hat{O}|\varphi\rangle$$

to obtain the expectation value of the operator $\hat{A}$ in the state $\hat{\rho}$:

$$\langle\hat{A}\rangle_\rho \;\equiv\; \sum_j a_j\,W(a_j) \;\overset{9.7}{=}\; \sum_j a_j\,\langle a_j|\hat{\rho}|a_j\rangle \;\overset{A.25}{=}\; \sum_j a_j\,\mathrm{tr}\,\hat{\rho}\,|a_j\rangle\langle a_j|$$

$$= \;\mathrm{tr}\left(\hat{\rho}\,\underbrace{\sum_j a_j\,|a_j\rangle\langle a_j|}_{=\hat{A}}\right) \;=\; \mathrm{tr}\left(\hat{\rho}\,\hat{A}\right).$$

This expectation value can also be expressed with the eigenstates $|\varphi_\nu\rangle$ of $\hat{\rho}$:

$$\langle\hat{A}\rangle_\rho \;\equiv\; \sum_j a_j\,W(a_j) \;\overset{9.7}{=}\; \sum_j a_j\,\sum_\nu p_\nu\,|\langle a_j|\varphi_\nu\rangle|^2$$

$$= \;\sum_\nu p_\nu\,\langle\varphi_\nu|\underbrace{\sum_j a_j|a_j\rangle\langle a_j|}_{\tilde{A}}|\varphi_\nu\rangle. \;=\; \sum_\nu p_\nu\,\langle\varphi_\nu|\hat{A}|\varphi_\nu\rangle.$$

Thus:

EXPECTATION VALUE OF AN OPERATOR $\hat{A}$ IN A STATE $\hat{\rho}$

$$\langle\hat{A}\rangle_\rho \;=\; \mathrm{tr}\left(\hat{\rho}\,\hat{A}\right) \;=\; \sum_\nu p_\nu\,\langle\varphi_\nu|\hat{A}|\varphi_\nu\rangle. \tag{9.8}$$

This relation is basis independent because if the invariance of the trace-operation. The special case $\hat{A} = \hat{\mathbb{1}}$ with $\langle\hat{\mathbb{1}}\rangle = 1$ shows that

$$\boxed{\mathrm{tr}\,\hat{\rho} \;=\; 1\,.} \tag{9.9}$$

9.2.1 Density operator for a pure state

The statistical operator for the special case of a pure state $|\psi\rangle$ is like $\hat{\rho}_\psi$ in eq. 9.4,

$$\boxed{\hat{\rho} = |\psi\rangle\langle\psi|} \qquad, \tag{9.10}$$

without a linear combination. The expectation value of some observable $\hat{A}$ then gets its familiar form again,

$$\langle\hat{A}\rangle = \langle\psi|\hat{A}|\psi\rangle\,. \tag{9.11}$$

How can one decide whether a given density operator $\hat{\rho}$ represents a pure state ? There are several possibilities. One unique criterion is the form (9.10), i.e., one of the eigenvalues of ρ is unity (and all others are zero). Conversely, the density operator for a non-pure state can only be written as a linear combination of *several* terms of the form (9.10).

Another necessary and sufficient condition for a pure state is

$$\boxed{\hat{\rho}^2 = \hat{\rho}} \qquad . \tag{9.12}$$

This condition is necessary, since it is immediately implied by eq. 9.10. The spectral decomposition $\hat{\rho}$ implies that it is also sufficient. Another necessary and sufficient condition is the weaker looking relation

$$\sum_\nu p_\nu^2 = \qquad \mathrm{tr}\,\hat{\rho}^2 = 1. \qquad \textit{(basis indep. !)} \tag{9.13}$$

The *matrix representation* of $\hat{\rho}$ (=density matrix) in a basis in which $|\psi\rangle$ is the first basis vector is simply

pure state

$$\rho \,\hat{=}\, \begin{pmatrix} 1 & 0 & \dots \\ 0 & 0 & \dots \\ \dots & \dots & \dots \end{pmatrix} \qquad . \tag{9.14}$$

