

as in all others): we only obtain probabilities from the quantum mechanical description, i.e., we cannot predict the result of individual measurements.

An extension of the von Neumann measurement that is sometimes used in the context of quantum information processing and communication is the positive operator-valued measure (POVM), where the states that form the basis for the measurement are not orthogonal. The corresponding projection operators must still sum up to unity.

## 4.4 Entanglement measures

### 4.4.1 General requirements

In section 4.2.3, we introduced a definition of entanglement:

A state of a bipartite system is called entangled if it cannot be written as a direct product of two states from the two subsystem Hilbert spaces.

Formally:

$$\Psi_{A \otimes B} \neq \Psi_A \otimes \Psi_B.$$

Entanglement defines a clear border between the classical and the quantum world. This is not the only differentiation, but certainly an important one.

In the context of quantum information, it is sometimes important to know more about a state than that it is not separable. One would like to measure the amount of entanglement and sometimes also the type of entanglement. Quantitative measures are particularly important in the context of quantum communication: some codes rely on sharing entangled quantum states and secrecy can only be guaranteed if the entanglement is sufficiently large.

The general goal of quantifying entanglement can be approached on different lines. A useful measure  $C$  of entanglement should fulfill some general requirements, including

- $C = 0$  for product states  $\rho = \rho_A \otimes \rho_B$ .
- $C$  should reach its maximum for maximally entangled states like the Bell states.
- $C$  is invariant under local unitary transformations. The measure should not depend on the choice of the local basis.

Out of the many measures that fulfill these requirements, we discuss only the most popular ones. Most of the definitions are not completely general, but they cover only certain systems, e.g. only bipartite systems or only pure states.

### 4.4.2 Entropy of entanglement

One of the simplest measures that fulfill these requirements for pure states is the entropy of entanglement. As discussed in section 4.2.4, the projection of an entangled pure state onto a subspace is mixed. This degree of mixing can be used as a measure of entanglement of the full state.

We start with the von Neumann entropy of a density operator

$$S(\rho) = -Tr\{\rho \log_2(\rho)\}$$

or sometimes the logarithm is taken with respect to the basis  $e$ ,  $\log_2 \rightarrow \ln$ . The von Neumann entropy vanishes for a pure state, where all populations are 0 or 1 and it reaches its maximum for the completely mixed state, where

$$S\left(\frac{1}{N}\mathbf{1}\right) = -\frac{1}{N}Tr(\log_2 \frac{1}{N}\mathbf{1}) = \log_2 N,$$

where  $N$  is the dimension of the Hilbert space. The von Neumann entropy is related to Shannon's measure of information, which is important in the context of information capacity, and to Gibbs' entropy from statistical mechanics. More details are given in chapter 13.

A useful interpretation of the von Neumann entropy is that it represents the minimum number of bits required to store the result of a random variable: A pure state  $\rho_1 = |\Psi\rangle\langle\Psi|$  of a single qubit can always be written in its eigenbase as

$$\rho_1 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}.$$

Its entropy vanishes,

$$S(\rho_1) = 1 \log_2(1) + 0 \log_2(0) = 0.$$

A suitable measurement of the observable  $\sigma_z$  always produces the result +1, and the information gain from such a measurement vanishes. For the maximally mixed state

$$\rho_2 = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

however, the entropy reaches its maximum value

$$\begin{aligned} S(\rho_2) &= -Tr\left\{\begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix} \log_2 \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}\right\} \\ &= \frac{1}{2}Tr\left\{\begin{pmatrix} \log_2 2 & 0 \\ 0 & \log_2 2 \end{pmatrix}\right\} = 1. \end{aligned}$$

Here, every binary observable generates completely random values. Every result must therefore be represented by one bit, compression is not possible.

The entropy of entanglement is defined for bipartite pure states as the von Neumann entropy of one of the reduced states:

$$E(\rho) = S(\rho_A) = S(\rho_B),$$

where  $\rho_A = Tr_B(\rho)$  and vice versa. If  $\rho$  is a product state, such as  $|\uparrow\uparrow\rangle$ ,  $\rho_A$  and  $\rho_B$  are pure states and the entropy vanishes. If the state is maximally entangled, e.g.

$$|\Psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle),$$

the subsystems become completely mixed,  $\rho_A = \rho_B = \frac{1}{2}\mathbf{1}$ . The corresponding entropy, the entanglement entropy of a maximally entangled 2-qubit state is then  $E(\rho) = S(\rho_A) = S(\rho_B) = 1$ .

