2 The Density Operator

In this chapter we introduce the density operator, which provides an alternative way to describe the state of a quantum mechanical system. So far we have only dealt with situations where the state of a system was perfectly known (in a quantum mechanical sense). But, as we will see, the density operator is especially well suited for applications when the information available on a given system is incomplete.

Most of the material presented in this chapter is taken from Auletta, Fortunato and Parisi, Chap. 5, and Cohen-Tannoudji, Diu and Laloë, Vol. I, Complement E_{III}.

2.1 Pure States

We already know for the material covered in Chapter 1 that the state of a quantum mechanical system can be described by a ket

$$|\psi(t)\rangle = \sum_j c_j(t) |u_j\rangle, \tag{2.1}$$

where $\{|u_j\rangle\}$ is a suitable basis for the corresponding space. In such cases the information on the system is complete. Because $|\psi(t)\rangle$ is normalized we also have

$$\sum_j |c_j(t)|^2 = 1. \tag{2.2}$$

We further know that the matrix elements of an operator $\hat{O}$ are given by

$$O_{ij} = \left\langle u_i \left| \hat{O} \right| u_j \right\rangle \tag{2.3}$$

and the expected value for the operator is calculated with

$$\begin{aligned} \left\langle \hat{O} \right\rangle_\psi(t) &= \left\langle \psi(t) \left| \hat{O} \right| \psi(t) \right\rangle \\ &= \sum_{i,j} c_i^*(t) c_j(t) O_{ij}. \end{aligned} \tag{2.4}$$

Finally, the dynamic evolution of the system is governed by the Schrödinger equation (see equation (1.52)).

A quick examination of equations (2.1) and (2.4) reveals that the product $c_i^*(t) c_j(t)$ is a matrix element of the operator $|\psi(t)\rangle\langle\psi(t)|$ since

$$\langle u_j \,|\, \psi(t) \rangle \langle \psi(t) \,|\, u_i \rangle = c_j(t)\, c_i^*(t). \tag{2.5}$$

We therefore introduce the **density operator**

$$\hat{\rho}(t) \equiv |\psi(t)\rangle\langle\psi(t)|. \tag{2.6}$$

Since $\hat{\rho}(t)$ is constructed from the ket defining the state of the system, we should not be surprised that it presents us with an alternative way calculating the relevant quantities characterizing that states (e.g., equations (2.2)-(2.4) above). Indeed, the following relations can be readily verified

$$
\begin{aligned}
\mathrm{Tr}\left(\hat{\rho}(t)\right) &= \sum_j \rho_{jj}(t) \\
&= \sum_j \langle u_j \,|\, \psi(t)\rangle \langle \psi(t) \,|\, u_j\rangle \\
&= \sum_j |c_j(t)|^2 \\
&= 1
\end{aligned}
\tag{2.7}
$$

for the normalization condition, and

$$
\begin{aligned}
\mathrm{Tr}\left(\hat{\rho}(t)\hat{O}\right) &= \sum_j \left\langle u_j \left| \hat{\rho}(t)\hat{O} \right| u_j \right\rangle \\
&= \sum_{j,k} \langle u_j \,|\, \hat{\rho}(t) \,|\, u_k\rangle \left\langle u_k \left| \hat{O} \right| u_j \right\rangle \\
&= \sum_{j,k} \rho_{jk}(t) \left\langle u_k \left| \hat{O} \right| u_j \right\rangle \\
&= \sum_{j,k} c_j(t)\, c_k^*(t) \left\langle u_k \left| \hat{O} \right| u_j \right\rangle \\
&= \left\langle \psi(t) \left| \hat{O} \right| \psi(t) \right\rangle \\
&= \left\langle \hat{O} \right\rangle_\psi (t)
\end{aligned}
\tag{2.8}
$$

for the average of an observable (note also that $\mathrm{Tr}\left(\hat{\rho}(t)\hat{O}\right) = \mathrm{Tr}\left(\hat{O}\hat{\rho}(t)\right)$).

The time evolution of $\hat{\rho}(t)$ is easily calculated by taking its time derivative and using the Schrödinger equation (equation (1.52))

$$\frac{d}{dt}\hat{\rho}(t) = \left(\frac{d}{dt}|\psi(t)\rangle\right)\langle\psi(t)| + |\psi(t)\rangle\left(\frac{d}{dt}\langle\psi(t)|\right)$$

$$= \frac{1}{i\hbar} \left[\hat{H}(t) |\psi(t)\rangle\langle\psi(t)| - |\psi(t)\rangle\langle\psi(t)| \hat{H}(t) \right]$$

$$= \frac{1}{i\hbar} \left[\hat{H}(t), \hat{\rho}(t) \right], \tag{2.9}$$

which is reminiscent of the Heisenberg equation (although not exactly the same; it is usually referred to as the **von Neumann equation**). Indeed, we should note that every relations derived done so far were calculated in the Schrödinger representation (i.e., $|\psi(t)\rangle \equiv |\psi_{\mathrm{S}}(t)\rangle$ and $\hat{\rho}(t) \equiv \hat{\rho}_{\mathrm{S}}(t)$). However, it is interesting to note that in the Heisenberg representation the density operator does not depend on time since

$$\begin{aligned} \hat{\rho}_{\mathrm{H}}(t) &= \hat{U}_t^\dagger \hat{\rho}(t) \hat{U}_t \\ &= \hat{U}_t^\dagger |\psi(t)\rangle\langle\psi(t)| \hat{U}_t \\ &= |\psi(0)\rangle\langle\psi(0)| \\ &= \hat{\rho}(0), \end{aligned} \tag{2.10}$$

where equations (1.177)-(1.181) were used.

Another important relation is for the probability that a measurement yields the eigenvalue o_j of $\hat{O}$, which can be calculated with

$$\begin{aligned} \mathcal{P}(o_j) &= |c_j|^2 \\ &= \langle \psi(t) \, | \, u_j \rangle \langle u_j \, | \, \psi(t) \rangle \\ &= \left\langle \psi(t) \left| \hat{P}_j \right| \psi(t) \right\rangle \\ &= \mathrm{Tr}\left(\hat{\rho}(t) \hat{P}_j \right), \end{aligned} \tag{2.11}$$

from equation (2.8) with $\hat{P}_j$ the projector on the subspace covered by the eigenvalue o_j.

