4 Quantum Mechanics

Before discussing the formal structure of quantum mechanics, we review how this field has become the foundation of most areas of physical science, including chemistry, materials science as well as much of life science. The following part focuses on the general formal structure of the theory. Later on we will treat some simple applications which have not yet become standard subject matter of a quantum mechanics course but which are relevant to quantum information processing. Throughout this course we shall almost exclusively employ Dirac's abstract bra and ket notation for quantum states. This is quite natural for a field which focuses more on algebraic structures and relations between states than on, for example, probability distributions in space related to individual states which are best discussed in the position representation, that is in terms of wave functions.

4.1 History

4.1.1 Before the quantum revolution

During the 19^{th} century, science made enormous progress, solving many puzzles and laying the foundations for the industrial revolution. Examples include thermodynamics as the basis of steam engines or electromagnetic theory as the basis of electrical engines and power generation. Atoms and molecules were generally thought to form the basis of matter, but very little was known about their structure. The periodic system was known, but no theoretical basis for it. In 1900, William Thomson (Lord Kelvin) gave a speech where he suggested that all of physics was known and only a few minor problems remained to be solved.

4.1.2 Open questions

Some of the open questions that Kelvin himself worked on was the age of the earth and the sun. His estimate was about 20 million years, which was not compatible with the theory of evolution. Other problems included the nature of heat, which was the basis of (phenomenological) thermodynamics, the nature of radioactivity, or the fundamentals for materials science: what determines if a material is an insulator or a metal.

One of the biggest problems was the question about the stability of matter: how could arrangements of opposite charges avoid approaching each other until the distance reached zero, thereby releasing an infinite amount of energy according to Coulomb's law.

4.1.3 The first quantum revolution

Soon after Kelvin's 1900 speech, the fundamentals of physics were changed completely with the development of quantum mechanics. Some important milestones were

- 1900 Planck : Theory of blackbody radiation
- 1905 Einstein : Photoelectric effect
- 1910s de Broglie : Wave-particle duality
- 1925-1926 Heisenberg, Schrödinger, Born, Jordan : Mathematical formalism [37, 38, 39, 40]
- 1927 Heisenberg : Uncertainty principle
- 1920s-1930s : Bohr, Heisenberg : The Copenhagen interpretation
- 1930s-1940s Feynman, Schwinger, Tomonaga : Quantum Field Theory
- 1970s : Standard model of particle physics

Some of the central points for quantum information are

- The existence of stationary states (eigenstates of the Hamiltonian)
- The quantisation of electromagnetic energy
- The evolution of quantum systems under the Schrödinger equation
- The measurement process and the related back-action

4.1.4 Is quantum mechanics weird?

Quantum mechanics is often described as being weird or counterintuitive. Indeed, some aspects are different from everyday experience:

- Wave-particle duality: The behaviour of quantum-mechanical objects can often not be described in terms of particles of waves but must refer to both.
- Entanglement: particles can show correlations that are stronger than anything permitted by classical theory, even if they are far apart from each other.
- Uncertainty principle: certain pairs of physical properties, like position and momentum, cannot be simultaneously known to arbitrary precision. The process of measuring either of these properties affects the state of the system.
- Pairs of identical particles can not be in identical states (Fermions). However, different types of particles prefer to be in identical states (Bosons).

In vast parts of scientific and popular culture, some of these properties are described in misleading ways. A common example are statements like "entanglement is very fragile and is lost very quickly at temperatures significantly higher than absolute zero". Counterexamples include, e.g., the pairs of electrons in the ground states of the H_2 molecule or atomic Helium, which remain entangled in the singlet state for billions of years.

4.1.5 Is quantum mechanics relevant?

Quantum mechanics is often regarded as being relevant only on the sub-atomic scale. Evidence for this is that the Planck constant is one of the smallest constants used in physics (depending of course on the units used). Nevertheless, manifestations of quantum mechanical principles abound in our daily lives. This includes fundamental questions like the source of energy for the sun, chemical reactions, or on a very fundamental scale why object usually do not overlap[41]. This is closely related to the question why atoms are so big that they consist mostly of empty space, plus a tiny nucleus and point-like electrons.

In the context of condensed matter physics, quantum mechanics explains why some objects (like glass) are transparent, while others are opaque and why some objects support electrical currents (like graphite), while others do not (like diamond) although they consist of the same constituents. Another example is the existence of (ferro-)magnetic materials, which can not be explained by classical physics.

4.2 General structure

4.2.1 Spectral lines and stationary states

In a way, quantum mechanics started almost two hundred years ago when scientists like Wollaston and Fraunhofer first observed distinct lines in optical spectra. Later on Kirchhoff and Bunsen showed that the spectral lines were characteristic for the different chemical elements and thus established a connection between optics and what later became atomic physics. About a hundred years ago early quantum theory established that:

1. electromagnetic radiation is emitted and absorbed in quanta, or photons, whose energy is proportional to their frequency, and
2. atoms possess certain stationary states with fixed energies. The differences of these en-

ergy values are equal to the energies of the photons emitted or absorbed in transitions.

Schrödinger showed that the stationary states could be described by wave functions whose dynamics was determined by an equation that was later named after him. The possible (quantized) energy values arose from an eigenvalue problem related to the Schrödinger equation. It did not take long to show that Schrödinger's theory was completely equivalent to approaches by Heisenberg and by Pauli which involved an algebraic eigenvalue problem.

4.2.2 Vectors in Hilbert space

One of the most strikingly counter-intuitive features of quantum mechanics is the linear structure of its state space. As it turns out this property is also extremely important for the application of quantum mechanics to information processing. In classical mechanics the state of a finite number of interacting point particles is uniquely specified by a vector of generalized coordinates and momenta. In quantum mechanics, the state of the system is also uniquely specified, this time by a vector in Hilbert space. In both cases, linear combinations of two admissible vectors are again admissible vectors. The difference lies in the meaning and interpretation of the vector components. Classically the components are coordinates and momenta which have definite values in every admissible state, leading to definite predictions for the outcomes of all conceivable physical measurements. In the quantum case, Hilbert space vector components denote probability amplitudes related to the possible outcomes of certain measurements. This leads to the standard probabilistic interpretation of superpositions of Hilbert space vectors.

The superposition principle is one of the most fundamental concepts of quantum mechanics, but not all of its consequences are fully explored. It relates not only to the states themselves, but also to the evolution under the Hamiltonian. Whether it remains valid in the context of general relativity is an open question: a superposition of two position states of a massive particle implies that the space-time structure, which is distorted by the particle's mass, also is in a superposition state.

It is important to note that even the Hilbert spaces of very simple systems can have infinite dimension. A single hydrogen atom in free space has countably infinitely many bound states plus a continuum of scattering states. For the time being we neglect the continuous spectrum, assuming that we can suppress transitions into continuum states. For mathematical simplicity we even assume that the dimension d of the Hilbert space is finite. $d = 2$ will be the important special case of a single quantum bit, or qubit.

The Hilbert space thus is a d-dimensional complex linear space: every linear combination of states (Hilbert space vectors) is a state too; scalar product, norm, etc., can be defined as usual. The common quantum mechanical abbreviation for a complex column vector is a Dirac ket:

$$|a\rangle = \begin{pmatrix} a_1 \\ a_2 \\ \cdot \\ \cdot \\ a_d \end{pmatrix}.$$

The corresponding row vector is a Dirac bra:

$$\langle a| = (a_1^*, a_2^*, \ldots, a_d^*),$$

where the asterisk denotes complex conjugation.

In view of the probabilistic interpretation of quantum mechanics, it suffices to consider normalized states $|\psi\rangle$, that is, $|||\psi\rangle||^2 := \langle\psi|\psi\rangle = 1$. Furthermore the states $|\psi\rangle$ and $e^{i\alpha}|\psi\rangle(\alpha$ real) are physically equivalent: overall phase factors do not matter. However, *relative* phases between components of a state are *extremely* important:$|\phi\rangle + |\psi\rangle$ and $|\phi\rangle + e^{i\alpha}|\psi\rangle$ (for $\alpha \neq 0$) may have completely different physical properties, and many of the most interesting quantum mechanical phenomena are interference effects related to such relative phases.

4.2.3 Operators in Hilbert space

Operators map states to each other linearly; they thus are $d \times d$ complex matrices operating on the d-dimensional Hilbert space:

$$\mathbf{R}|\psi\rangle = |\phi\rangle.$$

Operators will be denoted by boldface letters. An *eigenstate* (or eigenvector) $|\phi_q\rangle$ of an operator $\mathbf{Q}$ fulfills the eigenvalue equation

$$\mathbf{Q}|\phi_q\rangle = q|\phi_q\rangle,$$

where the complex number q is called the *eigenvalue*. The eigenvalues of different eigenstates can be equal; this is called *degeneracy*. A trivial example is the unit operator $\mathbf{1}$ ($d \times d$ unit matrix) all of whose eigenvalues are equal to unity.

Observables (measurable quantities) correspond to *self-adjoint* or *Hermitian* matrices, that is,

$$\mathbf{A}^\dagger = \mathbf{A}; \quad (\mathbf{A}^\dagger)_{ij} := (\mathbf{A})^*_{ji}. \tag{4.1}$$

Self-adjoint operators possess real eigenvalues (the eigenvalues are the possible outcomes of a measurement and thus have to be real); the eigenstates $|a_i\rangle$ corresponding to the eigenvalues a_i of the operator $\mathbf{A}$ are pairwise orthogonal (or can be orthogonalized in the case of degeneracy). Thus they form a *basis* in Hilbert space,

$$\begin{aligned} \mathbf{A}|a_i\rangle &= a_i|a_i\rangle \quad \langle a_i|a_j\rangle = \delta_{ij} \\ & (i,j = 1,\ldots,d), \end{aligned} \tag{4.2}$$

where δ_{ij} is the familiar Kronecker symbol. (It should be kept in mind that we are operating in a finite-dimensional Hilbert space where all states can be normalized to unity.)