### 4.4.3 Concurrence

- Concurrence, a legal term referring to the need to prove both *actus reus* and *mens rea*
- Concurring opinion (also called a "concurrency"), a legal opinion which supports the conclusion, though not always the reasoning, of the majority.
- Concurrence (computer science), a property of systems in which several processes are executing at the same time
- Concurrence (road), an instance of one physical road bearing two or more different route numbers
- Concurrent DOS, Digital Research's multiuser multitasking operating system, with "Concurrent" once being their registered trademark
- Concurrent estate, a concept in property law
- Concurrent computing, the simultaneous execution of multiple interacting computational tasks
- Concurrent lines, a mathematical term for multiple lines or curves intersecting at a single point
- Concurrent enrollment, the process in which high school students enroll at a university or college usually to attain college credit
- Concurrent resolution, a legislative measure passed by both the United States Senate and the United States House of Representatives
- Concurrent Computer Corporation, a computer company originally known as Interdata
- Concurrent Design Facility, an assessment center of the European Space Agency using concurrent engineering methods
- Concurrence (quantum computing), a measure of quantum entanglement used in quantum information theory

Figure 4.4: Meanings of the term "Concurrence" in different fields (from wikipedia).

As discussed in section 4.2.6, the concurrence for pure 2-qubit states

$$|\Psi\rangle = \alpha|\uparrow\uparrow\rangle + \beta|\uparrow\downarrow\rangle + \gamma|\downarrow\uparrow\rangle + \delta|\downarrow\downarrow\rangle$$

is

$$C := 2|\alpha\delta - \beta\gamma| \geq 0. \quad (4.67)$$

If we consider a typical product state, e.g.

$$\Psi_1 = |\uparrow\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

we find  $C(\Psi_1) = 0$ , i.e. the state is not entangled. Similarly, for

$$\Psi_2 = \frac{1}{2}(|\uparrow\rangle + |\downarrow\rangle) \otimes (|\uparrow\rangle + |\downarrow\rangle) = \frac{1}{2} \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix},$$

we find again  $C(\Psi_2) = 0$ . Since  $\Psi_1$  and  $\Psi_2$  are identical under local transformations (here: rotations  $z \rightarrow x$ ), this is consistent with the general requirements for entanglement measures.

We now consider the effect of an ‘‘entangling gate’’, such as

$$\text{CN} = \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & \cos \frac{\varphi}{2} & -\sin \frac{\varphi}{2} \\ & & \sin \frac{\varphi}{2} & \cos \frac{\varphi}{2} \end{pmatrix},$$

which is close to the CNOT gate if  $\varphi = \pi$ . If we apply it to  $\Psi_2$ , we find

$$\Psi_3 = \text{CN} \cdot \Psi_2 = \frac{1}{2} \begin{pmatrix} 1 \\ 1 \\ \cos \frac{\varphi}{2} - \sin \frac{\varphi}{2} \\ \cos \frac{\varphi}{2} + \sin \frac{\varphi}{2} \end{pmatrix}.$$

This corresponds to the ‘pre-measurement’ in the theory of the quantum measurement process, which entangles the system with the apparatus.

For this state, the concurrence is

$$\begin{aligned} C(\Psi_3) &= \frac{1}{2} \left| \cos \frac{\varphi}{2} + \sin \frac{\varphi}{2} - (\cos \frac{\varphi}{2} - \sin \frac{\varphi}{2}) \right| \\ &= \left| \sin \frac{\varphi}{2} \right|. \end{aligned}$$

The state is therefore entangled for any finite angle  $\varphi$ . The entanglement reaches its maximum of  $C = 1$

for  $\varphi = \pi$ , where  $\text{CN} \approx \text{CNOT}$ , apart from the – sign, and returns to 0 for  $\varphi = 2\pi$ .

We can also calculate the entanglement entropy for this state. The full density operator has the form

$$\rho_3 = \frac{1}{4} \begin{pmatrix} 1 & 1 & c_- & c_+ \\ 1 & 1 & c_- & c_+ \\ c_- & c_- & 1 - \sin \varphi & \cos \frac{\varphi}{4} \\ c_+ & c_+ & \cos \frac{\varphi}{4} & 1 + \sin \varphi \end{pmatrix},$$

where

$$c_{\pm} = \cos \frac{\varphi}{2} \pm \sin \frac{\varphi}{2}.$$

For the subsystems, this yields

$$\rho_A = \text{Tr}_B(\rho) = \frac{1}{2} \begin{pmatrix} 1 & \cos \frac{\varphi}{2} \\ \cos \frac{\varphi}{2} & 1 \end{pmatrix}$$

and

$$\rho_B = \text{Tr}_A(\rho) = \frac{1}{2} \begin{pmatrix} 1 - \frac{1}{2} \sin \varphi & \cos^2 \frac{\varphi}{2} \\ \cos^2 \frac{\varphi}{2} & 1 + \frac{1}{2} \sin \varphi \end{pmatrix},$$

where we used the trigonometric identity  $1 + \cos(\varphi/4) = 2 \cos^2(\varphi/2)$ . The difference between  $\rho_A$  and  $\rho_B$  reflects the asymmetric role that control and target bit play in the CNOT gate.