It is interesting to note some of the properties of the density operator. Namely, the relations involving it are linear in its dependency (see equations (2.7)-(2.11)), contrarily to the ket $|\psi(t)\rangle$ that appears twice in the corresponding expressions. Also, we can verify that $\hat{\rho}(t)$ is an Hermitian operator since

$$\begin{aligned} \rho_{ij}^\dagger(t) &= \rho_{ji}^*(t) \\ &= \langle u_j \, | \, \hat{\rho}(t) \, | \, u_i \rangle^* \\ &= \left[\langle u_j \, | \, \psi(t) \rangle \langle \psi(t) \, | \, u_i \rangle \right]^* \\ &= \langle \psi(t) \, | \, u_j \rangle \langle u_i \, | \, \psi(t) \rangle \\ &= \langle u_i \, | \, \psi(t) \rangle \langle \psi(t) \, | \, u_j \rangle \\ &= \rho_{ij}(t). \end{aligned} \tag{2.12}$$

This last property implies that, although the matrix associated to the density operator contains off-diagonal elements when expressed in the basis $\{|u_j\rangle\}$ since

$$\begin{aligned}
\hat{\rho}\,(t) &= |\psi\,(t)\rangle\langle\psi\,(t)| \\
&= \sum_{i,j} c_i^*\,(t)\,c_j\,(t)\,|u_i\rangle\langle u_j|\,,
\end{aligned} \tag{2.13}$$

it is always possible possible to diagonalize it through a unitary transformation to another basis $\{|v_j\rangle\}$ such that

$$\hat{\rho}\,(t) = \sum_{j} p_j\,(t)\,|v_j\rangle\langle v_j|\,, \tag{2.14}$$

with $p_j\,(t)$ the "weight" or eigenvalue associated to the subspace j (see equation (1.21) in Chapter 1).

Finally, we can also verify that

$$\begin{aligned}
\hat{\rho}^2\,(t) &= \hat{\rho}\,(t) \tag{2.15} \\
\mathrm{Tr}\,\big(\hat{\rho}^2\,(t)\big) &= 1\,, \tag{2.16}
\end{aligned}$$

which can evidently be extended to higher exponents.

2.2 Statistical Mixtures of States (Mixed States)

It is often the case that only partial information is available on a quantum mechanical system, in contrast with the situation covered in the last section. More precisely, the coefficient $c_j\,(t)$ in the expansion for $|\psi\,(t)\rangle$ in equation (2.1) will not be known. Rather, probabilities p_j that a system is in a given state $|\psi_j\rangle$ are to be relied upon to statistically describe its state and evolution. It is important to note that the fact that we do not know the coefficients $c_j\,(t)$ makes it impossible to establish a "statistical average" for the state $|\psi\,(t)\rangle$. However, perhaps a generalization of the density operator introduced for pure states in the previous section can be used in such a fashion.

In general, there can be a number of probabilities p_j and associated states $|\psi_j\rangle$ known to be occupied by the system $|\psi\,(t)\rangle$, with the condition that

$$\sum_{j} p_j = 1\,. \tag{2.17}$$

It is important to note that the different states $|\psi_j\rangle$ are not required to be orthogonal to one another, as is the case for pure states. This description of a quantum mechanical system is said to result from a ***statistical mixture of states*** or ***mixed states***, for short.

As was done with the calculations leading to equation (2.11), we could inquire as to what would the probability $\mathcal{P}\,(o_k)$ be of measuring the eigenvalue o_k for an observable $\hat{O}$. When the system is in the $|\psi_j\rangle$ state this probability would be, using equation (2.11),

$$
\begin{aligned}
\mathcal{P}_j\left(o_k\right) &= \left\langle \psi_j \left| \hat{P}_k \right| \psi_j \right\rangle \\
&= \operatorname{Tr}\left(\hat{\rho}_j \hat{P}_k\right),
\end{aligned}
\tag{2.18}
$$

where $\hat{\rho}_j = |\psi_j\rangle\langle\psi_j|$. Using this equation and our limited knowledge concerning the state of the system we can write the probability $\mathcal{P}\left(o_k\right)$ of measuring the eigenvalue o_k as the following weighted average

$$
\begin{aligned}
\mathcal{P}\left(o_k\right) &= \sum_j p_j \mathcal{P}_j\left(o_k\right) \\
&= \sum_j p_j \operatorname{Tr}\left(\hat{\rho}_j \hat{P}_k\right) \\
&= \sum_{j,m,n} p_j\left(\hat{\rho}_j\right)_{mn}\left(\hat{P}_k\right)_{nm} \\
&= \sum_{m,n}\left(\sum_j p_j \hat{\rho}_j\right)_{mn}\left(\hat{P}_k\right)_{nm} \\
&= \operatorname{Tr}\left(\sum_j p_j \hat{\rho}_j \hat{P}_k\right).
\end{aligned}
\tag{2.19}
$$

Referring once again to equation (2.11) for the case of a pure state, we now write

$$
\mathcal{P}\left(o_k\right) = \operatorname{Tr}\left(\hat{\tilde{\rho}} \hat{P}_k\right),
\tag{2.20}
$$

where we introduced the density operator for a statistical mixture of states

$$
\hat{\tilde{\rho}} = \sum_j p_j \hat{\rho}_j.
\tag{2.21}
$$

We therefore see that the mixed state density operator $\hat{\tilde{\rho}}$ is a weighted average of the pure state density operators $\hat{\rho}_j$.

This mixed states density operator shares many properties of its counterpart for a pure state. More precisely, we can easily verify that

$$
\begin{aligned}
\operatorname{Tr}\left(\hat{\tilde{\rho}}\right) &= \operatorname{Tr}\left(\sum_j p_j \hat{\rho}_j\right) \\
&= \sum_j p_j \operatorname{Tr}\left(\hat{\rho}_j\right) \\
&= \sum_j p_j \\
&= 1,
\end{aligned}
\tag{2.22}
\tag{2.23}
$$

where we used equations (2.7) and (2.17), and

$$
\begin{aligned}
\left\langle \hat{O} \right\rangle &= \sum_k o_k \mathcal{P}_k \left(o_k \right) \\
&= \sum_k o_k \mathrm{Tr} \left(\hat{\tilde{\rho}} \hat{P}_k \right) \\
&= \mathrm{Tr} \left(\hat{\tilde{\rho}} \sum_k o_k \hat{P}_k \right) \\
&= \mathrm{Tr} \left(\hat{\tilde{\rho}} \hat{O} \right),
\end{aligned}
\tag{2.24}
$$

where equations (2.20) and (1.21) were used.

We have so far avoided any explicit mention of dynamical evolution and, therefore, assumed that the previous calculations were effected at a given time t_0 such that $|\psi_j\rangle \equiv |\psi_j (t_0)\rangle$. If $\hat{H}(t)$ is the Hamiltonian of the system, then the initial state $|\psi_j (t_0)\rangle$ at t_0 will evolve into $|\psi_j (t)\rangle$ at time t according to the Schrödinger equation. That is, at time $t = t_0 + dt$ we have (to first order) $|\psi_j (t)\rangle = |\psi_j (t_0)\rangle + d |\psi_j (t_0)\rangle$, with

$$
d |\psi_j (t_0)\rangle = \frac{1}{i\hbar} \hat{H}(t_0) |\psi_j (t_0)\rangle \, dt,
\tag{2.25}
$$

and so on as time evolves. Accordingly, the time-dependent density operator will be

$$
\hat{\tilde{\rho}}(t) = \sum_j p_j \hat{\rho}_j (t),
\tag{2.26}
$$

where $\hat{\rho}_j (t) = |\psi_j (t)\rangle \langle \psi_j (t)|$. It should be clear from equation (2.25) that, in general, $|\psi_j (t)\rangle \neq |\psi_j (t_0)\rangle$ and thus $\hat{\tilde{\rho}}(t) \neq \hat{\tilde{\rho}}(t_0)$. It follows that, combining equation (2.9) for the time evolution of $\hat{\rho}_j (t)$ for the corresponding pure state with the linearity property of $\hat{\tilde{\rho}}(t)$ in equation (2.26), we have

$$
\frac{d}{dt} \hat{\tilde{\rho}}(t) = \frac{1}{i\hbar} \left[\hat{H}(t), \hat{\tilde{\rho}}(t) \right].
\tag{2.27}
$$

The mixed state density operator has therefore the same time evolution equation (in form) as its pure state counterpart. It is straightforward to show that because of its linearity property the mixed state density operator is also Hermitian

$$
\begin{aligned}
\tilde{\rho}_{ij}^\dagger (t) &= \sum_k p_k^* \left(\hat{\rho}_k^\dagger \right)_{ij} (t) \\
&= \sum_k p_k \left(\hat{\rho}_k \right)_{ij} (t) \\
&= \tilde{\rho}_{ij} (t),
\end{aligned}
\tag{2.28}
$$

since the probabilities p_k are real and $\rho^\dagger (t) = \rho (t)$.