In another basis, $|\psi\rangle$ will be a linear combination, e.g.,

$$|\psi\rangle = c_1 |1\rangle + c_2 |2\rangle . \tag{9.15}$$

The density operator of this pure state is

$$\hat{\rho}_0 = |\psi\rangle\langle\psi| = \left(c_1 |1\rangle + c_2 |2\rangle \right)\left(c_1^* \langle 1| + c_2^* \langle 2| \right)$$

$$\hat{=}\, \begin{pmatrix} |c_1|^2 & c_1 c_2^* \\ c_1^* c_2 & |c_2|^2 \end{pmatrix}, \tag{9.16}$$

where the last expression is the matrix representation in the basis $|1\rangle, |2\rangle$. **Interference** can appear in some observable $\hat{A}$ via mixed matrix elements like $\langle 1|\hat{A}|2\rangle = \mathrm{tr}\left(\hat{A} |2\rangle\langle 1| \right)$ i.e. via the off-diagonal matrix elements $c_1 c_2^*$ and $c_1^* c_2$.

$$\mathrm{tr}\left(\hat{\sigma} |\psi\rangle\langle\varphi| \right) = \langle\varphi|\hat{\sigma}|\psi\rangle$$

9.2.2 Schrödinger equation for a mixed state

The time evolution of pure states $|\psi\rangle$ implies the evolution of the mixed states. We begin with the density operator for a pure state $\hat{\rho} = |\psi\rangle\langle\psi|$ and use $\hat{H} = \hat{H}^\dagger$.

$$
\begin{aligned}
i\hbar\frac{d}{dt}\hat{\rho} = i\hbar\frac{d}{dt}\left(|\psi\rangle\langle\psi|\right) &= \left(i\hbar\frac{d}{dt}|\psi\rangle\right)\langle\psi| + |\psi\rangle\left(i\hbar\frac{d}{dt}\langle\psi|\right) \\
&= \left(i\hbar\frac{d}{dt}|\psi\rangle\right)\langle\psi| - |\psi\rangle\left(i\hbar\frac{d}{dt}|\psi\rangle\right)^\dagger \\
&= \hat{H}\left(|\psi\rangle\langle\psi|\right) - |\psi\rangle\left(\hat{H}|\psi\rangle\right)^\dagger \\
&= \hat{H}\left(|\psi\rangle\langle\psi|\right) - \left(|\psi\rangle\langle\psi|\right)\hat{H}^\dagger \\
&= \hat{H}\hat{\rho} - \hat{\rho}\hat{H}^\dagger = \left[\hat{H},\hat{\rho}\right] \quad .
\end{aligned}
$$

$H^\dagger = H$

The density operator for a general mixed state is a linear combination of density operators for pure states. Therefore the Schrödinger equation for a general density operator has the same form:

TIME EVOLUTION OF A DENSITY OPERATOR $\hat{\rho}$

$$
i\hbar\frac{d}{dt}\hat{\rho}(t) = [\hat{H},\hat{\rho}(t)] \quad . \tag{9.17}
$$

9.3 Unpolarized state

How can one now describe an unpolarized state ? The proper description is the *mixed state*

$$
\hat{\rho} = \frac{1}{2}|e_x\rangle\langle e_x| + \frac{1}{2}|e_y\rangle\langle e_y| . \tag{9.18}
$$

The probabilities (9.7) $W(x) = \langle e_x|\hat{\rho}|e_x\rangle = \frac{1}{2}$ and $W(y) = \langle e_y|\hat{\rho}|e_y\rangle = \frac{1}{2}$ are then indeed equal.

Note that in eq. 9.18 the density operator $\hat{\rho}$ for an unpolarized ensemble is just the (suitably normalized) *identity operator* ! Therefore one can also write it in every other basis:

$$\hat{\rho} = \frac{1}{2}\hat{\mathbb{1}} = \frac{1}{2}|e_{x'}\rangle\langle e_{x'}| + \frac{1}{2}|e_{y'}\rangle\langle e_{y'}| . \qquad (9.19)$$

The polarization in this mixed state is therefore zero with respect to any basis.