The sets of eigenstates and eigenvalues characterize an observable $\mathbf{A}$ completely, because any arbitrary state can be expanded in eigenstates of $\mathbf{A}$, which obey (4.2). This leads to the *spectral representation* of $\mathbf{A}$. To define that representation we need a further class of operators: *projection operators* or *projectors* for short. The projector $\mathbf{P}_i$ onto the eigenstate $|a_i\rangle$ (or, more correctly, to the subspace spanned by $|a_i\rangle$) is defined by

$$\mathbf{P}_i := |a_i\rangle\langle a_i|.$$

Application of $\mathbf{P}_i$ to an arbitrary state $|\psi\rangle$ yields a multiple of $|a_i\rangle$

$$\mathbf{P}_i|\psi\rangle = |a_i\rangle\langle a_i|\psi\rangle = \langle a_i|\psi\rangle|a_i\rangle,$$

where $|\langle a_i|\psi\rangle|$is the "length" of the projection of $|\psi\rangle$ onto the unit vector $|a_i\rangle$. Since the vectors $|a_i\rangle$ are orthonormal (4.2), we have

$$\mathbf{P}_i\mathbf{P}_j = \delta_{ij}\mathbf{P}_j; \text{ especially } \mathbf{P}_i^2 = \mathbf{P}_i.$$

These equations have obvious geometrical interpretations: two subsequent projections yield zero when they project onto different orthogonal subspaces; when they project onto the same subspace the second projection has no effect. From $\mathbf{P}^2 = \mathbf{P}$ we see immediately that the only possible eigenvalues of a projector are zero and unity. The projector to the subspace spanned by $|a_i\rangle$ and $|a_j\rangle$ is simply $\mathbf{P}_i + \mathbf{P}_j$. This projector also has the characteristic property of being equal to its square. As the $\mathbf{P}_i$ cover "all directions" of Hilbert space we obtain a completeness relation:

$$\sum_{i=1}^{d} \mathbf{P}_i = \sum_{i=1}^{d} |a_i\rangle\langle a_i| = \mathbf{1}.$$

Now the *spectral representation* of $\mathbf{A}$ can be defined:

$$\mathbf{A} = \sum_{i=1}^{d} a_i\mathbf{P}_i = \sum_{i=1}^{d} a_i|a_i\rangle\langle a_i|.$$

4.2.4 The Schrödinger equation

The stationary states of a quantum system are eigenstates of a special operator, the Hamiltonian operator (or Hamiltonian, for short), whose eigenvalues are the energy values of the stationary states. This follows from the *Schrödinger equation* (often called the "time-dependent" Schrödinger equation) governing the evolution of an arbitrary state $|\psi(t)\rangle$,

$$\frac{d}{dt}|\psi(t)\rangle = -\frac{i}{\hbar}\mathcal{H}|\psi(t)\rangle, \tag{4.3}$$

where $\mathcal{H}$ is the Hamiltonian. If the Hamiltonian is time-independent and $|\phi_i\rangle$ is an eigenstate of the Hamiltonian with energy eigenvalue ε_i:

$$\mathcal{H}|\phi_i\rangle = \varepsilon_i|\phi_i\rangle, \tag{4.4}$$

then $|\phi_i\rangle$ will evolve into

$$|\psi(t)\rangle = \exp\left(-i\frac{\varepsilon_i t}{\hbar}\right)|\phi_i\rangle.$$

So $|\psi(t)\rangle$ is a solution of the time-dependent Schrödinger equation with initial condition

$$|\psi(t=0)\rangle = |\phi_i\rangle.$$

Obviously $|\psi(t)\rangle$ is a *stationary* state, as a global phase factor has no physical significance.

The eigenvalue equation (4.4) is often called the "time-independent Schrödinger equation". As any initial state $|\psi(t=0)\rangle$ can be expressed as a linear combination of eigenstates $|\phi_i\rangle$ of $\mathcal{H}$, the initial value problem is solved (at least in principle).

4.2.5 Time evolution

Formally the solution for *time-independent* $\mathcal{H}$ can be written as

$$\begin{aligned} |\psi(t)\rangle &= \mathbf{U}(t)|\psi(t=0)\rangle \qquad (4.5)\\ &:= \exp\left(-i\frac{\mathcal{H}t}{\hbar}\right)|\psi(t=0)\rangle. \end{aligned}$$

The *time evolution operator* $\mathbf{U}(t)$ may be interpreted in two ways:
(i) as a power series

$$\begin{aligned} \exp\left(-i\frac{\mathcal{H}t}{\hbar}\right) &= \mathbf{1} + \left(-i\frac{\mathcal{H}t}{\hbar}\right) + \frac{1}{2}\left(-i\frac{\mathcal{H}t}{\hbar}\right)^2 \\ &\quad + \frac{1}{6}\left(-i\frac{\mathcal{H}t}{\hbar}\right)^3 + \cdots \qquad (4.6) \end{aligned}$$

(ii) by means of the spectral representation

$$\exp\left(-i\frac{\mathcal{H}t}{\hbar}\right) = \sum_{i=1}^{d} \exp\left(-i\frac{\varepsilon_i t}{\hbar}\right)|\phi_i\rangle\langle\phi_i|.$$

Version (ii) is easy to use of the eigenvalues are known. (i) does not require diagonalization but convergence is only guaranteed for short times, $\mathcal{H}t/\hbar < 1$.

For a more general Hamiltonian $\mathcal{H}(t)$ depending on time, the time evolution operator $\mathbf{U}(t)$ (as defined by $|\psi(t)\rangle = \mathbf{U}(t)|\psi(0)\rangle$) obeys an operator differential equation; for a general time dependence of $\mathcal{H}$ the solution of that equation is not known, even for $d = 2$, but it can be approximated numerically.

All eigenvalues $\exp\left(-i\frac{\varepsilon_i t}{\hbar}\right)$ of $\mathbf{U}(t)$ have unit modulus; operators with this property are called *unitary*. A unitary operator $\mathbf{U}$ preserves all scalar products, that is, the scalar product of $|\psi\rangle$ and $|\chi\rangle$ equals that of $\mathbf{U}|\psi\rangle$ and $\mathbf{U}|\chi\rangle$; consequently *norms* are preserved too. The general property characterizing unitarity is

$$\mathbf{U}^\dagger\mathbf{U} = \mathbf{1} \Leftrightarrow \mathbf{U}^\dagger = \mathbf{U}^{-1}.$$

For time-independent $\mathcal{H}$ we have

$$(\mathbf{U}(t))^{-1} = \mathbf{U}(-t),$$

that is, unitary time evolution is *reversible.*The states $|a_i\rangle$ are now the eigenstates of $\mathbf{A}$ and a_i its eigenvalues. Physically this means that an arbitrary state is first decomposed into components along eigenstates of $\mathbf{A}$, and then each of these components is treated according to its eigenstate property (4.2). It should be noted that the spectral representation is possible not only for observables (4.1) but for the larger class of *normal* operators $\mathbf{B}$ with $\mathbf{B}^\dagger\mathbf{B} = \mathbf{B}\mathbf{B}^\dagger$.

4.2.6 Measurements

The process of measurement in quantum mechanics is difficult to grasp since it involves phenomena at the border between the quantum system and its environment, including the observer. In this section we will stay quite formal and just state the *projection postulate* which is usually employed to describe the measurement process. A more physical discussion of the postulate and its interpretation will follow in Section 4.5 .

The situation to which the postulate refers is that of a quantum system prepared in a state $|\psi\rangle$. After preparation a single measurement of the observable $\mathbf{A}$ is performed. This cycle of preparation and measurement is repeated many times so that the notion of probability used in the postulate makes sense. Alternatively we may imagine an ensemble containing a large number of independent copies of the quantum system, all prepared in the same state $|\psi\rangle$. $\mathbf{A}$ is measured for all system copies independently.

> POSTULATE: A single measurement of the observable $\mathbf{A}$ in the normalized state $|\psi\rangle$ yields one of the eigenvalues a_i of $\mathbf{A}$ with probability $|\langle a_i|\psi\rangle|^2$ ($\sum_i |\langle a_i|\psi\rangle|^2 = 1$ due to normalization).

Immediately after the measurement the system is in the (normalized) state

$$\frac{\mathbf{P}_i|\psi\rangle}{||\mathbf{P}_i|\psi\rangle||}, \tag{4.7}$$

where $\mathbf{P}_i$ is the projection operator onto the subspace of eigenstates of $\mathbf{A}$ with eigenvalue a_i. This subspace is one-dimensional if the eigenvalue a_i is non-degenerate. Any measurement thus leads to a *reduction of the wave function*.

In general it is not possible to predict the outcome of a single measurement. A measurement of $\mathbf{A}$ on an ensemble of systems as discussed above yields the *average* (expectation value)

$$\langle \mathbf{A} \rangle := \langle \psi|\mathbf{A}|\psi\rangle$$

with deviations described by the *variance* (the square of the standard deviation)

$$\langle (\mathbf{A} - \langle \mathbf{A} \rangle)^2 \rangle \geq 0.$$

The variance vanishes if and only if $|\psi\rangle$ is an eigenstate of $\mathbf{A}$.

This chapter describes two fundamentally different kinds of change of state: the time evolution governed by the Hamiltonian, which is unitary, deterministic and reversible (at least for a time-independent Hamiltonian), and the measurement process, which is probabilistic and irreversible. From an aesthetic point of view this is a very unpleasant situation. After all, quantum mechanics is supposed to be valid for the whole system, including the measurement apparatus, at least in principle, and then it is hard to see why a measurement (an interaction between the apparatus and the system) should be fundamentally different from other dynamical processes in the system. This is one of the questions that have kept the measurement process discussion going for many decades. In Section 4.5 we will return to the measurement process in order to discuss in a little more detail those aspects that are relevant for quantum information processing.

4.3 Quantum states

4.3.1 The two-dimensional Hilbert space: qubits, spins, and photons

In many situations, only two states of a quantum system are important. Examples include the ground and first excited states of an atom and a single spin-1/2 particle fixed in space. A photon can be in one of two mutually orthogonal polarization states: horizontal and vertical if it is linearly polarized, or left and right if it is circularly polarized.

In order to keep the analogy to classical bits as close as possible, it is convenient to choose such two-state systems for the discussion of quantum computing. Any quantum system with a two-dimensional Hilbert space can store a *quantum bit* or *qubit*. Any two mutually orthogonal states in this Hilbert space can be chosen as the computational basis states $|0\rangle$ and $|1\rangle$; they correspond to the states “logical 0” and “logical 1” of a classical bit. In contrast to a classical bit, however, a qubit can also exist in any arbitrary linear combination of the computational basis states.

We briefly discuss some properties of single qubits in this section. For definiteness we assume that the qubits are represented by spin-1/2 particles possessing a magnetic moment which can be influenced by an external magnetic field $\vec{B}$. This analogy between qubits and spin-1/2 particles was first noted by Feynman, Vernon and Hellwarth [42]. It allows one to treat any two-dimensional Hamiltonian subspace as a virtual spin-1/2, often called a pseudo-spin.