In fact, the only properties of $\hat{\tilde{\rho}}(t)$ (mixed states) that differ from those of $\hat{\rho}(t)$ (pure state) are $\hat{\tilde{\rho}}^2(t) \neq \hat{\tilde{\rho}}(t)$ and $\mathrm{Tr}\left(\hat{\tilde{\rho}}^2(t)\right) \leq 1$. The first of these relations can be proven starting with

$$
\begin{aligned}
\hat{\tilde{\rho}}^2(t) &= \sum_{j,k} p_j p_k \hat{\rho}_j(t) \hat{\rho}_k(t) \\
&= \sum_{j,k} p_j p_k \left|\psi_j(t)\right\rangle \left\langle\psi_j(t) \,\middle|\, \psi_k(t)\right\rangle \left\langle\psi_k(t)\right|.
\end{aligned}
\tag{2.29}
$$

If we define, with $\{|u_m\rangle\}$ some basis,

$$
\left|\psi_j(t)\right\rangle = \sum_m c_{j,m}(t) \left|u_m\right\rangle,
\tag{2.30}
$$

then

$$
\begin{aligned}
\left\langle\psi_j(t) \,\middle|\, \psi_k(t)\right\rangle &= \sum_m c_{j,m}^*(t) c_{k,m}(t) \\
&\leq 1,
\end{aligned}
\tag{2.31}
$$

for $\sum_m c_{j,m}^*(t) c_{k,m}(t) = 1$ when $j = k$, and $\sum_m c_{j,m}^*(t) c_{k,m}(t) = 0$ when $|\psi_j(t)\rangle$ and $|\psi_k(t)\rangle$ are orthogonal. Inserting these two relations in equation (2.29) we have

$$
\hat{\tilde{\rho}}^2(t) = \sum_j p_j^2 \hat{\rho}_j(t) + \sum_{j,k \neq j} p_j p_k \left[\sum_m c_{j,m}^*(t) c_{k,m}(t)\right] |\psi_j(t)\rangle\langle\psi_k(t)|.
\tag{2.32}
$$

It is clear from this equation that (e.g., $p_j \neq p_j^2 \leq 1$)

$$
\hat{\tilde{\rho}}^2(t) \neq \hat{\tilde{\rho}}(t).
\tag{2.33}
$$

The second relation follows from

$$
\begin{aligned}
\mathrm{Tr}\left(\hat{\tilde{\rho}}^2(t)\right) &= \mathrm{Tr}\left(\sum_{j,k} p_j p_k \left|\psi_j(t)\right\rangle \left\langle\psi_j(t) \,\middle|\, \psi_k(t)\right\rangle \left\langle\psi_k(t)\right|\right) \\
&= \sum_{j,k} p_j p_k \left[\sum_m c_{j,m}^*(t) c_{k,m}(t)\right] \mathrm{Tr}\left(|\psi_j(t)\rangle\langle\psi_k(t)|\right) \\
&= \sum_{j,k} p_j p_k \left[\sum_m c_{j,m}^*(t) c_{k,m}(t)\right] \left[\sum_{p,q} c_{j,p}(t) c_{k,q}^*(t) \mathrm{Tr}\left(|u_p\rangle\langle u_q|\right)\right] \\
&= \sum_{j,k} p_j p_k \left[\sum_m c_{j,m}^*(t) c_{k,m}(t)\right] \left[\sum_{p,q} c_{j,p}(t) c_{k,q}^*(t) \delta_{pq}\right]
\end{aligned}
$$

$$= \sum_{j,k} p_j p_k \left[\sum_m c_{j,m}^* (t) \, c_{k,m} (t) \right] \left[\sum_p c_{j,p} (t) \, c_{k,p}^* (t) \right]$$

$$= \sum_{j,k} p_j p_k \left| \sum_m c_{j,m}^* (t) \, c_{k,m} (t) \right|^2$$

$$\leq \sum_{j,k} p_j p_k$$

$$\leq \left(\sum_j p_j \right)^2$$

$$\leq 1 \tag{2.34}$$

since $\left| \sum_m c_{j,m}^* (t) \, c_{k,m} (t) \right|^2 \leq 1$.

Finally, given an arbitrary vector $|\varphi\rangle$ we find

$$\begin{aligned} \left\langle \varphi \left| \hat{\tilde{\rho}} (t) \right| \varphi \right\rangle &= \sum_j p_j \left\langle \varphi \,|\, \hat{\rho}_j (t) \,|\, \varphi \right\rangle \\ &= \sum_j p_j \left| \left\langle \varphi \,|\, \psi_j (t) \right\rangle \right|^2 \\ &\geq 0, \end{aligned} \tag{2.35}$$

which implies that the expectation value of mixed density operator is positive (and real).

2.3 Physical Interpretation of the Density Matrix

Since the properties of the density operator are basically the same whether it relates to pure or mixed states, we will refrain from differentiating between the two types and use $\hat{\rho} (t)$ whatever the case. It is, however, understood that the notation $\hat{\rho}_j (t)$ refers to a pure state, which can be part of an overarching density operator in the manner of equation (2.26) (replacing $\hat{\tilde{\rho}} (t)$ by $\hat{\rho} (t)$ for now on).