9.4 Incomplete preparation

A real quantum mechanical system usually has many degrees of freedom. A typical preparation fixes only some of them (e.g. location at a slit) but not others (e.g. the polarization of a beam which goes through a double slit experiment).

In order to simplify the notation, in this section we will concentrate on the double-slit setup and treat only the degrees of freedom of the slit (basis vectors $|s_1\rangle, |s_2\rangle$) and polarisation (basis vectors $|e_x\rangle, |e_y\rangle$). How can one describe an ensemble of particles which have passed through slit 1 and are not polarized ? If both slit 1 *and* a polarization, say $|e_x\rangle$, had been measured, then the system would be in the pure state $|e_x, s_1\rangle$, equivalently described by the density operator $|e_x, s_1\rangle\langle e_x, s_1| .$

In order to describe the unpolarized situation, we need to sum over polarizations like in section 9.3. Thus the unpolarized beam through slit 1 is represented by the mixed state with density matrix

$$\hat{\rho} = \frac{1}{2}\sum_i |e_i, s_1\rangle\langle e_i, s_1| = \frac{1}{2}\left(\sum_i |e_i\rangle\langle e_i|\right) \otimes |s_1\rangle\langle s_1| \qquad (9.20)$$

This state is a *product* of a state in the space of polarizations (mixed) and a state in real space (slit, pure). When one only looks at location and does not measure polarizations, the this state can be treated as the pure state $|\psi_s\rangle = |s_1\rangle$ (see also ch. 9.5.2). The same is true for a linear combination of pure states $|\psi_s\rangle = c_1|s_1\rangle + c_2|s_2\rangle$, as long as location and spin are not entangled. This is why we were able to ignore polarisation in the original treatment of the double slit experiment.

9.5 Reduced density matrix

We will now treat the general case, with many degrees of freedom. Let us describe the total system as consisting of an "environment" with quantum numbers (degrees of freedom) $u^{(1)}, u^{(2)}, \ldots$ and the actual smaller "system" of interest, with degrees of freedom $s^{(1)}, s^{(2)}, \ldots$. In order to simplify notation, we shall write u for $u^{(1)}, u^{(2)}, \ldots$ and s for $s^{(1)}, s^{(2)}, \ldots$. Note that the strength of interaction and entanglement between "system" and "environment" is arbitrary. The most general state of the total system is represented by the density operator

$$\hat{\rho}_{us} = \sum_{u,u'} \sum_{s,s'} \rho_{uu'ss'} \, |u,s\rangle\langle u',s'| \; . \tag{9.21}$$

with $|u,s\rangle \equiv |u\rangle|s\rangle$ and $\langle u,s|u',s'\rangle = \delta_{uu'}\,\delta_{ss'}$. We now consider an operator $\hat{A}$, which only acts on the "system" s, i.e., $\hat{A}|u\rangle|s\rangle = |u\rangle\left(\hat{A}|s\rangle\right)$ and $\hat{A} = \hat{\mathbb{1}}_u \otimes \left(\sum_{ss'} A_{ss'}|s\rangle\langle s'|\right)$. For such an operator, the expectation value can be simplified. We shall write tr_u for the trace in the space of environment variables u, and similarly tr_s, resp. tr_{us}. Then

$$\langle \hat{A}\rangle_s = \mathrm{tr}_{us}\,\hat{\rho}_{us}\,\hat{A} = \mathrm{tr}_s\left(\mathrm{tr}_u\,\hat{\rho}_{us}\hat{A}\right) = \mathrm{tr}_s\underbrace{\left(\mathrm{tr}_u\,\hat{\rho}_{us}\right)}_{\tilde{\rho}_s}\hat{A} \; .$$

$$\boxed{\langle \hat{A}\rangle_s = \mathrm{tr}_s\,\tilde{\rho}_s\,\hat{A} \; .} \tag{9.22}$$