The Hilbert space of a single spin-1/2 particle is spanned by two basis states, which we choose in the following way:

$$\begin{aligned} \begin{pmatrix} 1 \\ 0 \end{pmatrix} &= |\uparrow\rangle = |0\rangle \qquad (4.8) \\ \begin{pmatrix} 0 \\ 1 \end{pmatrix} &= |\downarrow\rangle = |1\rangle. \end{aligned}$$

(The identification with the computational basis states $|0\rangle$ and $|1\rangle$ follows the convention of [35].) All operators in this Hilbert space can be combined from the four fundamental operators

$$\begin{aligned} \mathbf{P}_\uparrow &= \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = |\uparrow\rangle\langle\uparrow| \qquad (4.9) \\ \mathbf{P}_\downarrow &= \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = |\downarrow\rangle\langle\downarrow| \end{aligned}$$

$$\begin{aligned} \mathbf{S}^+ &= \hbar\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \hbar|\uparrow\rangle\langle\downarrow| \qquad (4.10) \\ \mathbf{S}^- &= \hbar\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \hbar|\downarrow\rangle\langle\uparrow|. \end{aligned}$$

$\mathbf{S}^+$ and $\mathbf{S}^-$ are called the raising and lowering operator, respectively. More convenient for the purposes of physics are the following combinations:

$$\mathbf{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \mathbf{P}_\uparrow + \mathbf{P}_\downarrow \qquad (4.11)$$

$$\mathbf{S}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \frac{\hbar}{2}(\mathbf{P}_\uparrow - \mathbf{P}_\downarrow) = \frac{\hbar}{2}\mathbf{Z} \qquad (4.12)$$

$$\mathbf{S}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \frac{1}{2}(\mathbf{S}^+ + \mathbf{S}^-) = \frac{\hbar}{2}\mathbf{X} \qquad (4.13)$$

$$\mathbf{S}_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \frac{i}{2}(\mathbf{S}^- - \mathbf{S}^+) = \frac{\hbar}{2}\mathbf{Y}. \qquad (4.14)$$

The spin matrices $\mathbf{S}_\alpha$ obey the usual angular momentum commutation relations

$$[S_x, S_y] = i\hbar S_z,$$

and they are their own inverses (up to a factor):

$$\mathbf{S}_x^2 = \mathbf{S}_y^2 = \mathbf{S}_z^2 = \frac{\hbar^2}{4}\mathbf{1}.$$

The matrices $\mathbf{X}, \mathbf{Y}$, and $\mathbf{Z}$ have eigenvalues ±1 and are commonly known as *Pauli matrices*.

4.3.2 Hamiltonian and evolution

The $\mathbf{S}_\alpha$ can be used to write the Hamiltonian of a spin-1/2 particle (fixed in space) in an external field with components B_x, B_y, B_z:

$$\mathcal{H} = -\vec{B}\cdot\vec{\mathbf{S}} = -(B_x\mathbf{S}_x + B_y\mathbf{S}_y + B_z\mathbf{S}_z). \qquad (4.15)$$

Usually the Hamiltonian (4.15) contains pre-factors related to the nature of the particle, like the g factor and the Bohr magneton. At this point, however, those pre-factors do not matter and are eliminated by using appropriate units for $\vec{B}$. Note that (4.15) is, apart from trivial modifications, the most general Hermitian single-qubit operator.

It is evident why $\mathbf{X}$ is also often called the “NOT gate” in the language of quantum computing: it maps the two computational basis states onto each other. Any unitary 2 × 2 matrix is a valid quantum gate, for example the $\mathbf{Z}$ gate, which generates a π relative phase between the computational basis states.

We will also frequently encounter the Hadamard gate

$$\mathbf{H} = \frac{1}{\sqrt{2}}(\mathbf{X} + \mathbf{Z}) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \qquad (4.16)$$

H (hopefully not to be confused with the Hamiltonian $\mathcal{H}$) is at the same time unitary and Hermitian, implying that $\mathbf{H}^2 = \mathbf{1}$. Nevertheless **H** is sometimes called the "square-root of NOT" gate, because it turns $|0\rangle$ into a state "halfway between" $|0\rangle$ and $|1\rangle$ and similarly for $|1\rangle$. However, in contrast to real $\sqrt{\text{NOT}}$, applying it twice does not result in a NOT.

We can describe the time evolution via the evolution operator $\mathbf{U}(t)$ for a $\vec{B}$ field along one of the coordinate axes $\alpha = x, y, z$.

$$\begin{aligned} \mathbf{U}(t) &= \exp\left(-\frac{i\mathcal{H}t}{\hbar}\right) && (4.17)\\ &= \exp\left(\frac{iB_\alpha t}{2}\frac{2\mathbf{S}_\alpha}{\hbar}\right). \end{aligned}$$

The solution can be obtained by expanding the exponential function

$$\begin{aligned} e^x &= 1 + x + \frac{x^2}{2!} + \cdots = \sum_{n=0}^{\infty}\frac{x^n}{n!}\\ \exp\left(-\frac{i\mathcal{H}t}{\hbar}\right) &= \mathbf{1} - \frac{i\mathcal{H}t}{\hbar} - \frac{1}{2}\left(\frac{\mathcal{H}t}{\hbar}\right)^2 + \ldots \end{aligned}$$

As the square of the operator $2\mathbf{S}_\alpha/\hbar$ is equal to the unit operator, all even terms of the power series expansion (4.6) of the exponential in $\mathbf{U}(t)$ are proportional to $\mathbf{1}$, whereas all odd terms are proportional to $2\mathbf{S}_\alpha$, and thus

$$\mathbf{U}(t) = \cos\left(\frac{B_\alpha t}{2}\right)\mathbf{1} + i\sin\left(\frac{B_\alpha t}{2}\right)\frac{2\mathbf{S}_\alpha}{\hbar}. \quad (4.18)$$

For $\alpha = z$ we have

$$\mathbf{U}(t) = \begin{pmatrix} \exp\left(i\frac{B_z t}{2}\right) & 0 \\ 0 & \exp\left(-i\frac{B_z t}{2}\right) \end{pmatrix}.$$

For the initial state, we choose, as a simple example,

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

Applying $\mathbf{U}(t)$ to this state yields

$$\mathbf{U}(t)|\uparrow\rangle = |\psi(t)\rangle = \exp\left(i\frac{B_z t}{2}\right)|\psi(0)\rangle,$$

which is a stationary state, as expected, because the initial state was an eigenstate of $\mathbf{S}_z$ (and thus of $\mathcal{H}$).

The case $\alpha = x$ is different; (4.18) leads to

$$\mathbf{U}(t) = \begin{pmatrix} \cos\left(\frac{B_x t}{2}\right) & i\sin\left(\frac{B_x t}{2}\right) \\ i\sin\left(\frac{B_x t}{2}\right) & \cos\left(\frac{B_x t}{2}\right) \end{pmatrix}, \quad (4.19)$$

consequently

$$\begin{aligned} |\psi(t)\rangle &= \begin{pmatrix} \cos\left(\frac{B_x t}{2}\right) \\ i\sin\left(\frac{B_x t}{2}\right) \end{pmatrix} && (4.20)\\ &= \cos\left(\frac{B_x t}{2}\right)|\uparrow\rangle + i\sin\left(\frac{B_x t}{2}\right)|\downarrow\rangle. \end{aligned}$$

This state runs through a continuum of states periodically and thus performs a kind of "uniform rotation in Hilbert space". The result for $\alpha = y$ is similar.

4.3.3 Vector representation

The most general state in the Hilbert space of a single qubit is an arbitrary normalized linear combination of $|\uparrow\rangle$ and $|\downarrow\rangle$ which may be parametrized, for example, by two angles:

$$\begin{aligned} |\theta,\phi\rangle : &= \exp(-i\phi/2)\cos\frac{\theta}{2}|\uparrow\rangle && (4.21)\\ &\quad + \exp(i\phi/2)\sin\frac{\theta}{2}|\downarrow\rangle\\ &\quad (0 \le \theta \le \pi; 0 \le \phi \le 2\pi). \end{aligned}$$

Thus a qubit in a sense contains two (bounded) *real* numbers' worth of information, in contrast to the single binary number contained in a classical bit. Unfortunately, however, not all of this information is accessible and robust. The question of how to read, write, and manipulate part of this information will keep us busy throughout this course.

Figure 4.1 shows how the two angles (θ, ϕ) parametrize the surface of a sphere, the *Bloch sphere*, which is often helpful in visualizing state changes of single qubit systems. Every Hilbert

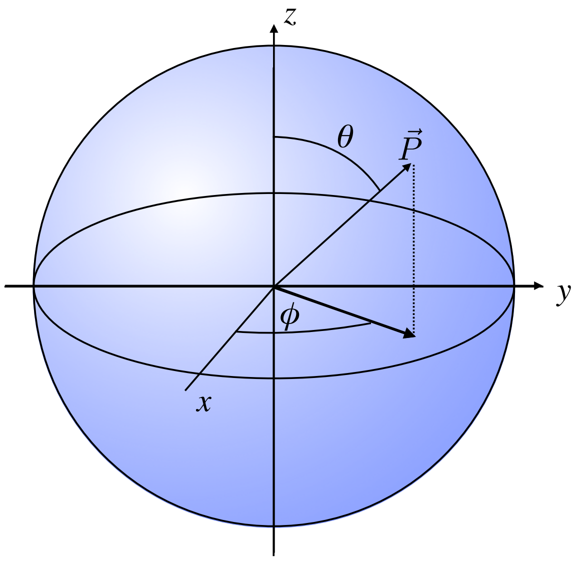


Figure 4.1: Polarization vector $\vec{P}$ in the Bloch sphere.

space vector (or pure state) of a single qubit is represented by a point on the surface of the Bloch sphere. Every unitary single-qubit operator is (apart from a global phase factor) a rotation of the Bloch sphere, as will be discussed in more detail in Chapter 5. In the next subsection we will encounter a different kind of states, called mixed states. The mixed states of a single qubit will be seen to populate the interior of the Bloch sphere. (→ section 4.4.3).

4.3.4 Coupling to environment

> “Stepping up from one qubit to two is a bigger leap than you might expect. Much that is weird and wonderful about quantum mechanics can be appreciated by considering the properties of the quantum states of two qubits.” (John Preskill [32]).

In the real world there are no isolated spin-1/2 particles; quantum systems always couple to the “environment” which we often cannot or do not want to take into account in our quantum mechanical considerations. However, if we consider a quantum system which is in reality only part of a larger system, the following “articles of faith” to which we have become accustomed when dealing with isolated quantum systems are no longer always true:

- States are vectors in Hilbert space.
- Measurements are orthogonal projections onto the final state.
- Time evolution is unitary.