To get a better understanding of the physical meaning behind the elements $\rho_{ij} (t)$ of the density matrix associated to the operator $\hat{\rho} (t)$, we choose a basis $\{|u_j\rangle\}$ consider the following equations

$$\begin{aligned} \rho_{jj} (t) &= \sum_m p_m \left[\hat{\rho}_m (t) \right]_{jj} \\ &= \sum_m p_m \left\langle u_j \,|\, \psi_m (t) \right\rangle \left\langle \psi_m (t) \,|\, u_j \right\rangle \\ &= \sum_m p_m \left| c_{m,j} (t) \right|^2 \end{aligned} \tag{2.36}$$

and

$$
\begin{aligned}
\rho_{jk}(t) &= \sum_m p_m \left[\hat{\rho}_m(t)\right]_{jk} \\
&= \sum_m p_m \langle u_j \mid \psi_m(t)\rangle \langle \psi_m(t) \mid u_k\rangle \\
&= \sum_m p_m c_{m,j}(t)\, c_{m,k}^*(t),
\end{aligned}
\tag{2.37}
$$

where $c_{m,j}(t) = \langle u_j \mid \psi_m(t)\rangle$. Equation (2.36) shows that the diagonal elements $\rho_{jj}(t)$ are the probability of finding the system in the state $|u_j\rangle$ ($|c_{m,j}(t)|^2$ is the probability of finding a system in the state $|\psi_k(t)\rangle$ in the eigenstate $|u_j\rangle$). The elements are therefore called the **populations** of the $|u_j\rangle$ state. On the other hand, the terms $c_{m,j}(t)\, c_{m,k}^*(t)$ found in the off-diagonal elements $\rho_{jk}(t)$ are responsible for the interference behaviour characteristic of quantum mechanical systems (see the A and B coefficients in equation (1.94) for the double slit experiment). For this reason, they are called **coherences**.

The time evolution of these matrix elements is determined by equation (2.9) (or (2.27)). For example, when the basis $\{|u_j\rangle\}$ consists of eigenvectors of the Hamiltonian $\hat{H}$ we have (i.e., $\hat{H}|u_j\rangle = E_j|u_j\rangle$)

$$
\frac{d}{dt}\rho_{jj}(t) = 0
\tag{2.38}
$$

$$
\frac{d}{dt}\rho_{jk}(t) = \frac{1}{i\hbar}(E_j - E_k)\,\rho_{jk}(t),
\tag{2.39}
$$

which imply that

$$
\rho_{jj}(t) = \rho_{jj}(0)
\tag{2.40}
$$

$$
\rho_{jk}(t) = \rho_{jk}(0)\, e^{i(E_j - E_k)t/\hbar}.
\tag{2.41}
$$

We therefore find that the populations are constant, while the coherences oscillate at the interference frequencies $\omega_{jk} = (E_j - E_k)/\hbar$.

Finally, keeping with the same basis $\{|u_j\rangle\}$ of Hamiltonian eigenvectors, it is possible to show that

$$
\rho_{jj}\rho_{kk} \geq |\rho_{jk}|^2,
\tag{2.42}
$$

which implies that coherences can only be present between states having non-zero populations (see the First Problem List).

Exercise 2.1. Thermodynamic equilibrium. Let us consider the density operator

$$
\hat{\rho} = Z^{-1} e^{-\hat{H}/kT},
\tag{2.43}
$$

where the normalization factor is the reciprocal of $Z = \mathrm{Tr}\left(e^{-\hat{H}/kT}\right)$, while k and T are, respectively, the Boltzmann constant and the temperature. Find the populations and coherences for this operator using the basis $\{|u_j\rangle\}$ containing the eigenvectors of the Hamiltonian $\hat{H}$.

Solution.

The populations are given by

$$
\begin{aligned}
\rho_{jj} &= \left\langle u_j \left| e^{-\hat{H}/kT} \right| u_j \right\rangle / Z \\
&= e^{-E_j/kT}/Z
\end{aligned}
\tag{2.44}
$$

with the so-called partition function given by

$$
\begin{aligned}
Z &= \mathrm{Tr}\left(e^{-\hat{H}/kT}\right) \\
&= \sum_j \left\langle u_j \left| e^{-\hat{H}/kT} \right| u_j \right\rangle \\
&= \sum_j e^{-E_j/kT}.
\end{aligned}
\tag{2.45}
$$

Furthermore, we have

$$
\begin{aligned}
\rho_{jk} &= \left\langle u_j \left| e^{-\hat{H}/kT} \right| u_k \right\rangle / Z \\
&= e^{-E_j/kT} \langle u_j \,|\, u_k \rangle / Z \\
&= 0.
\end{aligned}
\tag{2.46}
$$

We therefore recover the Boltzmann formula, which states that the level populations decrease exponentially with their energy, while there is no coherence between the levels.

Exercise 2.2. Rabi oscillations. Let us consider an initially undisturbed degenerate two-level system of energy E_0, which is subsequentally subjected to a constant perturbation $H_{12} = H_{12}^* = H_{21}$. To simplify matters, let us assume that the system is initially set such that $\rho_{11}(0) = 1$ and $\rho_{12}(0) = \rho_{22}(0) = 0$. The basis $\{|u_1\rangle, |u_2\rangle\}$ used to build the density operator are the eigenvectors of the unperturbed Hamiltonian. Calculate the the time evolution of the density matrix elements.

Solution.

Using equation (2.9) we can write (with $H_{11} = H_{22} = E_0$)

$$
\frac{d}{dt}\rho_{ij}(t) = \frac{1}{i\hbar} \sum_{k=1}^{2} \left[H_{ik}\rho_{kj}(t) - \rho_{ik}(t) H_{kj} \right]
\tag{2.47}
$$

and

$$\begin{aligned}
\frac{d}{dt}\rho_{11}(t) &= \frac{1}{i\hbar}\left[E_0\rho_{11}(t) + H_{12}\rho_{21}(t) - \rho_{11}(t)E_0 - \rho_{12}(t)H_{21}\right] \\
&= \frac{H_{12}}{i\hbar}\left[\rho_{12}^*(t) - \rho_{12}(t)\right] \quad\quad\quad (2.48)
\end{aligned}$$

$$\begin{aligned}
\frac{d}{dt}\rho_{12}(t) &= \frac{1}{i\hbar}\left[E_0\rho_{12}(t) + H_{12}\rho_{22}(t) - \rho_{11}(t)H_{12} - \rho_{12}(t)E_0\right] \\
&= \frac{H_{12}}{i\hbar}\left[\rho_{22}(t) - \rho_{11}(t)\right] \quad\quad\quad (2.49)
\end{aligned}$$

$$\frac{d}{dt}\rho_{22}(t) = -\frac{d}{dt}\rho_{11}(t), \quad\quad\quad\quad\quad\quad (2.50)$$

where we used $\rho_{21}(t) = \rho_{12}^*(t)$ and the fact that $\rho_{11}(t) + \rho_{22}(t) = 1$ for the last equation (see equation (2.7)). Inserting equations (2.48) and (2.50) in the time derivative of equation (2.49) we have

$$\begin{aligned}
\frac{d^2}{dt^2}\rho_{12}(t) &= -\frac{2H_{12}}{i\hbar}\frac{d}{dt}\rho_{11}(t) \\
&= \frac{2H_{12}^2}{\hbar^2}\left[\rho_{12}^*(t) - \rho_{12}(t)\right] \\
&= -i\frac{4H_{12}^2}{\hbar^2}\text{Im}\left\{\rho_{12}(t)\right\}. \quad\quad\quad (2.51)
\end{aligned}$$