We see: $\langle \hat{A}\rangle$ can be written like an expectation value in an isolated "system" (!), with a trace only over the degrees of freedom of the system, but with the

---

REDUCED DENSITY OPERATOR

$$\tilde{\rho}_s = \mathrm{tr}_u\,\hat{\rho}_{us}\,, \quad \text{with matrix elements } \tilde{\rho}_{ss'} = \sum_u \rho_{uuss'}\,, \tag{9.23}$$

---

which contains the influence of the environment in the matrix elements $\tilde{\rho}_{ss'}$.[4] Note that this simplification is independent of the strength of interaction between system and environment !

We shall now look at some examples of reduced density matrices.

---

[4]When ρ_{us} is diagonal in the basis $|u,s\rangle$, i.e. $\rho_{uu'ss'} = p_{us}\,\delta_{uu'}\,\delta_{ss'}$, then $\tilde{\rho}_{ss'} = \sum_u p_{us}\,\delta_{ss'}$.

9.5.1 Heat bath

We consider a system in contact with an external "heat bath" at fixed temperature T. Often one can neglect the details of the interaction with the bath, except for the effect of the temperature, which is to weight all states of the system by

$$\widetilde{p}_i \; \propto \; \exp(-\frac{E_i}{k_B T}) \tag{9.24}$$

(Boltzmann weight) depending on the energy E_i of the state. This can again be interpreted as a statistical mixture.

9.5.2 Independent system

The special situation in which the "system" and "environment" are in completely independent states is describe by weights $\rho_{uu'ss'}$ which factorize

$$\rho_{uu'ss'} \; = \; \rho_{uu'} \, \rho_{ss'} \, . \tag{9.25}$$

One can normalize them separately, $\mathrm{tr}_u \rho_{uu'} = \mathrm{tr}_s \rho_{ss'} = 1$. Then

$$\hat{\rho}_{us} \; = \; \widetilde{\hat{\rho}}_u \, \widetilde{\hat{\rho}}_s \, , \tag{9.26}$$

with $\widetilde{\rho}_{uu'} = \rho_{uu'}$ and $\widetilde{\rho}_{ss'} = \rho_{ss'}$. The environment now has no influence at all on the reduced density matrix and on expectation values of operators which act only on the system; it can therefore be ignored. Environment and system each can be in pure or mixed states. We considered an example in ch. 9.4.

When the system and environment do not interact, then the Hamilton operator has the form $\hat{H} = \hat{H}_u \otimes \hat{\mathbb{1}}_s + \hat{\mathbb{1}}_u \otimes \hat{H}_s$. Then the reduced density matrix obeys (see eq. 9.17)

$$i\hbar \frac{d}{dt} \widetilde{\rho}_s(t) \; = \; [\hat{H}_s, \widetilde{\rho}_s(t)] \tag{9.27}$$

and system and environment will remain independent.[5] In earlier chapters we implicitly assumed such an independence.

---

[5]Note, however, that in general, the reduced density matrix does *not* have a simple unitary time evolution !

257

9.5.3 Product state

A special case of independent systems occurs when the total system is in a pure state which is a product state between environment and subsystem:

$$|\psi\rangle = |\psi_u\rangle |\psi_s\rangle . \qquad (9.28)$$

Then the reduced density operator is simply

$$\widetilde{\rho}_s = \mathrm{tr}_u \left(|\psi_u\rangle|\psi_s\rangle\langle\psi_s|\langle\psi_u| \right) = \langle\psi_u|\psi_u\rangle |\psi_s\rangle\langle\psi_s| = |\psi_s\rangle\langle\psi_s| , \quad (9.29)$$

i.e., the "system" is again independent, and even in a pure state itself.

9.5.4 Entangled state

We will treat once more an example similar to ch. 9.1, this time with a reduced density matrix.