The simplest example is given by one qubit A which we call “system”, and to which we have access and another qubit B which we call “environment” and to which we have no access. The two pairs of states $\{|\uparrow\rangle_A, |\downarrow\rangle_A\}$ and $\{|\uparrow\rangle_B, |\downarrow\rangle_B\}$ are orthonormal bases for the Hilbert spaces of the two subsystems. The two qubit system with its four-dimensional Hilbert space is the simplest possible setting for a discussion of the concepts of pure and mixed states of a single subsystem, and of entanglement between subsystems.

If the subsystems A and B are in states $|\psi\rangle_A$ and $|\phi\rangle_B$, respectively, the combined system is in a direct product state which we denote by $|\psi\rangle_A \otimes |\phi\rangle_B$. Direct product states are often simply called product states and later on we will often use shorthand notations like $|\uparrow\uparrow\rangle$ for $|\uparrow\rangle_A \otimes |\uparrow\rangle_B$. Presently, however, we will stick to the somewhat clumsy but unambiguous notation with the subscripts A and B and the direct product sign $\otimes$.

Product states are the simplest, but by no means the only possible states of the combined system. According to the general superposition principle of quantum mechanics, any linear combination of product states, like $|\psi\rangle_A \otimes |\phi\rangle_B + |\chi\rangle_A \otimes |\lambda\rangle_B$ is a possible state of the combined system.

4.3.5 Entangled with environment

This leads us straight to the definition of entanglement for a bipartite system. 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. A word of caution is in order here: a state which does not look like a product state at first sight may be one after all. An entangled state cannot be written as a product state in *any* basis. In contrast, a state which can be written as a product state in *some* basis is called *separable*.

We consider the two-qubit state

$$|\psi\rangle = a\,|\uparrow\rangle_A \otimes |\uparrow\rangle_B + b\,|\downarrow\rangle_A \otimes |\downarrow\rangle_B . \quad (4.22)$$

($|a|^2 + |b|^2 = 1$) which for general values of a and b is entangled. A measurement of the state of qubit A (in the computational basis) leaves the system in the state $|\uparrow\rangle_A \otimes |\uparrow\rangle_B$ with probability $|a|^2$ and in $|\downarrow\rangle_A \otimes |\downarrow\rangle_B$ with probability $|b|^2$. In both cases, after the measurement on A, the state of B is *fixed*.

Now we consider a measurement with a general observable $\mathbf{M}_A \otimes \mathbf{1}_B$, which acts only on A. The expectation value of this observable for a state $|\psi\rangle$ (4.22) is easily calculated since $\mathbf{1}_B$ does not change $|...\rangle_B$ states and since ${}_B\langle\uparrow|\downarrow\rangle_B = 0$:

$$\begin{aligned}
&= \langle \mathbf{M}_A \rangle \\
&= \langle \psi | \mathbf{M}_A \otimes \mathbf{1}_B | \psi \rangle \\
&= \Big[a^* \; {}_A\langle\uparrow| \otimes_B \langle\uparrow| + b^* \; {}_A\langle\downarrow| \otimes_B \langle\downarrow| \Big] \\
&\quad \mathbf{M}_A \otimes \mathbf{1}_B \\
&\quad \Big[a\,|\uparrow\rangle_A \otimes |\uparrow\rangle_B + b\,|\downarrow\rangle_A \otimes |\downarrow\rangle_B \Big] \\
&= |a|^2 \; {}_A\langle\uparrow|\mathbf{M}_A|\uparrow\rangle_A + |b|^2 \; {}_A\langle\downarrow|\mathbf{M}_A|\downarrow\rangle_A
\end{aligned}$$

4.3.6 Density operator

The expression ${}_A\langle\uparrow|\mathbf{M}_A|\uparrow\rangle_A$ can be written as $\mathrm{Tr}_A(\mathbf{P}_{\uparrow A}\mathbf{M}_A)$, and correspondingly for $|\downarrow\rangle$. Here $\mathbf{P}_{\uparrow A}$ and $\mathbf{P}_{\downarrow A}$ are the projectors (4.9) for the system A; Tr_A denotes the trace (sum of the diagonal elements) in the Hilbert space of A, that is,

$$\mathrm{Tr}_A\,\mathbf{O} = {}_A\langle\uparrow|\mathbf{O}|\uparrow\rangle_A + {}_A\langle\downarrow|\mathbf{O}|\downarrow\rangle_A \quad (4.23)$$

for any operator $\mathbf{O}$. With this notation, the expectation value becomes

$$\begin{aligned}
\langle \mathbf{M}_A \rangle &= \mathrm{Tr}_A \left(|a|^2\, \mathbf{P}_{\uparrow A}\, \mathbf{M}_A + |b|^2\, \mathbf{P}_{\downarrow A}\, \mathbf{M}_A \right) \\
&= \mathrm{Tr}_A \left(\left[|a|^2\, \mathbf{P}_{\uparrow A} + |b|^2\, \mathbf{P}_{\downarrow A} \right] \mathbf{M}_A \right) \\
&= \mathrm{Tr}_A \left(\boldsymbol{\rho}_A \mathbf{M}_A \right).
\end{aligned}$$

The quantity

$$\boldsymbol{\rho}_A = |a|^2 \mathbf{P}_{\uparrow A} + |b|^2 \mathbf{P}_{\downarrow A} = \begin{pmatrix} |a|^2 & 0 \\ 0 & |b|^2 \end{pmatrix} \quad (4.24)$$

is the *density operator* (density matrix) of the system A. It is Hermitian (4.1), positive (no negative eigenvalues) and its trace is unity (due to normalization). It is important to note that *every* operator with these properties is a density operator, be it diagonal or not, in the basis which we have chosen accidentally or thoughtfully! Due to these properties every density operator can be written as a *convex combination* (a linear combination with positive coefficients whose sum equals unity) of orthogonal projectors. [1]

If $\boldsymbol{\rho}_A^2 = \boldsymbol{\rho}_A$ (for example if $|a| = 1$ in our example) $\boldsymbol{\rho}_A$ is a single projector onto a vector in Hilbert space. (Projectors onto higher-dimensional subspaces are excluded by $\mathrm{Tr}_A\,\boldsymbol{\rho} = 1$.) In that case $\boldsymbol{\rho}_A$ is called a *pure state*; otherwise it is called a *mixed state*. (Mixed states are also often called "incoherent superpositions" by people with an optics background.) In our example, $\boldsymbol{\rho}_A$ (4.24) is a mixed state if both a and b are nonzero, that is if and only if $|\psi\rangle$ (4.22) is an entangled state. This connection between entanglement and mixing turns out to hold beyond our simple example.

4.3.7 Product states

As a second example let us now consider a state in which the systems A and B are not entangled,

---

[1] In fact, this is the standard way to introduce the density operator in statistical mechanics. There, an ensemble of many copies of a given quantum system is considered. Each system can be in any one of a set of quantum states $|\psi_i\rangle$, with probability p_i. The density operator describing that ensemble is $\boldsymbol{\rho} = \sum_i p_i |\psi_i\rangle\langle\psi_i|$.

that is, a product state (in fact, the most general two-qubit product state):

$$|\Phi\rangle = \Big(a|\uparrow\rangle_A + b|\downarrow\rangle_A\Big) \otimes \Big(c|\uparrow\rangle_B + d|\downarrow\rangle_B\Big) \tag{4.25}$$

with $|a|^2 + |b|^2 = |c|^2 + |d|^2 = 1$. For that state the expectation value becomes

$$\begin{aligned}
&= \langle \mathbf{M}_A \rangle \\
&= \langle \Phi | \mathbf{M}_A \otimes \mathbf{1}_B | \Phi \rangle \\
&= \Big[a^* \ {}_A\langle\uparrow| + b^* \ {}_A\langle\downarrow|\Big] \mathbf{M}_A \Big[a\,|\uparrow\rangle_A + b\,|\downarrow\rangle_A\Big] \\
&\quad \Big[c^* \ {}_B\langle\uparrow| + d^* \ {}_B\langle\downarrow|\Big] \mathbf{1}_B \Big[c\,|\uparrow\rangle_B + d\,|\downarrow\rangle_B\Big] \\
&= |a|^2 \ {}_A\langle\uparrow|\mathbf{M}_A|\uparrow\rangle_A + |b|^2 \ {}_A\langle\downarrow|\mathbf{M}_A|\downarrow\rangle_A \\
&\quad + a^* b \ {}_A\langle\uparrow|\mathbf{M}_A|\downarrow\rangle_A + b^* a \ {}_A\langle\downarrow|\mathbf{M}_A|\uparrow\rangle_A \\
&= \mathrm{Tr}_A \Bigg(\mathbf{M}_A \Big[|a|^2 \mathbf{P}_{\uparrow A} + |b|^2 \mathbf{P}_{\downarrow A} \\
&\quad + a^* b \frac{\mathbf{S}_A^-}{\hbar} + b^* a \frac{\mathbf{S}_A^+}{\hbar}\Big]\Bigg) \\
&= \mathrm{Tr}_A \left(\mathbf{M}_A \boldsymbol{\rho}_A\right).
\end{aligned}$$

Again $\boldsymbol{\rho}_A$ is Hermitian and of unit trace, but obviously *not* diagonal; in the usual basis (4.8) it is

$$\boldsymbol{\rho}_A = \begin{pmatrix} |a|^2 & b^* a \\ a^* b & |b|^2 \end{pmatrix}.$$

Nevertheless $\boldsymbol{\rho}_A^2 = \boldsymbol{\rho}_A$, as we can easily verify, i.e. the system is in a pure state.

4.4 Quantum vs. classical

4.4.1 Entanglement and mixing

As we have seen above, the density matrix of A is a pure state if the (pure) state of the combined system $A + B$ is a product state (that is, not entangled). If the (pure) state of the combined system $A + B$ is entangled, the summation over all possibilities for the state of B ("partial trace over the Hilbert space of B") leads to the loss of the phases of the complex numbers a and b and we end up with a mixed state, as observed in the previous example involving the state (4.22).

The following general picture for the loss of coherence (as encoded in the phases of the initial pure state probability amplitudes) thus emerges: in the beginning, system (A) and environment (B) are not entangled. The system's density matrix is initially pure. By interaction, the system and environment become entangled (we will see examples in later chapters) and the system's density matrix becomes mixed.