It follows from this equation that the real and imaginary parts of the coherence $\rho_{12}(t)$ must verify

$$\frac{d^2}{dt^2}\text{Re}\left\{\rho_{12}(t)\right\} = 0 \quad\quad\quad\quad\quad\quad (2.52)$$

$$\frac{d^2}{dt^2}\text{Im}\left\{\rho_{12}(t)\right\} = -\frac{4H_{12}^2}{\hbar^2}\text{Im}\left\{\rho_{12}(t)\right\}, \quad\quad\quad (2.53)$$

which, enforcing $\rho_{12}(0) = 0$, yields

$$\rho_{12}(t) = At + iB\sin\left(\frac{2H_{12}}{\hbar}t\right), \quad\quad\quad (2.54)$$

with A and B are real constants to be evaluated. Inserting this result in equation (2.48) reveals that

$$\frac{d}{dt}\rho_{11}(t) = -\frac{2H_{12}}{\hbar}B\sin\left(\frac{2H_{12}}{\hbar}t\right) \quad\quad\quad (2.55)$$

and

$$\rho_{11}(t) \;=\; B\cos\left(\frac{2H_{12}}{\hbar}t\right) + C \tag{2.56}$$

$$\rho_{22}(t) \;=\; 1 - C - B\cos\left(\frac{2H_{12}}{\hbar}t\right). \tag{2.57}$$

Inserting these relations in equation (2.49) reveals that $A = 0$ and

$$\rho_{12}(t) = i\sin\left(\frac{2H_{12}}{\hbar}t\right), \tag{2.58}$$

as well as $B = C = 1/2$ for

$$\rho_{11}(t) \;=\; \frac{1}{2}\left[1 + \cos\left(\frac{2H_{12}}{\hbar}t\right)\right] \tag{2.59}$$

$$\rho_{22}(t) \;=\; \frac{1}{2}\left[1 - \cos\left(\frac{2H_{12}}{\hbar}t\right)\right]. \tag{2.60}$$

We therefore see that the populations are periodically completely transferred between the two levels at the so-called **Rabi frequency** $\Omega = 2H_{12}/\hbar$ (the corresponding oscillations are referred to as **Rabi oscillations**). Interestingly, this happens independently of the strength of the perturbation H_{12}, although the rate at which the transfer proceeds does.

2.4 Compound Systems and Entanglement

It is often the case that two (or more) quantum mechanical systems combine to form a larger system. For example, suppose we have a first subsystem for which the set of kets $\{|u_j(1)\rangle\}$ forms a basis and a second for which $\{|v_k(2)\rangle\}$ plays the same role. It follows that for the larger, compound system the set of all possible direct products $\{|u_j(1)\,v_k(2)\rangle\}$

$$|u_j(1)\,v_k(2)\rangle \equiv |u_j(1)\rangle \otimes |v_k(2)\rangle \tag{2.61}$$

provides a basis on its product space. Likewise, any observable in one space can be extended to the product space with

$$\hat{\mathbb{A}}(1) \;=\; \hat{A}(1) \otimes \hat{1}(2) \tag{2.62}$$

$$\hat{\mathbb{B}}(2) \;=\; \hat{1}(1) \otimes \hat{B}(2). \tag{2.63}$$

For the mathematical description of the compound system, we must distinguish between two cases, which we now discuss.

2.4.1 Separable Systems

Let us consider cases when the state $|\Psi(1,2)\rangle$ of the compound system can be written as a direct product of the type

$$|\Psi(1,2)\rangle = |\psi(1)\rangle \otimes |\varphi(2)\rangle, \tag{2.64}$$

where $|\psi(1)\rangle$ and $|\varphi(2)\rangle$ are state vectors for the first and second subsystems, respectively. The density operator for the product space then follows naturally with

$$
\begin{aligned}
\hat{\rho} &= |\Psi(1,2)\rangle\langle\Psi(1,2)| \\
&= |\psi(1)\rangle\langle\psi(1)| \otimes |\varphi(2)\rangle\langle\varphi(2)| \\
&= \hat{\rho}(1) \otimes \hat{\rho}(2), \tag{2.65}
\end{aligned}
$$

with $\hat{\rho}(i)$ the density operator of subsystem i, confined to its own space. Whenever the state of a system can be expressed by direct products such as in equations (2.64) or (2.65), then we say that it is **separable**. It is straightforward to verify that $\hat{\rho}$ is Hermitian

$$
\begin{aligned}
\hat{\rho}^\dagger &= [|\Psi(1,2)\rangle\langle\Psi(1,2)|]^\dagger \\
&= [\langle\Psi(1,2)|]^\dagger [|\Psi(1,2)\rangle]^\dagger \\
&= |\Psi(1,2)\rangle\langle\Psi(1,2)| \\
&= \hat{\rho}.
\end{aligned}
$$

Conversely, it is easy to verify that, when performed on the density operator of the compound space, the partial trace on, say, the second subspace recovers the density operator of the first subspace

$$
\begin{aligned}
\mathrm{Tr}_2(\hat{\rho}) &= \sum_k \langle v_k(2)\,|\,\hat{\rho}\,|\,v_k(2)\rangle \\
&= \sum_k \langle v_k(2)\,|\,\Psi(1,2)\rangle\langle\Psi(1,2)\,|\,v_k(2)\rangle \\
&= |\psi(1)\rangle\langle\psi(1)| \otimes \sum_k \langle v_k(2)\,|\,\varphi(2)\rangle\langle\varphi(2)\,|\,v_k(2)\rangle \\
&= \hat{\rho}(1) \otimes \sum_k |c_k(2)|^2 \\
&= \hat{\rho}(1), \tag{2.66}
\end{aligned}
$$

where $c_k(2)$ are the expansion coefficients for (the normalized) $|\varphi(2)\rangle$ state in the basis $\{|v_k(2)\rangle\}$. Similarly, we can calculate that

$$\mathrm{Tr}_1(\hat{\rho}) = \hat{\rho}(2) \tag{2.67}$$

and

$$
\begin{aligned}
\mathrm{Tr}\,(\hat{\rho}) &= \mathrm{Tr}_1\,(\mathrm{Tr}_2\,(\hat{\rho})) \\
&= \mathrm{Tr}_2\,(\mathrm{Tr}_1\,(\hat{\rho})) \\
&= 1.
\end{aligned}
\tag{2.68}
$$

If we now attempt to determine the expectation value $\left\langle \hat{\mathbb{A}}\,(1) \right\rangle$ of the observable defined for the first subsystem, but extended to the compound system, in the same manner as we did for a standalone system (see equation (2.8)), we then have

$$
\begin{aligned}
\left\langle \hat{\mathbb{A}}\,(1) \right\rangle &= \mathrm{Tr}\left(\hat{\rho}\hat{\mathbb{A}}\,(1) \right) \\
&= \sum_{j,k} \langle u_j\,(1)\,v_k\,(2)|\,\hat{\rho}\hat{\mathbb{A}}\,(1)\,|u_j\,(1)\,v_k\,(2)\rangle \\
&= \sum_{j,k}\sum_{m,n} \langle u_j\,(1)\,v_k\,(2)|\,\hat{\rho}\,|u_m\,(1)\,v_n\,(2)\rangle \\
&\qquad\qquad \langle u_m\,(1)\,v_n\,(2)|\,\hat{\mathbb{A}}\,(1)\,|u_j\,(1)\,v_k\,(2)\rangle ,
\end{aligned}
\tag{2.69}
$$