To calculate the logarithm, it is useful to convert the matrices into their eigenbases. The diagonal form of  $\rho_A$  is

$$\rho_A^d = \frac{1}{2} \begin{pmatrix} 1 - \cos \frac{\varphi}{2} & 0 \\ 0 & 1 + \cos \frac{\varphi}{2} \end{pmatrix}.$$

The entropy is thus

$$\begin{aligned} S(\rho_A) &= -\frac{1}{2} \left[ (1 - \cos \frac{\varphi}{2}) \log_2 \left( \frac{1 - \cos \frac{\varphi}{2}}{2} \right) \right. \\ &\quad \left. + (1 + \cos \frac{\varphi}{2}) \log_2 \left( \frac{1 + \cos \frac{\varphi}{2}}{2} \right) \right]. \end{aligned}$$

For  $\rho_B$ , we obtain

$$\rho_B^d = \frac{1}{2} \begin{pmatrix} 1 - \cos \frac{\varphi}{2} & 0 \\ 0 & 1 + \cos \frac{\varphi}{2} \end{pmatrix} = \rho_A^d$$

and therefore  $S(\rho_B) = S(\rho_A)$ . It also reaches its maximum at  $\varphi = \pi$ :

$$S(\rho_A, \pi) = -\log_2 \left( \frac{1}{2} \right) = 1.$$

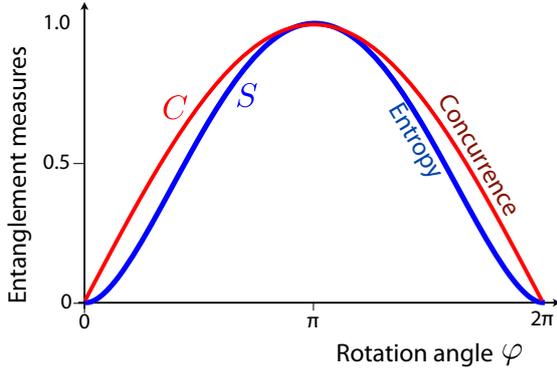


Figure 4.5: Entanglement entropy  $S$  and concurrence  $C$  of  $\rho_3$  as a function of the rotation angle  $\varphi$ .

Figure 4.5 shows the resulting entanglement entropy  $E(\rho_3) = S(\rho_A) = S(\rho_B)$  as a function of the rotation angle  $\varphi$ . Clearly, the dependence is different from that of the concurrence  $C(\Psi_3)$  for the same state, which starts linearly with  $\varphi$ . However, both entanglement measures reach their maximum for the same state and vanish when the state is separable.

For density matrices, i.e. partially mixed states of two qubits, the concurrence is defined as

$$C(\rho) = \max(0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4), \quad (4.68)$$

where  $\lambda_i$  are the eigenvalues, in decreasing order, of the Hermitian operator

$$R = \sqrt{\sqrt{\rho} \tilde{\rho} \sqrt{\rho}},$$

where

$$\tilde{\rho} = (\sigma_y \otimes \sigma_y) \rho^* (\sigma_y \otimes \sigma_y).$$

Equivalently, the  $\lambda_i$  may be calculated as the square roots of the eigenvalues of the non-Hermitian matrix  $\rho \tilde{\rho}$ . For pure states,  $\rho^2 = \rho$ , this yields the same result as the definition (4.67).

#### 4.4.4 Tangle

Concurrence and entropy quantify the entanglement between 2 qubits. In a 3-qubit system  $ABC$ , different types of entanglement exist. The qubits can be

pairwise entangled, i.e.  $A$  can be entangled with  $B$  or with  $C$ . Alternatively, there are three-way entangled states that are not pairwise entangled. These different types of entanglement can be quantified by several entanglement measures called “tangle”.

We consider a pure three-qubit state and start with the average two-tangle

$$\tau_2 = \frac{C_{12}^2 + C_{23}^2 + C_{13}^2}{3},$$

where the concurrence  $C_{ik}$  measures the pairwise entanglement between qubits  $i$  and  $k$ . Each of these is determined by tracing over the third qubit and then using eq. (4.68) to calculate the concurrence for the resulting 2-qubit state, which may be pure or mixed.