We stress that the pure or mixed character of a density operator is independent of the choice of basis for the Hilbert space of interest. It is thus completely unrelated to whether the density operator is diagonal or not. If $\boldsymbol{\rho}_A$ is a pure state, $\boldsymbol{\rho}_A^2 = \boldsymbol{\rho}_A$ holds in *any* basis. Fortunately it is not necessary to compute all matrix elements of $\boldsymbol{\rho}_A^2$ to check if $\boldsymbol{\rho}_A$ is pure. It suffices to check if the trace of $\boldsymbol{\rho}_A^2$ equals unity, because for mixed states that trace is strictly smaller than unity. (To see this, consider the basis in which $\boldsymbol{\rho}_A$ is diagonal, keeping in mind that the trace does not depend on the basis.)

Often, especially in experimental contexts, the diagonal elements of a density operator are called *populations* and the off-diagonal elements are called *coherences*. While a given density operator may be diagonal in one basis but non-diagonal in a different basis, distinguishing between diagonal and off-diagonal elements is meaningful if we use the eigenbasis of the Hamiltonian. In this basis, the diagonal elements represent populations of stationary states, while off-diagonal elements correspond, e.g., to precessing magnetization or oscillating electric dipole moments.

The "pedestrian" method of determining the density matrix $\boldsymbol{\rho}_A$ that we have used for the two simple examples above may be phrased more compactly, and more generally at the same time. Given a pure state $|\chi\rangle$ of the combined system $A + B$, the density operator of system A is obtained as

$$\boldsymbol{\rho}_A = \mathrm{Tr}_B\, |\chi\rangle\langle\chi| \qquad (4.26)$$

where Tr_B denotes the trace in the Hilbert space of B. The generalization to a mixed state of the compound system $A+B$ is obvious;

$$\boldsymbol{\rho}_A = \mathrm{Tr}_B\, \boldsymbol{\rho} \qquad (4.27)$$

is then usually called the *reduced density matrix* of A.

4.4.2 Bell states

Entanglement can be quantified beyond the crude yes/no level considered above. There exist several measures of entanglement, which will be discussed in section 4.6. A special class of states are the *maximally entangled* states, where the partial density operators are maximally mixed. For $a = \pm b = \frac{1}{\sqrt{2}}$ the state $|\psi\rangle$ (4.22) is maximally entangled. The four maximally entangled states

$$\begin{aligned} &\frac{1}{\sqrt{2}}\Big[|\uparrow\rangle_A \otimes |\uparrow\rangle_B \pm |\downarrow\rangle_A \otimes |\downarrow\rangle_B\Big] \\ &\frac{1}{\sqrt{2}}\Big[|\uparrow\rangle_A \otimes |\downarrow\rangle_B \pm |\downarrow\rangle_A \otimes |\uparrow\rangle_B\Big] \qquad (4.28) \end{aligned}$$

are known as *Bell states*; they are a basis (the Bell basis) of the two-qubit Hilbert space. The Bell states illustrate nicely how information can be hidden from local measurements, involving only one of the qubits A and B. In any of the states (4.28), any measurement of a single qubit will give completely random and (on average) identical results; these states cannot be distinguished by single-qubit measurements.

Entanglement between two quantum systems can only be created if they interact. Section 7.2.5 below, discusses an example where an initial product state of two spins-1/2 develops into a Bell state under the influence of an exchange interaction between the spins.

Up to now we have only considered pure states of the combined system $A+B$. We have discussed and quantified the entanglement between subsystems A and B, and we have defined the density operator for subsystem A by discarding the information on subsystem B. All this is also possible for mixed states of the combined system $A+B$; for example, the definition of the concurrence may be generalized to mixed two-qubit states [43, 44]. Thus mixed states of two qubits as well as pure states may be entangled to varying (but not arbitrary, see [45]) degrees. More general entanglement measures, extending, for example, beyond two qubits are a topic of ongoing research (see [46] and other articles in the same journal issue devoted to Quantum Information Theory). Some of them are discussed in section 4.6.1.

4.4.3 Bloch sphere

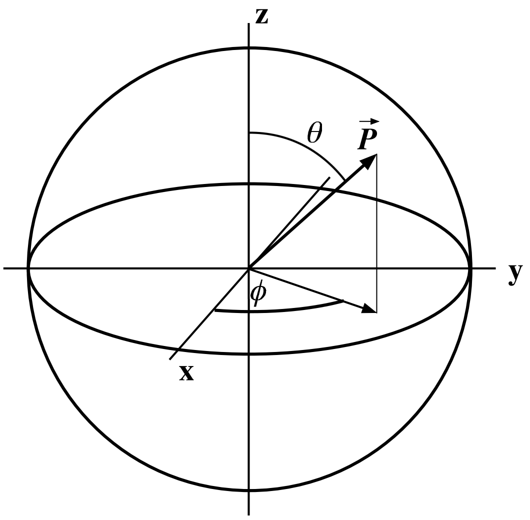


Figure 4.2: Polarization vector $\vec{P}$ on the Bloch sphere.

There is a useful graphic representation for single-qubit states; to derive it, note that every operator in the single-qubit Hilbert space can be written as a combination of the unit operator and the three spin matrices $\mathbf{S}_\alpha$ (eqs. (4.11) to (4.14)). As the spin matrices are Hermitian and traceless, the sum of $\frac{1}{2}\mathbf{1}$ plus any linear combination (with real coefficients) of the $\mathbf{S}_\alpha$ is Hermitian and has unit trace. Every 2×2 matrix with these properties can be written as

$$\frac{1}{2}\left(\mathbf{1}+\frac{2}{\hbar}\vec{P}\cdot\vec{\mathbf{S}}\right)=\frac{1}{2}\left(\begin{array}{cc}1+P_z & P_x-iP_y\\ P_x+iP_y & 1-P_z\end{array}\right) \tag{4.29}$$

where $\vec{P}$ is a real three-component vector. The eigenvalues of this matrix are

$$\lambda_\pm=\frac{1}{2}(1\pm|\vec{P}|), \tag{4.30}$$

that is, the matrix is positive if $|\vec{P}|\leq 1$. Thus the general single-qubit density matrix is

$$\boldsymbol{\rho}(\vec{P})=\frac{1}{2}\left(\mathbf{1}+\frac{2}{\hbar}\vec{P}\cdot\vec{\mathbf{S}}\right);\quad |\vec{P}|\leq 1. \tag{4.31}$$

The set of possible *polarization vectors* $\vec{P}$ is called the *Bloch sphere*; pure states have $|\vec{P}|=1$, since in that case one of the eigenvalues(4.30) vanishes. The physical meaning of the polarization vector is

$$\frac{1}{2}P_\alpha=\frac{1}{\hbar}\operatorname{Tr}\boldsymbol{\rho}\mathbf{S}_\alpha=\frac{1}{\hbar}\langle\mathbf{S}_\alpha\rangle. \tag{4.32}$$

In spherical coordinates, the polarization vector is

$$\vec{P}=r(\sin\theta\cos\phi,\sin\theta\sin\phi,\cos\theta). \tag{4.33}$$

4.4.4 Purity

For pure states $|\theta,\phi\rangle$ (4.21), $r=1$, while for mixed states $0\leq r<1$.

There is a simple general relation between the polarization vector $\vec{P}$ of the single-qubit density matrix $\boldsymbol{\rho}_A$ and the “purity” of $\boldsymbol{\rho}_A$. Among the many possible quantitative measures of purity of a single qubit density matrix we choose the quantity

$$\eta:=2\operatorname{Tr}\boldsymbol{\rho}^2-1. \tag{4.34}$$

A pure density matrix has $\eta=1$ and the “maximally mixed” density matrix $\boldsymbol{\rho}=\frac{1}{2}\mathbf{1}$ has $\eta=0$.

The quantity η can be written in terms of the eigenvalues of $\boldsymbol{\rho}$, and by (4.30), in terms of $\vec{P}$:

$$\eta=2(\lambda_+^2+\lambda_-^2)-1=|\vec{P}|^2=r^2. \tag{4.35}$$

The density matrix of the system A corresponding to the pure 2-qubit state $|\chi\rangle$ is in the usual basis (4.8)

$$\begin{aligned}\boldsymbol{\rho}_A(\chi) &= \operatorname{Tr}_B|\chi\rangle\langle\chi| \qquad (4.36)\\ &= \left(\begin{array}{cc}|\alpha|^2+|\beta|^2 & \alpha\gamma^*+\beta\delta^*\\ \alpha^*\gamma+\beta^*\delta & |\gamma|^2+|\delta|^2\end{array}\right).\end{aligned}$$

The determinant of $\boldsymbol{\rho}_A(\chi)$ is related to the concurrence C of $|\chi\rangle$:

$$\det\boldsymbol{\rho}_A(\chi)=\frac{1}{4}C^2, \tag{4.37}$$

and it can be expressed by the eigenvalues (4.30):

$$\det\boldsymbol{\rho}=\lambda_+\lambda_-=\frac{1}{4}(1-|\vec{P}|^2), \tag{4.38}$$

from which we conclude the desired relation

$$C^2=1-|\vec{P}|^2=1-\eta. \tag{4.39}$$

4.4.5 Time-dependence

Since there are no truly isolated systems (if there were we would have no way to notice!) the Schrödinger equation (4.3) is only an approximation which should be generalized to describe the dynamics of mixed states. This generalization is given by the *von Neumann equation* (often also called *Liouville–von Neumann equation* since it also generalizes the Liouville equation of classical statistical mechanics)

$$i\hbar\frac{d}{dt}\boldsymbol{\rho}=[\mathcal{H},\boldsymbol{\rho}]. \tag{4.40}$$

This equation is equivalent to Schrödinger’s equation (4.3) if $\boldsymbol{\rho}$ is a pure state. For time-independent $\mathcal{H}$ a formal solution analogous to (4.5) may be found:

$$\boldsymbol{\rho}(t)=\mathbf{U}(t)\boldsymbol{\rho}(t=0)\mathbf{U}(t)^\dagger \tag{4.41}$$

where

$$\mathbf{U}(t)=\exp\left(-i\frac{\mathcal{H}t}{\hbar}\right)$$

is again the time evolution operator.

A word of warning is in order at this point: all considerations above are only valid if $\mathcal{H}$ involves only degrees of freedom of the "system" and not of the "environment". As soon as system and environment are coupled by $\mathcal{H}$ the density operator $\boldsymbol{\rho}$ (of the system) is no longer sufficient to describe the dynamics consistently, and additional information or simplifying assumptions are necessary.