where we used the unit operator $\hat{1}\,(1)\otimes\hat{1}\,(2) = \sum_{m,n}|u_m\,(1)\,v_n\,(2)\rangle\,\langle u_m\,(1)\,v_n\,(2)|$ in the last equation, and

$$
\begin{aligned}
\left\langle \hat{\mathbb{A}}\,(1) \right\rangle &= \sum_{j,k}\sum_{m,n} \langle u_j\,(1)\,v_k\,(2)|\,\hat{\rho}\,|u_m\,(1)\,v_n\,(2)\rangle \\
&\qquad\qquad \left\langle u_m\,(1)\,\left|\,\hat{A}\,(1)\,\right|\,u_j\,(1) \right\rangle \langle v_n\,(2)\,|\,v_k\,(2)\rangle \\
&= \sum_{j,m} \langle u_j\,(1)|\left[\sum_k \langle v_k\,(2)\,|\,\hat{\rho}\,|\,v_k\,(2)\rangle \right]|u_m\,(1)\rangle \left\langle u_m\,(1)\,\left|\,\hat{A}\,(1)\,\right|\,u_j\,(1) \right\rangle \\
&= \sum_{j,m} \langle u_j\,(1)\,|\,\mathrm{Tr}_2\,(\hat{\rho})\,|\,u_m\,(1)\rangle \left\langle u_m\,(1)\,\left|\,\hat{A}\,(1)\,\right|\,u_j\,(1) \right\rangle \\
&= \sum_{j,m} \langle u_j\,(1)\,|\,\hat{\rho}\,(1)\,|\,u_m\,(1)\rangle \left\langle u_m\,(1)\,\left|\,\hat{A}\,(1)\,\right|\,u_j\,(1) \right\rangle \\
&= \sum_j \left\langle u_j\,(1)\,\left|\,\hat{\rho}\,(1)\,\hat{A}\,(1)\,\right|\,u_m\,(1) \right\rangle \\
&= \mathrm{Tr}_1\left(\hat{\rho}\,(1)\,\hat{A}\,(1) \right).
\end{aligned}
\tag{2.70}
$$

The probability $\mathcal{P}\,(a_j\,(1))$ of measuring the eigenvalue $a_j\,(1)$ is calculated in the same manner (i.e., by simply replacing $\hat{\mathbb{A}}\,(1)$ by $\hat{\mathbb{P}}_j\,(1)$ and $\hat{A}\,(1)$ by $\hat{P}_j\,(1)$ in equation (2.70))

$$
\begin{aligned}
\mathcal{P}\,(a_j\,(1)) &= \mathrm{Tr}\left(\hat{\rho}\hat{\mathbb{P}}_j\,(1) \right) \\
&= \mathrm{Tr}_1\left(\hat{\rho}\,(1)\,\hat{P}_j\,(1) \right).
\end{aligned}
$$

We thus find that calculations of expectation values and probabilities of an extended observable on the compound system yields the same value as those restricted to its original subsystem.

Exercise 2.3. Let us consider two two-level subsystems that are combined to form a larger compound system. The bases are $\{|u_1(1)\rangle, |u_2(1)\rangle\}$ and $\{|v_1(2)\rangle, |v_2(2)\rangle\}$, and the two subsystem states are given by

$$
\begin{aligned}
|\psi(1)\rangle &= c_1(1)|u_1(1)\rangle + c_2(1)|u_2(1)\rangle & (2.71)\\
|\varphi(2)\rangle &= c_1(2)|v_1(2)\rangle + c_2(2)|v_2(2)\rangle. & (2.72)
\end{aligned}
$$

Calculate the density operators $\hat{\rho}(1)$ and $\hat{\rho}(2)$ in operator and matrix forms, then do the same for the compound operator $\hat{\rho}$. Using the matrix form for $\hat{\rho}$, how would you calculate $\mathrm{Tr}_1(\hat{\rho})$ and $\mathrm{Tr}_2(\hat{\rho})$?

Solution.

For the first subsystem we write for its state

$$
|\psi(1)\rangle = \sum_{j=1}^{2} c_j(1)|u_j(1)\rangle \tag{2.73}
$$

and for its density operator

$$
\begin{aligned}
\hat{\rho}(1) &= |\psi(1)\rangle\langle\psi(1)| \\
&= \sum_{j,k=1}^{2} c_k(1)c_j^*(1)|u_k(1)\rangle\langle u_j(1)| \tag{2.74}\\
&= |c_1(1)|^2|u_1(1)\rangle\langle u_1(1)| + c_1(1)c_2^*(1)|u_1(1)\rangle\langle u_2(1)| \\
&\quad + c_2(1)c_1^*(1)|u_2(1)\rangle\langle u_1(1)| + |c_2(1)|^2|u_2(1)\rangle\langle u_2(1)|. \tag{2.75}
\end{aligned}
$$

We already know that $\rho_{jk}(1) = c_j^*(1)c_k(1)$ such that the corresponding matrix is

$$
\hat{\rho}(1) = \begin{pmatrix} |c_1(1)|^2 & c_1(1)c_2^*(1) \\ c_2(1)c_1^*(1) & |c_2(1)|^2 \end{pmatrix}. \tag{2.76}
$$

Relations similar to equations (2.74)-(2.76) also holds for $\hat{\rho}(2)$ (with the needed substitutions).

The density operator of the compound system is therefore

$$
\begin{aligned}
\hat{\rho} &= \hat{\rho}(1) \otimes \hat{\rho}(2) \\
&= \left[\sum_{j,k=1}^{2} c_k(1)c_j^*(1)|u_k(1)\rangle\langle u_j(1)|\right] \otimes \left[\sum_{m,n=1}^{2} c_n(2)c_m^*(2)|v_n(2)\rangle\langle v_m(2)|\right] \\
&= \sum_{j,k,m,n=1}^{2} c_k(1)c_j^*(1)c_n(2)c_m^*(2)|u_k(1)v_n(2)\rangle\langle u_j(1)v_m(2)| \tag{2.77}
\end{aligned}
$$

The matrix form for $\hat{\rho}$ can be obtained from equation (2.76) and the corresponding one for $\hat{\rho}(2)$ to yield

$$
\hat{\rho} = \begin{pmatrix} |c_1(1)|^2 & c_1(1)\,c_2^*(1) \\ c_2(1)\,c_1^*(1) & |c_2(1)|^2 \end{pmatrix} \otimes \begin{pmatrix} |c_1(2)|^2 & c_1(2)\,c_2^*(2) \\ c_2(2)\,c_1^*(2) & |c_2(2)|^2 \end{pmatrix} \tag{2.78}
$$

$$
= \left(\begin{array}{c|c} |c_1(1)|^2\,\hat{\rho}(2) & c_1(1)\,c_2^*(1)\,\hat{\rho}(2) \\ \hline c_2(1)\,c_1^*(1)\,\hat{\rho}(2) & |c_2(1)|^2\,\hat{\rho}(2) \end{array} \right)
$$