Entanglement between one qubit and both others can be measured by the bipartite concurrence

$$C_{i(jk)} = \sqrt{2 - 2 \text{Tr}(\rho_i^2)},$$

where  $\rho_i$  is the subsystem of qubit  $i$  obtained by tracing over the two other qubits. If the pure 3-qubit state is a product state,  $\rho_i$  is pure and therefore  $\rho_i = \rho_i^2$  and  $\text{Tr}(\rho_i^2) = 1$  and  $C_{i(jk)} = 0$ . For an entangled state,  $\text{Tr}(\rho_i^2) < 1$  and  $C_{i(jk)} > 0$ . For a maximally entangled state,  $\rho_i = \frac{1}{2} \mathbf{1}$  and  $C_{i(jk)} = 1$ .

While the bipartite concurrence tells us if qubit  $i$  is entangled with the two others, this entanglement could be with only one of them or with both. This can be quantified by the three-tangle  $\tau_3$ , which subtracts the pairwise entanglement of qubit  $i$  with qubits  $j$  and  $k$  from the bipartite concurrence to obtain the essential three-way entanglement of a pure three-qubit state:

$$\tau_3 = C_{i(jk)}^2 - (C_{ij}^2 + C_{ik}^2). \quad (4.69)$$

The difference between pure 2-way and 3-way entanglement can be seen by considering the GHZ and W-states:

$$\begin{aligned} |W\rangle_{001} &= \frac{1}{\sqrt{3}}(|001\rangle + |010\rangle + |100\rangle) \\ |\text{GHZ}_{\pm}\rangle &= \frac{1}{\sqrt{2}}(|000\rangle \pm |111\rangle). \end{aligned}$$

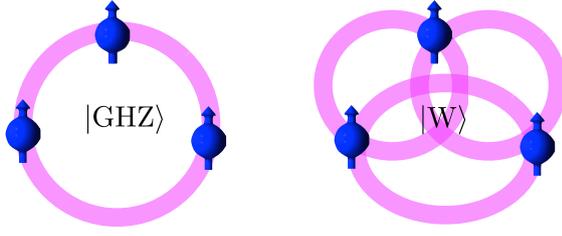


Figure 4.6: Different types of entanglement in 3-partite states.

The essential difference between these states becomes obvious if we perform a measurement on one of the three qubits. In the case of the GHZ state, if we measure an arbitrary qubit and obtain the result 0, the system collapses into the state  $|000\rangle$ . Clearly, this is no longer an entangled state. Measuring any one of the qubits therefore completely destroys the entanglement. This is therefore “essential three-way entanglement”. In contrast, if we measure the third qubit of the W state and obtain the result 0, we are left with the state  $|010\rangle + |100\rangle$ , in which the first two qubits are still maximally entangled. This type of entanglement is therefore called pairwise entanglement.

The different types of entanglement are complementary: If a system is strongly three-way entangled, its bipartite entanglement cannot be large. This can be quantified. For a three-qubit system,

$$\tau_3 + \tau_2^{(k)} + S_k^2 = 1.$$

Here,  $S_k$  quantifies the single-particle character of qubit  $k$  (for details, see Ref. [47]),  $\tau_2^{(k)}$  the two-way entanglement of qubit  $k$  with the other qubits, and  $\tau_3$  the ‘essential three-way entanglement’ defined by eq. (4.69).

#### 4.4.5 Positive Partial Transpose (PPT)

The Positive Partial Transpose (PPT) was introduced by Peres [48] and by the Horodeckis [49] as a necessary condition, for the joint density matrix  $\rho$  of two quantum mechanical systems  $A$  and  $B$  to be separable. It is directly formulated for density operators and therefore applicable to mixed states. It is not a

measure of entanglement, but a criterion that allows one to distinguish between entangled and separable states.