Let the total system be in a pure but entangled state, e.g.

$$|\psi\rangle = \frac{1}{\sqrt{2}} \left(|1_u, 0_s\rangle + |0_u, 1_s\rangle \right) . \qquad (9.30)$$

Then the density operator is

$$\hat{\rho}_{us} = |\psi\rangle\langle\psi| = \frac{1}{2} \left(|1_u, 0_s\rangle + |0_u, 1_s\rangle \right) \left(\langle 1_u, 0_s| + \langle 0_u, 1_s| \right)$$

and the reduced density matrix for the (sub-)system becomes (using $\langle u|u'\rangle = \delta_{uu'}$) (orthonormality of basis vectors)

$$\widetilde{\rho}_s = \mathrm{tr}_u \, \hat{\rho}_{us} = \sum_{u=0_u, 1_u} \langle u| \hat{\rho} |u\rangle = \frac{1}{2} \left(|0_s\rangle \langle 0_s| + |1_s\rangle \langle 1_s| \right) . \quad (9.31)$$

The matrix representation is

$$\widetilde{\rho}_s = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} .$$

Thus when the total system is in a pure state, but entangled between environment and sub-system, then the reduced density operator for the sub-system is **mixed** (since $\widetilde{\rho}^2 = \frac{1}{2}\widetilde{\rho} \neq \widetilde{\rho}$), without off-diagonal interference terms !

A.12.4 Pure states with several degrees of freedom

Real physical systems have many degrees of freedom. In real space each particle has three coordinates, and may also have spin and other internal degrees of freedom.

The total Hilbert space is then the **tensor product** of the individual spaces: Let $\{|e_A\rangle\}$, $\{|e_B\rangle\}, \ldots$ be orthonormal basis vectors for the property $A, B, \ldots$ (e.g. $\{|x\rangle\}$, $\{|y\rangle\}, \ldots$). Then

$$|e_A, e_B, \ldots\rangle \equiv |e_A\rangle \otimes |e_B\rangle \ldots \equiv |e_A\rangle |e_B\rangle \ldots \qquad (A.188)$$

are the basis states of the total Hilbert space (as already mentioned in ch. (4.4)), with the scalar product

$$\langle e_A, e_B, \ldots | e_{A'}, e_{B'}, \ldots \rangle = \langle e_A | e_{A'} \rangle \cdot \langle e_B | e_{B'} \rangle \ldots = \delta_{A,A'} \, \delta_{B,B'} \ldots , \qquad (A.189)$$

and **a general state in this Hilbert space is a linear combination of these basis vectors**. The operator

$$|e_A, e_B, \ldots\rangle\langle e_A, e_B, \ldots|$$

is a projection operator onto one of the basis states. The sum of all such projection operators is the identity operator in the total Hilbert space:

$$\sum_A \sum_B \sum_{\ldots} |e_A, e_B, \ldots\rangle\langle e_A, e_B, \ldots| = \hat{\mathbb{1}} . \qquad (A.190)$$

An **operator $\hat{O}_A$, which acts only in a subspace**

$$\hat{O}_A |e_A, e_B, \ldots\rangle = \left(\hat{O}_A |e_A\rangle \right) \otimes |e_B\rangle \otimes \ldots \qquad (A.191)$$

has the matrix elements

$$\langle e_A, e_B, \ldots | \hat{O}_A | e_{A'}, e_{B'}, \ldots \rangle = \langle e_A | \hat{O}_A | e_{A'} \rangle \cdot \underbrace{\langle e_B | e_{B'} \rangle}_{\delta_{B,B'}} \ldots . \qquad (A.192)$$

in the given basis. In general, however, an operator (e.g. the Hamilton operator) acts on several degrees of freedom, and it can create **entanglement** between them, like

$$\frac{1}{\sqrt{2}} \left(|\text{location}_1, \text{spin}_1\rangle + |\text{location}_2, \text{spin}_2\rangle \right) \qquad (A.193)$$

In this state, space and spin are correlated (entangled), similar to the Stern-Gerlach experiment.