$$
= \left(\begin{array}{cc|cc} |c_1(1)|^2\,|c_1(2)|^2 & |c_1(1)|^2\,c_1(2)\,c_2^*(2) & c_1(1)\,c_2^*(1)\,|c_1(2)|^2 & c_1(1)\,c_2^*(1)\,c_1(2)\,c_2^*(2) \\ |c_1(1)|^2\,c_2(2)\,c_1^*(2) & |c_1(1)|^2\,|c_2(2)|^2 & c_1(1)\,c_2^*(1)\,c_2(2)\,c_1^*(2) & c_1(1)\,c_2^*(1)\,|c_2(2)|^2 \\ \hline c_2(1)\,c_1^*(1)\,|c_1(2)|^2 & c_2(1)\,c_1^*(1)\,c_1(2)\,c_2^*(2) & |c_2(1)|^2\,|c_1(2)|^2 & |c_2(1)|^2\,c_1(2)\,c_2^*(2) \\ c_2(1)\,c_1^*(1)\,c_2(2)\,c_1^*(2) & c_2(1)\,c_1^*(1)\,|c_2(2)|^2 & |c_2(1)|^2\,c_2(2)\,c_1^*(2) & |c_2(1)|^2\,|c_2(2)|^2 \end{array} \right),
$$
$$\tag{2.79}$$

where vertical and horizontal lines were added to better visualize how a matrix stemming from a direct product of matrices is built. Comparing equations (2.77) and (2.79) we see that the j and k indices designate the quadrant of the matrix and the m and n indices the element within a quadrant. It is easy to verify that $\text{Tr}(\hat{\rho}) = 1$ and $\hat{\rho}^\dagger = \hat{\rho}$.

To recover the matrices for $\hat{\rho}(1) = \text{Tr}_2(\hat{\rho})$ and $\hat{\rho}(2) = \text{Tr}_1(\hat{\rho})$ it is advantageous to first represent the elements of $\hat{\rho}$ by $\rho_{jk,mn}$, where the first pair of indices (i.e., j and k) apply to the elements of $\hat{\rho}_1$ and the second (i.e., m and n) to $\hat{\rho}(2)$ (as in equation (2.77)). We can then write

$$
\rho_{jk}(1) = \sum_m \rho_{jk,mm} \tag{2.80}
$$

$$
\rho_{mn}(2) = \sum_j \rho_{jj,mn}. \tag{2.81}
$$

Thus for $\hat{\rho}(1)$ we first choose a quadrant in equation (2.79) and sum its (two) diagonal elements, recovering the leftmost matrix on the right-hand side of equation (2.78). For $\hat{\rho}_2$ we sum the element located on the mth row and n^{th} column in the first ($j = 1$) and fourth ($j = 2$) quadrants, recovering the rightmost matrix on the right-hand side of the same equation. This process of taking a partial trace on two indices corresponding to one subspace is commonly called a *contraction* (notably within the context of tensor calculus and general relativity).

2.4.2 Entangled Systems

It is not a rule that the state of all compound systems can be expressed as in equations (2.64) or (2.65). If fact, a quantum mechanical system is said to be **entangled** when (here, for the case of two subsystems)

$$
|\Psi(1,2)\rangle \neq |\psi(1)\rangle \otimes |\varphi(2)\rangle. \tag{2.82}
$$

This is similar to saying that the two subsystems are not statistically independent. To get a better sense as to what this means, let us take two two-level subsystems, with respective bases $\{|u_1(1)\rangle, |u_2(1)\rangle\}$ and $\{|v_1(2)\rangle, |v_2(2)\rangle\}$, which form a compound system described by, say, the state

$$|\Psi(1,2)\rangle = \frac{1}{\sqrt{2}}(|u_1(1)\,v_2(2)\rangle + |u_2(1)\,v_1(2)\rangle). \tag{2.83}$$

A close inspection of equation (2.83) will convince the reader that this ket cannot be factorized in a direct product of two kets, one from each subspace.

The density operator of the compound system is calculated in the usual manner to yield

$$
\begin{aligned}
\hat{\rho} &= |\Psi(1,2)\rangle\langle\Psi(1,2)| \\
&= \frac{1}{2}\left[|u_1(1)\,v_2(2)\rangle\langle u_1(1)\,v_2(2)| + |u_1(1)\,v_2(2)\rangle\langle u_2(1)\,v_1(2)|\right. \\
&\quad\left. + |u_2(1)\,v_1(2)\rangle\langle u_1(1)\,v_2(2)| + |u_2(1)\,v_1(2)\rangle\langle u_2(1)\,v_1(2)|\right].
\end{aligned} \tag{2.84}
$$

Let us now compute $\hat{\rho}(1)$, as we did in the previous section,

$$
\begin{aligned}
\hat{\rho}(1) &= \mathrm{Tr}_2(\hat{\rho}) \\
&= \langle v_1(2)\,|\,\hat{\rho}\,|\,v_1(2)\rangle + \langle v_2(2)\,|\,\hat{\rho}\,|\,v_2(2)\rangle \\
&= \frac{1}{2}\left[|u_2(1)\rangle\langle u_2(1)| + |u_1(1)\rangle\langle u_1(1)|\right].
\end{aligned} \tag{2.85}
$$

In a similar manner we have

$$
\begin{aligned}
\hat{\rho}(2) &= \mathrm{Tr}_1(\hat{\rho}) \\
&= \langle u_1(1)\,|\,\hat{\rho}\,|\,u_1(1)\rangle + \langle u_2(1)\,|\,\hat{\rho}\,|\,u_2(1)\rangle \\
&= \frac{1}{2}\left[|v_2(2)\rangle\langle v_2(2)| + |v_1(2)\rangle\langle v_1(2)|\right].
\end{aligned} \tag{2.86}
$$

If we now calculate the direct product of these two reduced density operators, we find that

$$
\begin{aligned}
\hat{\rho}' &= \hat{\rho}(1) \otimes \hat{\rho}(2) \\
&= \frac{1}{4}\left[|u_1(1)\,v_1(2)\rangle\langle u_1(1)\,v_1(2)| + |u_1(1)\,v_2(2)\rangle\langle u_1(1)\,v_2(2)|\right. \\
&= \quad\left. + |u_2(1)\,v_1(2)\rangle\langle u_2(1)\,v_1(2)| + |u_2(1)\,v_2(2)\rangle\langle u_2(1)\,v_2(2)|\right] \\
&\neq \hat{\rho}.
\end{aligned} \tag{2.87}
$$

This result is completely at odds with what we found for separable systems. That is, performing partial traces to inquire about only one of the two subsystems at a time,

independently of the other, has altered the overall compound system in a manner that we cannot recover its initial state from the reduced subsystems. This is a signature of the initial correlation (or entanglement) between the subsystems. In other words, *the two subsystems are not independent and must treated as one single quantum mechanical entity* (i.e., the compound system).