We consider a bipartite system  $AB$  and write the basis states of qubit  $A$  as  $|i\rangle$  and  $|j\rangle$  and for qubit  $B$  as  $|l\rangle$  and  $|k\rangle$ . The density operator of the full system can then be written as

$$\rho = \sum_{ijkl} p_{ijkl} |i\rangle\langle j| \otimes |k\rangle\langle l|. \quad (4.70)$$

The partial transpose with respect to one of the qubits, e.g.  $B$ , is obtained by interchanging the corresponding bras and kets,

$$(|k\rangle\langle l|)^T = |l\rangle\langle k|,$$

while the corresponding states of qubit  $A$  remain unchanged. Applying this transformation to the density operator (4.70) yields

$$\rho^{T_B} = (1 \otimes T)\rho = \sum_{ijkl} p_{ijkl} |i\rangle\langle j| \otimes |l\rangle\langle k|.$$

The PPT criterion states that if  $\rho^{T_B}$  has a negative eigenvalue, then  $\rho$  is entangled. A positive partial transpose is thus a necessary condition for a density operator to be separable. In the  $2 \times 2$  and  $2 \times 3$  dimensional cases the condition is also sufficient.

Unfortunately, the proof of this theorem is not trivial. However, it is easy to show that for separable states the eigenvalues of the partial transpose are positive. If the state is separable, it can be written as

$$\rho = \sum_i p_i \rho_i^A \otimes \rho_i^B$$

for some probabilities  $p_i \geq 0$ . The density operators  $\rho_i^{A,B}$  act on the Hilbert spaces of the individual qubits. If we take the partial transpose of one of them, their eigenvalues, which must all be positive or zero, do not change and therefore the eigenvalues of the product state must also be positive or zero.

#### 4.4.6 Examples

We now apply this test to 2 specific examples, one that we know to be a product state, the other a well-

known entangled state. The first example is the product state

$$\rho_1 = |\uparrow\uparrow\rangle\langle\uparrow\uparrow| = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

Clearly, the partial transpose leaves this state invariant,  $\rho_1^{T_B} = \rho_1$ , and the eigenvalues are (1,0,0,0). Since none of them is negative, this is compatible with a product state.

As the second example, we take one of the Bell states,  $\frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle)$ . It's density operator is

$$\begin{aligned} \rho_2 &= \frac{1}{2}(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle)(\langle\uparrow\uparrow| + \langle\downarrow\downarrow|) \\ &= \frac{1}{2}(|\uparrow\uparrow\rangle\langle\uparrow\uparrow| + |\uparrow\uparrow\rangle\langle\downarrow\downarrow| \\ &\quad + |\downarrow\downarrow\rangle\langle\uparrow\uparrow| + |\downarrow\downarrow\rangle\langle\downarrow\downarrow|) \\ &= \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}. \end{aligned} \quad (4.71)$$

The  $T_B$  operation does not affect the projectors  $|\uparrow\uparrow\rangle\langle\uparrow\uparrow|$  and  $|\downarrow\downarrow\rangle\langle\downarrow\downarrow|$ , but it changes

$$\begin{aligned} |\uparrow\uparrow\rangle\langle\downarrow\downarrow| &\xrightarrow{T_B} |\uparrow\downarrow\rangle\langle\downarrow\uparrow| \\ |\downarrow\downarrow\rangle\langle\uparrow\uparrow| &\xrightarrow{T_B} |\downarrow\uparrow\rangle\langle\uparrow\downarrow|. \end{aligned}$$

We therefore get

$$\begin{aligned} \rho_2^{T_B} &= \frac{1}{2}(|\uparrow\uparrow\rangle\langle\uparrow\uparrow| + |\uparrow\downarrow\rangle\langle\downarrow\uparrow| \\ &\quad + |\downarrow\uparrow\rangle\langle\uparrow\downarrow| + |\downarrow\downarrow\rangle\langle\downarrow\downarrow|) \\ &= \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \end{aligned}$$

To obtain the eigenvalues of this state, we have to diagonalize the central 2x2 matrix, which corresponds to  $\sigma_x/2$  and therefore has the same eigenvalues as  $\sigma_z/2$ ,  $\lambda_{2,3} = \pm 1/2$ . We have therefore found one negative eigenvalue and are correspondingly assured that  $\rho_2$  is entangled, as we expect for a Bell state.

#### 4.4.7 Decay of entanglement

Superposition states like  $\rho_2$  generally are not stable, but decay over time. A typical evolution is that the populations equilibrate on a time scale  $T_1$ , while the off-diagonal elements decay to zero on a time scale  $T_2$ ,  $\rho_{ik} = \rho_{ik}(0)e^{-t/T_2}$ . The state  $\rho_2$  would thus evolve as

$$\rho_2(t) = \begin{pmatrix} p_+ & 0 & 0 & \frac{1}{2}e^{-t/T_2} \\ 0 & p_- & 0 & 0 \\ 0 & 0 & p_- & 0 \\ \frac{1}{2}e^{-t/T_2} & 0 & 0 & p_+ \end{pmatrix}$$

with

$$p_{\pm} = \frac{1}{4}(1 \pm e^{-t/T_1}).$$

Clearly,  $\rho(t=0)$  is equal to  $\rho_2$  of eq. (4.71).