4.4.6 EPR correlations

Some aspects of quantum mechanics are radically different from classical mechanics. This can be illustrated by the *Einstein–Podolsky–Rosen* thought experiment [47] invented in 1935 by Albert Einstein, Boris Podolsky, and Nathan Rosen, with the intention of showing that quantum mechanics does not provide a complete description of nature. Ironically the discussion started by Einstein, Podolsky, and Rosen led to the discovery by John Bell in 1964 [48] that indeed correlations between separated quantum systems which are entangled due to interactions in the past can be stronger than is possible from any classical mechanism. This result was experimentally confirmed by several groups, most notably the group of Alain Aspect [49], showing that nature prefers quantum mechanics to a "complete description" in the sense of Einstein *et al.* At the same time these results show that there are "quantum tasks" which cannot be performed by any classical system.

To discuss these matters, we consider once more two qubits A and B, which will be under the control of two scientists named Alice and Bob. (These are the names of the standard characters in quantum information processing. David Mermin once remarked that, in the present context, the names Albert and Boris would be more appropriate.) We will refer to the qubits as spins-$\frac{1}{2}$, keeping in mind that real experiments usually involve photons, whose polarization states form a two-dimensional Hilbert space. The combined system $A + B$ is initially prepared in the maximally entangled state

$$|\psi_s\rangle = \frac{1}{\sqrt{2}}\Big[|\uparrow\rangle_A \otimes |\downarrow\rangle_B - |\downarrow\rangle_A \otimes |\uparrow\rangle_B\Big], \tag{4.42}$$

a member of the Bell basis (4.28). $|\psi\rangle$ is often called the *singlet* state because it is an eigenstate of the total spin $\mathbf{S}_T^2 := (\vec{\mathbf{S}}_A + \vec{\mathbf{S}}_B)^2$ with eigenvalue zero (see Appendix 14).

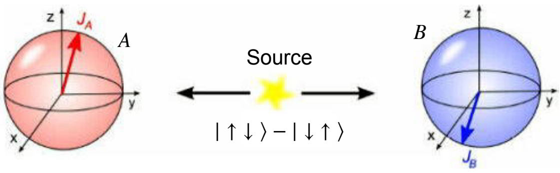


Figure 4.3: A version of the EPR experiment.

The state $|\psi_s\rangle$ having been prepared, the two qubits are separated spatially, as shown in Figure 4.3. Alice and Bob perform measurements of the z spin components of their respective qubits. (The argument does not change if any other axis in spin space is chosen, as long as both partners agree on its direction.) Let us assume that Alice measures first and that she obtains $S_z = +\frac{\hbar}{2}$ for her qubit. According to the postulates of quantum mechanics then the state of the combined system collapses to $|\uparrow\rangle_A \otimes |\downarrow\rangle_B$ and Alice can predict with certainty, the outcome of Bob's subsequent measurement, $S_z = -\frac{\hbar}{2}$. The argument is symmetric: if Bob does the measurement, he knows what result Alice will get - no matter who measures first.

This was called a "spooky action at a distance" (*spukhafte Fernwirkung*) by Einstein, and it is not surprising that he did not like it, having made considerable efforts to eliminate actions at a distance from physics in his theory of relativity. One attempt to reconcile the prediction of quantum mechanics with classical thinking is the assumption of an underlying classical mechanism which determines the outcome of the experiment but which scientists have not yet been able to unravel. This line of thinking goes under the label *hidden-variable theory*.

4.4.7 Bell's theorem

John Bell showed that the assumption of hidden classical variables leads to certain restrictions (the, by now, famous Bell inequalities) for the results of certain measurements. These inequalities are violated by quantum mechanical theory and, as it finally turned out, also by experiment.

As an example we will discuss an inequality due to Clauser, Horne, Shimony, and Holt [50] (the CHSH inequality) which was also independently found by Bell who did not publish it. We start the discussion with a purely classical reasoning assuming that the outcomes of the measurements performed by Alice and Bob on the state $|\psi\rangle$ (4.42) can be described by an underlying classical probability distribution.

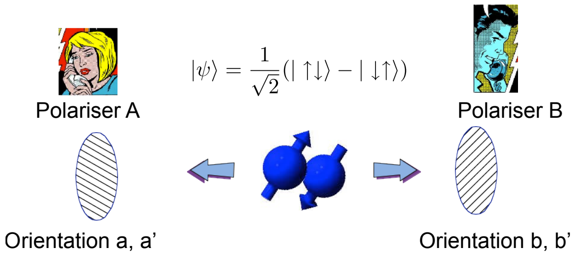


Figure 4.4: Experimental scheme for testing the Bell inequalities.

As shown in Figure 4.4, we assume that Alice can choose to measure one of the components

$$\mathbf{a} = \frac{2}{\hbar}\vec{\mathbf{S}}_A \cdot \vec{a} \text{ or } \mathbf{a}' = \frac{2}{\hbar}\vec{\mathbf{S}}_A \cdot \vec{a}', \tag{4.43}$$

defined by two unit vectors $\vec{a}$ and $\vec{a}'$, respectively. In any single experiment, $\mathbf{a}$ and $\mathbf{a}'$ can assume the values ± 1. Bob can perform similar measurements with respect to directions $\vec{b}$ and $\vec{b}'$ of his qubit.

A large number of singlet states is prepared and shared between Alice and Bob, each of whom performs a single measurement on each qubit, deciding randomly (and independently) which of the two possible measurements to perform. The pairs of measurements take place at such space–time points as to exclude any influence of one measurement on the other.

According to the classical point of view the quantities $\mathbf{a}$, $\mathbf{a}'$, $\mathbf{b}$, and $\mathbf{b}'$ have definite values independent of observation, for each of the large number of measurements performed. These values are governed by a joint probability distribution $p(a, a', b, b')$ about which nothing is known except that it is non-negative and normalized to unity. Now consider the quantity

$$\mathbf{f} := (\mathbf{a} + \mathbf{a}')\mathbf{b} - (\mathbf{a} - \mathbf{a}')\mathbf{b}'. \tag{4.44}$$

Since $\mathbf{a}$ and $\mathbf{a}'$ are either equal or opposite to each other, one summand of f is zero and the other is ± 2; thus $|f| = 2$ and consequently

$$\bar{\mathbf{f}} := \sum_{a,a',b,b'} p(a, a', b, b')\mathbf{f} \leq 2, \tag{4.45}$$

where the overbar denotes the average (expectation value) with respect to the probability distribution defined by $p(a, a', b, b')$. The average may be performed separately for each term in $\mathbf{f}$, leading to

$$\overline{\mathbf{ab}} + \overline{\mathbf{a'b}} - \overline{\mathbf{ab'}} + \overline{\mathbf{a'b'}} \leq 2, \tag{4.46}$$

the CHSH inequality. Every single measurement pair performed by Alice and Bob, as described above, contributes to one of the four averages of products in the CHSH inequality and, for a large number of measurements, the inequality may be checked to arbitrary precision.

4.4.8 The quantum mechanical prediction

Now let us consider the situation from a quantum mechanical point of view. We choose the following directions of measurement for Alice and Bob:

$$\begin{aligned} \vec{a} &= \hat{z}, \quad \vec{a}' = \hat{x}, \quad \vec{b} = \frac{1}{\sqrt{2}}(-\hat{z} - \hat{x}), \\ \vec{b}' &= \frac{1}{\sqrt{2}}(\hat{z} - \hat{x}) \end{aligned}$$

where $\hat{x}$ denotes the unit vector in x direction, etc. This leads to (see (4.12, 4.13))

$$\begin{aligned} \mathbf{a} &= \mathbf{Z}_A, \quad \mathbf{a}' = \mathbf{X}_A, \\ \mathbf{b} &= -\frac{1}{\sqrt{2}}(\mathbf{Z}_B + \mathbf{X}_B), \quad \mathbf{b}' = \frac{1}{\sqrt{2}}(\mathbf{Z}_B - \mathbf{X}_B). \end{aligned} \tag{4.47}$$

The calculation then proceeds by observing that

$$\begin{aligned} \mathbf{a} \otimes \mathbf{b} |\uparrow\rangle_A \otimes |\downarrow\rangle_B &= |\uparrow\rangle_A \otimes \frac{1}{\sqrt{2}}(|\downarrow\rangle_B - |\uparrow\rangle_B), \\ \mathbf{a} \otimes \mathbf{b} |\downarrow\rangle_A \otimes |\uparrow\rangle_B &= -|\downarrow\rangle_A \otimes \frac{1}{\sqrt{2}}(-|\uparrow\rangle_B - |\downarrow\rangle_B) \end{aligned}$$

so that the quantum mechanical expectation value of $\mathbf{a} \otimes \mathbf{b}$ in the singlet state (4.42) is

$$\langle \mathbf{ab} \rangle = \langle \psi | \mathbf{a} \otimes \mathbf{b} | \psi \rangle = \frac{1}{\sqrt{2}}. \tag{4.48}$$

The other expectation values are calculated in a similar manner, leading to

$$\langle \mathbf{a}'\mathbf{b} \rangle = \frac{1}{\sqrt{2}}, \quad \langle \mathbf{ab}' \rangle = -\frac{1}{\sqrt{2}}, \quad \langle \mathbf{a}'\mathbf{b}' \rangle = \frac{1}{\sqrt{2}}, \tag{4.49}$$

and consequently

$$\langle \mathbf{ab} \rangle + \langle \mathbf{a}'\mathbf{b} \rangle - \langle \mathbf{ab}' \rangle + \langle \mathbf{a}'\mathbf{b}' \rangle = 2\sqrt{2} \tag{4.50}$$

in obvious contradiction to the classical Bell-CHSH inequality (4.46).

4.4.9 The Aspect experiment

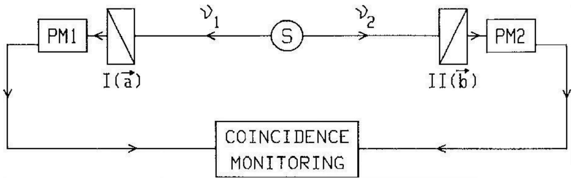


Figure 4.5: Experimental setup of Aspect for testing the Bell inequalities.

The quantum mechanical result (4.50) was confirmed by Alain Aspect *et al.* [49] using the setup shown in Figure 4.5. This changed the status of the Einstein, Podolsky, and Rosen scenario from a *Gedankenexperiment* to a real experiment. In the experiment the spin-1/2 states from the above analysis are replaced by photon polarization states: the two mutually orthogonal $\mathbf{S}_z$ eigenstates are mapped to linear polarizations at 0 deg and 90 deg (in some fixed coordinate system), and the $\mathbf{S}_x$ eigenstates correspond to ±45 deg. polarizations. This translates the algebraic relations between Hilbert space vectors, such as $|+\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$ (where $\mathbf{S}_x|+\rangle = +\frac{\hbar}{2}|+\rangle$) to relations between electric fields of polarized photons.