It is also instructive to contemplate entanglement from the point of the state of a system (i.e., not through the density operator). We once again consider a compound system $|\Psi(1,2)\rangle$ made from two subsystems $|\psi(1)\rangle$ and $|\varphi(2)\rangle$ (without necessarily assuming them to be two-level systems). Performing a measurement to find the probability of finding the non-degenerate eigenvalue a_j of the observable $\hat{A}(1)$ (or $\hat{\mathbb{A}}(1)$) on the first subsystem, irrespective of the state of the second subsystem, we have

$$
\begin{aligned}
\mathcal{P}(a_j) &= \left\langle \Psi(1,2) \left| \hat{\mathbb{P}}_j(1) \right| \Psi(1,2) \right\rangle \\
&= \sum_k |\langle u_j(1) v_k(2) | \Psi(1,2) \rangle|^2.
\end{aligned}
\tag{2.88}
$$

The state $|\Psi'(1,2)\rangle$ of the compound system after the measurement is given by

$$
\begin{aligned}
|\Psi'(1,2)\rangle &= \frac{\hat{\mathbb{P}}_j(1) |\Psi(1,2)\rangle}{\sqrt{\left\langle \Psi(1,2) \left| \hat{\mathbb{P}}_j(1) \right| \Psi(1,2) \right\rangle}} \\
&= \frac{\sum_k |u_j(1) v_k(2)\rangle\langle u_j(1) v_k(2)| |\Psi(1,2)\rangle}{\sqrt{\sum_k |\langle u_j(1) v_k(2) | \Psi(1,2) \rangle|^2}}.
\end{aligned}
\tag{2.89}
$$

It should be clear that the choice of the $\{|v_k(2)\rangle\}$ basis is totally arbitrary and could not affect the outcome of the measurement on the first subsystem. If the original compound state was separable to start with such that

$$
|\Psi(1,2)\rangle = |\psi(1)\rangle \otimes |\varphi(2)\rangle
\tag{2.90}
$$

then

$$
\begin{aligned}
|\Psi'(1,2)\rangle &= \frac{\hat{\mathbb{P}}_j(1) |\Psi(1,2)\rangle}{\sqrt{\left\langle \Psi(1,2) \left| \hat{\mathbb{P}}_j(1) \right| \Psi(1,2) \right\rangle}} \\
&= \frac{\left(\hat{P}_j(1) \otimes \hat{1}(2) \right) (|\psi(1)\rangle \otimes |\varphi(2)\rangle)}{\sqrt{\left\langle \Psi(1,2) \left| \hat{\mathbb{P}}_j(1) \right| \Psi(1,2) \right\rangle}} \\
&= \frac{\hat{P}_j(1) |\psi(1)\rangle}{\sqrt{\left\langle \psi(1) \left| \hat{P}_j(1) \right| \psi(1) \right\rangle}} \otimes |\varphi(2)\rangle,
\end{aligned}
\tag{2.91}
$$

while

$$
\begin{aligned}
\mathcal{P}\left(a_j\right) &= \left\langle \Psi\left(1,2\right) \middle| \hat{\mathbb{P}}_j\left(1\right) \middle| \Psi\left(1,2\right) \right\rangle \\
&= \left\langle \Psi\left(1,2\right) \middle| \left[\hat{P}_j\left(1\right) \otimes \hat{1}\left(2\right)\right] \middle| \Psi\left(1,2\right) \right\rangle \\
&= \left\langle \psi\left(1\right) \middle| \hat{P}_j\left(1\right) \middle| \psi\left(1\right) \right\rangle \left\langle \varphi\left(2\right) \middle| \hat{1}\left(2\right) \middle| \varphi\left(2\right) \right\rangle \\
&= \left| \left\langle u_j\left(1\right) \middle| \psi\left(1\right) \right\rangle \right|^2 .
\end{aligned}
\tag{2.92}
$$

These equations are, indeed, independent of the basis used to expand $|\varphi\left(2\right)\rangle$. We also note, as we should have expected, that the state emerging after the measurement is also separable. Importantly, the probability of obtaining a given outcome on a measurement on one subsystem only depends on that system, as is clearly seen in equation (2.92). The two subsystems are therefore uncorrelated (both before and after the measurement).

It is interesting to note that the final state of the compound system after a measurement is also separable even when the original compound system is entangled, as can be verified by transforming equation (2.89) to

$$
\left| \Psi'\left(1,2\right) \right\rangle = \left| u_j\left(1\right) \right\rangle \otimes \frac{\sum_k \left| v_k\left(2\right) \right\rangle \left\langle u_j\left(1\right) v_k\left(2\right) \middle| \Psi\left(1,2\right) \right\rangle}{\sqrt{\sum_k \left| \left\langle u_j\left(1\right) v_k\left(2\right) \middle| \Psi\left(1,2\right) \right\rangle \right|^2}}.
\tag{2.93}
$$

The final compound state is the direct product of the final state $|u_j\left(1\right)\rangle$ of the first subsystem corresponding to the eigenvalue a_j with a modified state for the second subsystem. We therefore conclude that *a measurement on one subsystem leaves the compound system in a separable state irrespective of its nature before the measurement.*

For an entangled system the probability $\mathcal{P}\left(a_j\right)$ of the measurement on the first subsystem is seen from equation (2.88) to also depends on the state of the second subsystem. This is the signature of the existence of an initial correlation between the two subsystems, and evidence that they have interacted in the past. However, the measurement process will remove any correlation, since the outcome is a separable compound state.

Finally, we note the surprising fact that the final state of the second subsystem

$$
\left| \varphi'\left(2\right) \right\rangle = \frac{\sum_k \left| v_k\left(2\right) \right\rangle \left\langle u_j\left(1\right) v_k\left(2\right) \middle| \Psi\left(1,2\right) \right\rangle}{\sqrt{\sum_k \left| \left\langle u_j\left(1\right) v_k\left(2\right) \middle| \Psi\left(1,2\right) \right\rangle \right|^2}}
\tag{2.94}
$$

depends on the nature of the measurement made on the first subsystem (from the presence of $\langle u_j\left(1\right)|$ in this equation). For example, the two subsystems may have interacted at one point in the past, then move a large distance away from one another. But one subsystem would still be directly affected by a subsequent measurement made on the other subsystem, irrespective on how far from each other they are. This is the essence of the so-called Einstein-Podolsky-Rosen paradox.

Exercise 2.4. Let us consider two two-level subsystems that can exist in the states $|\uparrow\rangle$ and $|\downarrow\rangle$. The systems are brought together to form a larger one in the initial state

$$|\Psi(1,2)\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right). \tag{2.95}$$

A measurement is made on the first subsystem to find the probability $\mathcal{P}(\uparrow_1)$. What is the state of the second subsystem after the measurement?

Solution.

Referring to equation (2.94), the state of the second subsystem after the measurement on the first is

$$
\begin{aligned}
\left|\varphi'(2)\right\rangle &= \frac{|\downarrow_2\rangle\langle\uparrow\downarrow|\Psi(1,2)\rangle + |\uparrow_2\rangle\langle\uparrow\uparrow|\Psi(1,2)\rangle}{\sqrt{|\langle\uparrow\downarrow|\Psi(1,2)\rangle|^2 + |\langle\uparrow\uparrow|\Psi(1,2)\rangle|^2}} \\
&= |\downarrow_2\rangle. \tag{2.96}
\end{aligned}
$$

It follows that the measurement on the first subsystem has completely determined the final state of the second. That is, an observer who obtained $|\uparrow_1\rangle$ as the measurement outcome knows with certainty that $\varphi'(2) = |\downarrow_2\rangle$.