For sufficiently long times  $t \gg (T_1, T_2)$ , this state tends to

$$\rho_2(t \rightarrow \infty) = \frac{1}{4}\mathbf{1},$$

which corresponds to the maximally mixed state and is clearly not entangled.

If we apply the partial transpose to  $\rho_2(t)$ , we obtain

$$\rho_2(t) = \begin{pmatrix} p_+ & 0 & 0 & 0 \\ 0 & p_- & \frac{1}{2}e^{-t/T_2} & 0 \\ 0 & \frac{1}{2}e^{-t/T_2} & p_- & 0 \\ 0 & 0 & 0 & p_+ \end{pmatrix},$$

which has the eigenvalues

$$\lambda_i = (p_+, p_- + \frac{1}{2}e^{-t/T_2}, p_- - \frac{1}{2}e^{-t/T_2}, p_+).$$

While the eigenvalues  $\lambda_1$ ,  $\lambda_2$ , and  $\lambda_4$  are always positive,  $\lambda_3$  is negative for

$$\frac{1}{4}(1 - e^{-t/T_1}) < \frac{1}{2}e^{-t/T_2}$$

or

$$e^{-t/T_1} + 2e^{-t/T_2} > 1,$$

i.e. for sufficiently short times. For long times, however,  $t \gg T_1, T_2$ , it tends towards 1/4, the same as all

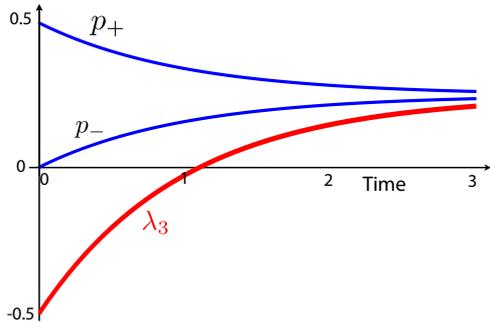


Figure 4.7: Time dependence of the populations and the eigenvalue  $\lambda_3$  of  $\rho_2$  for  $T_1 = T_2 = 1$ .

the other eigenvalues, and the resulting state fulfills the PPT criterion.

Fig. 4.7 shows the time dependence of the populations (blue) and of the third (negative) eigenvalue  $\lambda_3(t)$ . For long times, the populations approach their equilibrium values  $p_\infty = 1/4$ . The initially negative eigenvalue  $\lambda_3(t)$  increases and vanishes after a time  $\approx 1$  for the present example, where we arbitrarily assumed  $T_1 = T_2 = 1$ . At this point, the system is no longer entangled. With a certain tendency towards drama, this effect that the system becomes separable on a finite time scale has been termed “entanglement sudden death”.

The PPT criterion is not suited for the characterization of multipartite ( $>2$  parts) systems.

#### 4.4.8 Quantum discord

Another measure of nonclassical correlations between two subsystems is the quantum discord. The concept was introduced in 2001 by Ollivier and Zurek [50] and by Henderson and Vedral [51]. It measures correlations that can also be present in certain mixed separable states and are considered “quantum mechanical”. It is based on “quantum mutual information”, the quantum mechanical analog of Shannon mutual information. More precisely, discord is the difference between the total mutual information of the subsystems and the mutual information that can be extracted by local measurements. In the case of pure states, the quantum discord measures the entropy of entanglement.

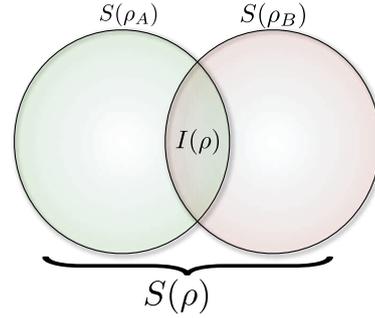


Figure 4.8: Schematic representation of the mutual information  $I(\rho)$  between subsystems  $A$  and  $B$ .

We first remember the von Neumann or information entropy  $S(\rho) = -\text{Tr}(\rho \log_2 \rho)$  defined in section 4.4.2. If we apply this definition to a system consisting of 2 qubits  $A$  and  $B$ , we can define the entropy of the individual subsystems  $S(\rho_A)$ ,  $S(\rho_B)$ , as well as the entropy  $S(\rho)$  of the combined system. From this, we calculate

$$I(\rho) = S(\rho_A) + S(\rho_B) - S(\rho),$$

which is known as the von Neumann mutual information between the two subsystems. If the subsystems  $\rho_A$  and  $\rho_B$  are completely independent, the sum of the information contents of the subsystems,  $S(\rho_A) + S(\rho_B)$  is equal to the information content  $S(\rho)$  of the combined system and the difference vanishes. If the two are entangled, then a measurement of one subsystem also contains information about the other and the total information content is smaller than the sum of the two subsystems. In the case of a maximally entangled system, such as the Bell states, the measurement of one subsystem contains also the complete information about the other subsystem. The mutual information thus measures the total correlations between the two subsystems.