A photon pair with entangled polarizations corresponding to the singlet state (4.42) can be created by a cascade of decays from an excited atomic state. Later measurements used nonlinear optical processes to generate entangled photons. Measurements of the spin components (4.47) then correspond to photon polarization measurements, and the 45° angle between the two spin space reference directions changes to a 22.5° angle between polarizations.

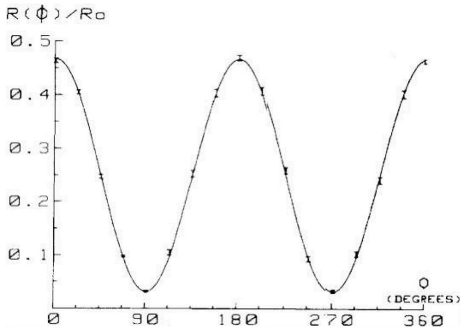


Figure 4.6: Summary of the results of Aspect for different angles. The curve shows the quantum mechanical prediction.

As shown in Figure 4.6, the experimental results clearly confirm the prediction of quantum mechanics and violate the Bell-CHSH inequality by several standard deviations. This and other experiments have demonstrated the impossibility of hidden-variable theories, and hence, the reality and importance of entanglement in several convincing ways.

4.4.10 CNOT as copy operator

In the classical world of our everyday work we take the possibility of copying something for granted: we distribute copies of our research papers to other scientists and we (hopefully) make backup copies of our important data files on a regular basis. In Chapter 3 we discussed the possibilities of copying classical bits, using either the classical irreversible NAND/NOT gate, or the reversible classical CNOT gate which performs the following operation on a pair of classical bits (x, y):

$$(x, y) \longrightarrow (x, x \text{ XOR } y).$$

With the target bit y initialized to zero, this yields

$$(x, 0) \longrightarrow (x, x), \tag{4.51}$$

as desired. As shall be discussed in Chapter 5, a quantum CNOT gate may be defined which performs exactly the same operation on the input states $|0\rangle$ and $|1\rangle$:

$$\begin{aligned} |0\rangle \otimes |0\rangle &\longrightarrow |0\rangle \otimes |0\rangle \\ |1\rangle \otimes |0\rangle &\longrightarrow |1\rangle \otimes |1\rangle \end{aligned} \tag{4.52}$$

Here the first qubit is assumed to be the source qubit and the second qubit is the target qubit, which after copying is supposed to be in the same state as the source qubit, provided it was properly initialized to a certain "blank" state (logical zero in our case) in the beginning. So, it seems to be possible to copy quantum states too! However, the problems start as soon as we initialize the source qubit to a state

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle. \tag{4.53}$$

In this case the CNOT gate (which is supposed to be a linear operator) maps

$$\begin{aligned} |\psi\rangle \otimes |0\rangle &= \alpha|0\rangle \otimes |0\rangle + \beta|1\rangle \otimes |0\rangle \\ &\longrightarrow \alpha|0\rangle \otimes |0\rangle + \beta|1\rangle \otimes |1\rangle \\ &\neq |\psi\rangle \otimes |\psi\rangle, \end{aligned} \tag{4.54}$$

because $|\psi\rangle \otimes |\psi\rangle$ contains "mixed terms" $|0\rangle \otimes |1\rangle$ and $|1\rangle \otimes |0\rangle$. This example shows that it may be possible to copy every member of a finite set of mutually orthogonal quantum states, but *not* every superposition of these states. The ability to copy classical objects may thus be interpreted as the ability to copy *special* quantum states.

4.4.11 The no-cloning theorem

In general it is not possible to make a copy (or clone) of an *unknown* (pure) quantum state by means of *unitary* operations. This is the famous *no-cloning theorem* of Wootters and Zurek [51] and also Dieks [52]. The proof is amazingly simple. Let $|\psi\rangle$ be a pure state from some Hilbert space $\mathfrak{H}_{\text{source}}$, and $|s\rangle$ some "standard" (or blank) initial state from a Hilbert space $\mathfrak{H}_{\text{target}}$ which has the same structure as $\mathfrak{H}_{\text{source}}$. A "quantum state cloner" would then be a unitary operator $\mathbf{U}$ (defined on the direct product $\mathfrak{H}_{\text{source}} \otimes \mathfrak{H}_{\text{target}}$) with the property

$$\mathbf{U}|\psi\rangle \otimes |s\rangle = |\psi\rangle \otimes |\psi\rangle \quad \forall |\psi\rangle \in \mathfrak{H}_{\text{source}}. \tag{4.55}$$

As $\mathbf{U}$ is supposed to clone every state from $\mathfrak{H}_{\text{source}}$ we now consider the cloning of a second state $|\phi\rangle$:

$$\mathbf{U}|\phi\rangle \otimes |s\rangle = |\phi\rangle \otimes |\phi\rangle. \tag{4.56}$$

For simplicity we assume that $|\psi\rangle$, $|\phi\rangle$, and $|s\rangle$ are normalized, and take the scalar product of the two equations above, keeping in mind that $\mathbf{U}$ is unitary, that is, it preserves scalar products:

$$\begin{aligned} \Big(\langle s| \otimes \langle\psi|\mathbf{U}^\dagger\Big)\Big(\mathbf{U}|\phi\rangle \otimes |s\rangle\Big) &= \langle s|s\rangle\langle\psi|\phi\rangle \\ &= \langle\psi|\phi\rangle \end{aligned} \tag{4.57}$$

As $\mathbf{U}$ is supposed to clone both states $|\psi\rangle$ and $|\phi\rangle$ we also have

$$\Big(\langle s| \otimes \langle\psi|\mathbf{U}^\dagger\Big)\Big(\mathbf{U}|\phi\rangle \otimes |s\rangle\Big) \tag{4.58}$$

$$\begin{aligned} &= \big(\langle\psi| \otimes \langle\psi|\big)\big(|\phi\rangle \otimes |\phi\rangle\big) \\ &= \big(\langle\psi|\phi\rangle\big)^2 \end{aligned} \tag{4.59}$$

and this is possible only if $\langle\psi|\phi\rangle = 0$ or $\langle\psi|\phi\rangle = 1$, that is, if the two states to be copied by the same operation are either identical or orthogonal. This proves the theorem while admitting copies of states from a set of mutually orthogonal Hilbert space vectors.

Several questions arise regarding the assumptions of the theorem:

- Can we allow non-unitary cloning operations? A possible idea might be to enlarge the Hilbert space by taking into account the environment's Hilbert space. It is not hard to see that this idea leads to the same problems as above.
- Can mixed states be cloned?
- Are less than perfect copies possible and useful?

All these questions have been addressed in the research literature, references to which can be found, for example, in [35].

The no-cloning theorem may be considered an obstacle in quantum computation, where it would be desirable to "store a copy in a safe place". It should be noted, however, that the theorem is at the very heart of the concept of secure quantum communication to be discussed in Chapter 13.

A similar operation is that of quantum teleportation; it transports a state ψ from one qubit to another:

$$U|\psi s\rangle = |s'\psi\rangle.$$

In contrast to the cloning case, the source qubit is modified by the teleportation operation. Details will be discussed in section 13.2.1.

4.5 Measurement revisited

4.5.1 Quantum mechanical projection postulate

The projection postulate (see Section 4.2.6) is one of the fundamental assumptions on which quantum mechanics is based. It assumes that an ideal measurement brings a particle into the eigenstate $|a_j\rangle$ of the measurement operator $\mathbf{A}$, where a_j is the corresponding eigenvalue, which we here assume to be non-degenerate for simplicity. We cannot predict in general which of the eigenstates will be realized, but the probability of the realization of each state $|a_j\rangle$ is

$$p_j = |\langle a_j|\psi\rangle|^2$$

for a system initially in state $|\psi\rangle$. According to the usual interpretation of quantum mechanics, this is a completely random process, whose outcome cannot be predicted. Accordingly, it can also be used as a basic random number generator.

The observable for this readout process must be adapted to the system used to implement the quantum computer as well as to the algorithm. A typical measurement distinguishes if qubit i is in state $|0\rangle$ or $|1\rangle$. The corresponding measurement operator may be written as $\mathbf{S}_z^i$, i.e., as the z-component of the spin operator acting on qubit i, with the positive eigenvalue indicating that the qubit is in state $|0\rangle$ and the negative eigenvalue labeling state $|1\rangle$.

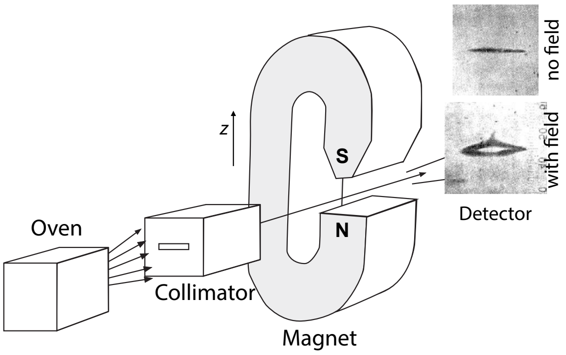


Figure 4.7: Stern–Gerlach experiment.

The usual treatment of measurement processes is due to von Neumann [53] and can be pictured as a generalized Stern–Gerlach experiment (see Figure 4.7). The measurement apparatus separates the particles according to their internal quantum states. In this picture it is obvious that the measurements are local, i.e., the results for the individual particles do not depend on the state of the other particles. Obviously the complete absence of interactions is not representative for a quantum computer.

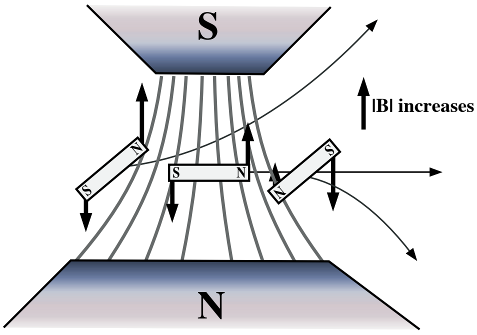


Figure 4.8: Pictorial representation of the coupling mechanism during the measurement process. Depending on their orientation, the magnetic dipoles are deflected in the inhomogeneous magnetic field.