We consider as an example the product state  $\Psi_1 = |\uparrow\uparrow\rangle$ . Here,  $S(\rho_A) = S(\rho_B) = S(\rho) = 0$ , and the mutual information vanishes,

$$I(|\Psi_1\rangle\langle\Psi_1|) = 0.$$

For the Bell state

$$\Psi_2 = \frac{1}{\sqrt{2}} (|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle),$$

the entropy of the combined system vanishes, but the subsystems are maximally mixed and their entropy reaches the maximal value of 1. Accordingly,

$$I(|\Psi_2\rangle\langle\Psi_2|) = 2.$$

In addition, we define the quantum conditional entropy

$$S(\rho_B|\rho_A) = \min_{\{\Pi_j^A\}} \sum S(\rho_{B|\Pi_j^A}),$$

where  $\{\Pi_j^A\}$  is the set of projective operators on subsystem  $A$  and  $\rho_{B|\Pi_j^A}$  are the resulting states. The quantum conditional entropy is also an entanglement measure: if it is negative, the state is entangled.

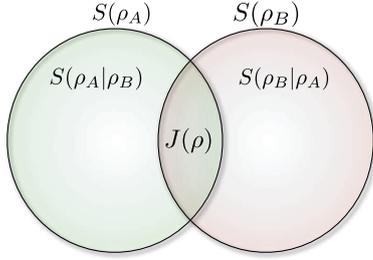


Figure 4.9: Schematic representation of  $J(\rho)$  for the classical case or for a specific set of observables.

From this we calculate the difference

$$J_A(\rho) = S(\rho_B) - S(\rho_B|\rho_A).$$

$J$  specifies the information gained about  $A$  as a result of a measurement on some set of observables on  $B$ . For a classical system,  $I(\rho) = J(\rho)$ .

The quantum discord is then defined as the difference

$$\mathcal{D}_A(\rho) = I(\rho) - J_A(\rho).$$

It vanishes for classical systems, but not generally for quantum mechanical systems. For a possible interpretation,  $I$  describes the correlation between the two subsystems,  $J$  the information gained about  $A$  by measurements on  $B$ . The difference  $\mathcal{D}_A(\rho)$  therefore measures information that can't be extracted by local measurements.

If we use the definitions of  $I$  and  $J$ , we can write

$$\begin{aligned} \mathcal{D}_A(\rho) &= I(\rho) - J_A(\rho) \\ &= S(\rho_A) - S(\rho) + S(\rho_B|\rho_A). \end{aligned}$$

The first 2 terms represent the entropy of entanglement before the measurements, the last term the conditional entropy between the two subsystems.

The quantum discord is not symmetric,  $\mathcal{D}_A(\rho) \neq \mathcal{D}_B(\rho)$  in general. As an example, consider the state

$$\rho_{AB} = \frac{1}{2} (|0\rangle\langle 0| \otimes |-\rangle\langle -| + |1\rangle\langle 1| \otimes |0\rangle\langle 0|).$$

Here, a measurement in the computational basis will not perturb subsystem  $A$ , while a measurement on  $B$  will always change the state.

A necessary and sufficient condition for a state  $\rho$  to have zero discord is that there exist a projective measure  $\{\Pi_k\}$  such that

$$\rho = \sum_k (\Pi_k \cdot \mathbf{1}) \rho (\Pi_k \cdot \mathbf{1}).$$

If  $\mathcal{D}_A(\rho) \neq 0$ , this means that measurements on the subsystem  $B$  perturb the subsystem  $A$ . This does not happen for classical systems, but can happen for quantum systems, even if they are not entangled. The discord can therefore also be interpreted as the difference between the total mutual information and the mutual information that can be extracted by local measurements. It can be nonzero for quantum mechanical systems in separable states. It therefore represents a measure of “quantumness” independent of entanglement.

The quantum discord has become quite popular recently. One possible reason for this is that it vanishes for pointer states, which correspond to the effectively classical states relevant for quantum measurements. In pure states, the quantum discord is nonzero only for entangled states.

Quantum discord can be measured by quantum discord witness operators. Since these operators are nonlinear, this is a nontrivial subject.

#### 4.4.9 Entanglement witnesses

Entanglement witnesses are functionals of the density operator that distinguish specific entangled states from separable ones. If they are linear functions, they can be represented as operators. The expectation value of these operators for an entangled state is strictly outside the range of possible expectation values of any separable state. Separable states are given by density operators of the type

$$\rho_s = \sum_i p_i \rho_i^A \otimes \rho_i^B,$$

where  $\rho_i^{A,B}$  are pure states of the subsystems  $A$  and  $B$  and the  $p_i \geq 0$  probabilities. Clearly, these states form a convex set, i.e. every linear combination

$$a\rho_A + (1-a)\rho_B \quad a \in [0, 1]$$

of 2 states  $\rho_A$  and  $\rho_B$  in the set is also inside.

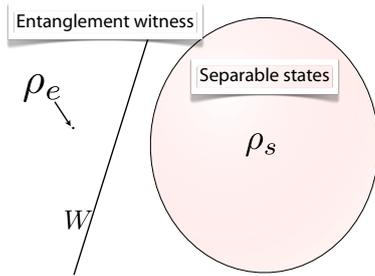


Figure 4.10: Schematic representation of an entanglement witness  $W$ , separating the entangled state  $\rho_e$  from the convex set of all separable states  $\rho_s$ .

This is compared to an entangled state  $\rho_e$ , which therefore must be outside of this convex set. It is then possible to find a (hyper-)plane located between the point and the convex set. This hyperplane can be represented as an operator  $W$  such that

$$\text{Tr}\{W\rho_e\} < 0 \quad \text{and} \quad \text{Tr}\{W\rho_s\} \geq 0.$$

Entanglement witness operators can always be found, but there is no general recipe for constructing them and they are not suitable for distinguishing between arbitrary entangled states and product states. However, for large systems with more than 3 qubits, there is often no other practical solution.

#### Further reading

There is a large number of excellent books on quantum mechanics and its applications at all levels. Dirac's classic book [52] is a concise and clear masterpiece. Cohen-Tannoudji *et al.* [53] is a detailed student-friendly textbook. Ballentine [54] has interesting modern applications, whereas Peres [55] concentrates on the conceptual structure of the theory.

#### Problems and Exercises

1. Show that  $\mathbf{H}^2 = \mathbf{1}$ , where  $\mathbf{H}$  is the Hadamard gate. Find  $\mathbf{X}^{\frac{1}{2}}$ , the square root of NOT. (Hint: use (4.18) for  $\alpha = x$  or (4.20) and choose appropriate values for the arguments of the sine and cosine functions.) Apply  $\mathbf{X}^{\frac{1}{2}}$  to  $|0\rangle$  and  $|1\rangle$ .
2. Calculate the time-dependent expectation value of the spin vector, with components  $\langle \mathbf{S}_\alpha \rangle$ , ( $\alpha = x, y, z$ ) for the time-dependent states (4.19) and (4.21) and visualize it in terms of a classical magnetic moment precessing in a magnetic field. This aspect will be discussed again in the context of nuclear magnetic resonance in chapter 10.
3. Check that the state  $|\theta, \phi\rangle$  (4.22) is an eigenstate of the operator

$$\cos \theta \mathbf{S}_z + \sin \theta \cos \phi \mathbf{S}_x + \sin \theta \sin \phi \mathbf{S}_y$$

with eigenvalue  $+\hbar/2$ .

4. Try to write the following two states as product states:

$$\text{a) } ac|\uparrow\uparrow\rangle + ad|\uparrow\downarrow\rangle + bc|\downarrow\uparrow\rangle + bd|\downarrow\downarrow\rangle$$

$$\text{b) } \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

5. Calculate the expectation values  $\langle \langle \mathbf{S}_\alpha \rangle \rangle$  and the variances  $\langle \langle (\mathbf{S}_\alpha - \langle \mathbf{S}_\alpha \rangle)^2 \rangle \rangle$  ( $\alpha = x, y, z$ ) for the pure state

$$|\chi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$$

and the mixed state

$$\rho = \frac{1}{2}(\mathbf{P}_\uparrow + \mathbf{P}_\downarrow)$$

Calculate the purity  $\eta$  (4.41) for the mixed state.

6. Calculate the quantum discord for the state

$$\rho = \frac{1-z}{4} \mathbf{1} + z |\Psi\rangle\langle\Psi|,$$

with  $|\Psi\rangle = \frac{1}{\sqrt{2}} (|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle)$ .