For this simple example, it is relatively straightforward to see how the inhomogeneous field separates the different particles according to their orientation. As shown in figure 4.8, a particle whose north pole is closer to the south pole of the magnet has a lower energy than the particle with the opposite orientation – its potential energy is negative. It can further lower its energy by moving farther into the high-field region and is therefore deflected upwards, while the oppositely oriented particle is deflected down. Transferred into the quantum mechanical context, particles will follow different trajectories, depending on their spin state.

If we want to describe the result of a sequence of measurements, where different realizations of eigenstates may occur, it is more convenient to use the density operator introduced in Section 4.3.4. Since the measurement projects the system into an eigenstate of the observable, the resulting density operator (which describes the ensemble of the measurement outcomes) is diagonal in the basis of these eigenstates. The measurement process corresponds to a non-unitary evolution

$$\boldsymbol{\rho} \to \sum_j \mathbf{P}_j \boldsymbol{\rho} \mathbf{P}_j ,$$

where the $\mathbf{P}_j = |a_j\rangle\langle a_j|$ are the projection operators onto the eigenstates a_j of the observable $\mathbf{A}$, i.e., operators with a single 1 on the diagonal and zeroes everywhere else.

As a simple example, we consider the density operator

$$\rho = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

and measure the $z-$component of the spin. The corresponding projection operators are

$$P_1 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} , \quad P_2 = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} .$$

The result of the measurement will then be

$$\begin{aligned} & \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \\ + & \frac{1}{2} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \\ & \qquad = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} . \end{aligned}$$

Apparently the measurement process simply eliminates all off-diagonal elements of the density operator in the basis of the observable (which is usually also an eigenbasis of the Hamiltonian). This implies that the result of the measurement process will be a mixed state, unless the system was already in an eigenstate of $\mathbf{A}$.

We will give some more details of the measurement process below; before that we put it in a historical and philosophical context.

4.5.2 The Copenhagen interpretation

The conventional interpretation of this measurement process is due to Bohr and coworkers and known as the “Copenhagen interpretation” of quantum mechanics. It can be summarized by a few fundamental assumptions.

- Quantum mechanics describes individual systems.
- Quantum mechanical probabilities are primary, i.e., they cannot be derived from a deterministic theory (like in classical statistical mechanics).
- The world must be divided into two parts. The object under study must be described quantum mechanically, the remaining part, which includes the measurement apparatus, is classical. The division between system and measurement apparatus can be made at an arbitrary position.
- The measurement process is irreversible.
- Complementary properties cannot be measured simultaneously.

The Copenhagen interpretation has the advantage that it is relatively simple and internally consistent. It cannot satisfy, from an aesthetic point of view, since it implies two different types of evolution: the "normal" unitary evolution of the Schrödinger equation and the non-unitary measurement process. In the strict sense, it implies that quantum mechanical systems cannot be attributed real properties; instead, it represents "only" an operational description of the possible outcomes of measurements and their probabilities.

These deficiencies have prompted many researchers to look for better alternatives and / or to check some of the fundamental assumptions for their validity. A more detailed model that tries to integrate the measurement process with the unitary evolution under the Schrödinger equation and avoids the splitting of the universe into a quantum mechanical and a classical part, is due to John (also known as János or Johann) von Neumann.

4.5.3 Von Neumann's model

In von Neumann's model, the system S is coupled to an apparatus A, which is also considered as a quantum mechanical system that can be described by a state vector. For a simple two-level system the basis states are $|\psi_a\rangle$ and $|\psi_b\rangle$, the eigenstates of a system observable $\mathbf{O}_S$. The measurement should determine if the system is in state $|\psi_a\rangle$ or $|\psi_b\rangle$. To obtain a quantum mechanical description of the measurement process, we also describe the apparatus A as a two-level system. The eigenstates are written as $|\xi_a\rangle$ and $|\xi_b\rangle$ and correspond to the apparatus indicating that the system is in state $|\psi_a\rangle$ and $|\psi_b\rangle$, respectively. A corresponding observable acting on the apparatus can be written as $\mathbf{O}_A$.

According to von Neumann, the measurement process involves coupling the system to the measurement apparatus through an interaction of the type

$$\mathcal{H}_{int} = \mathbf{O}_S \mathbf{B}_A,$$

where $\mathbf{O}_S$ is the observable to be measured and $\mathbf{B}_A$ is a variable of the measurement apparatus. The system thus drives the motion of the measurement apparatus and in the idealized process, the eigenvalues of $\mathbf{O}_S$ can be read off a "pointer variable" of the measurement apparatus, which is treated classically. One usually assumes that the observable $\mathbf{O}_S$ that one tries to measure, commutes with the Hamiltonian of the system. In the case of the Stern–Gerlach experiment, the observable $\mathbf{O}_S$ is the z-component of the spin operator, $\mathbf{S}_z$, and the pointer variable is the position z along the field direction.

Before the measurement process, the total (system and apparatus) can be described as a state without correlations between system and apparatus. The two parts can thus be described individually by the states $|\psi\rangle_S = c_a|\psi_a\rangle_S + c_b|\psi_b\rangle_S$ (which is not known) and the initial state $|\xi\rangle_A$ of the measurement device. The combined system is then in the product state

$$|\psi\rangle_S \otimes |\xi\rangle_A = (c_a|\psi_a\rangle_S + c_b|\psi_b\rangle_S) \otimes |\xi\rangle_A.$$

The interaction between system and apparatus must be such that it drives the evolution as

$$|\psi_a\rangle_S \otimes |\xi\rangle_A \rightarrow |\psi_a\rangle_S \otimes |\xi_a\rangle_A$$

and

$$|\psi_b\rangle_S \otimes |\xi\rangle_A \to |\psi_b\rangle_S \otimes |\xi_b\rangle_A$$

Since the evolution is linear, the superposition state evolves as

$$\begin{aligned} & (c_a|\psi_a\rangle_S + c_b|\psi_b\rangle_S) \otimes |\xi\rangle_A \\ \to \quad & c_a|\psi_a\rangle_S \otimes |\xi_a\rangle_A + c_b|\psi_b\rangle_S \otimes |\xi_b\rangle_A. \end{aligned}$$

Apparently the combined system (consisting of system and apparatus) is still in a superposition state, but the two parts are now entangled. Von Neumann's model does not generate a reduction of the wave function, such as is required by the projection postulate (compare equation (4.7)). This is a necessary consequence of the unitary evolution. The reduction only occurs if we assume in addition that the apparatus is a classical system, where a reduction *must* occur. A reduction of the wavefunction component for the apparatus into (e.g.) $|\xi_a\rangle_A$ then also causes a reduction of the system state into $|\psi_a\rangle_S$. The combined system is then in state

$$c_a|\psi_a\rangle_S \otimes |\xi_a\rangle_A.$$

4.5.4 Discussion

This formal result matches the expected outcome: the system is in a well-defined, pure state that matches the outcome of the measurement and the apparatus is also in the matching state. What remains open are the details of the wavefunction collapse. While the wavefunction reduction is therefore not explained, it has been shifted farther away from the system. According to von Neumann's understanding, the final reduction occurs in the mind of the observer. While this is therefore not a full resolution of the measurement paradox, it improves the situation. Since the apparatus is very complex in terms of a quantum mechanical description, the collapse of its wavefunction is very fast. Furthermore, since it does not directly involve the system, some inconsistency is easier to accept. Nevertheless, one major issue remains unresolved in von Neumann's model (as well as in all others): we only obtain probabilities from the quantum mechanical description, i.e., we cannot predict the result of individual measurements. In a wider context, this relates to the question if quantum mechanics can teach us something about the reality of quantum objects (ontic interpretation) or if it only relates to our knowledge of these objects and how they will behave under experimental conditions (epistemic interpretation). Today, textbooks as well as research papers focus on the epistemic approach, which is based on the Kopenhagen model. Ontic models of quantum mechanics include pilot-wave or hidden-variable models, which were proposed by David Bohm [54, 55] in the early 1950s. They assume that wavefunctions are real but there are also extra degrees of freedom representing the actual positions of particles, and it is the latter that get observed. The so-called "many-world" interpretation, introduced by Hugh Everett[56] in 1957 accepts that observers become entangled with the systems they measure. As a result, measurements do not collapse the wavefunction but lead to separate branches of the wavefunction, which are interpreted as parallel worlds.

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.

4.6 Entanglement measures

4.6.1 General requirements

In section 4.3.4, 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.

4.6.2 Entropy of entanglement

One of the simplest measures that fulfill these requirements for pure states is the entropy of entanglement. As discussed in section 4.3.6, 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

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

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

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

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 σ_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:

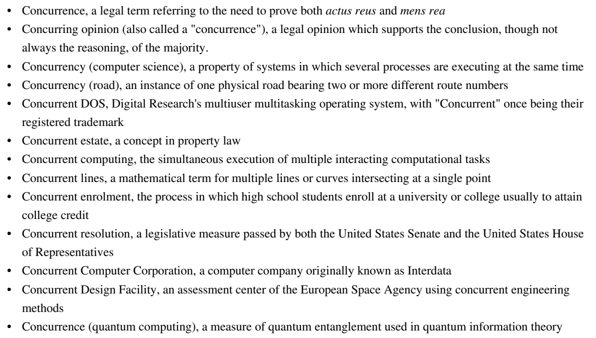
$$E(\rho) = S(\rho_A) = S(\rho_B),$$

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

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

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 $E(\rho) = S(\rho_A) = S(\rho_B) = 1$.

4.6.3 Concurrence : Definition



- Concurrence, a legal term referring to the need to prove both *actus reus* and *mens rea*
- Concurring opinion (also called a "concurrence"), a legal opinion which supports the conclusion, though not always the reasoning, of the majority.
- Concurrency (computer science), a property of systems in which several processes are executing at the same time
- Concurrency (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 enrolment, 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 4.9: Meanings of the term "Concurrence" in different fields (from wikipedia).

The term "concurrence" has been used in many different contexts. In quantum information, it was introduced as a measure of 'quantumness'. For pure 2-qubit states

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

it is defined as

$$C := 2|\alpha\delta - \beta\gamma| \geq 0. \tag{4.60}$$

The concurrence is bounded from above:

$$C \leq 1. \tag{4.61}$$

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

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

we find again $C(\Psi_2) = 0$. Since Ψ_1 and Ψ_2 are identical under local transformations (here: rotations $z \to x$), this is consistent with the general requirements for entanglement measures.

4.6.4 Generating entanglement

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

$$\mathrm{CN} = \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & \cos\frac{\varphi}{2} & -\sin\frac{\varphi}{2} \\ & & \sin\frac{\varphi}{2} & \cos\frac{\varphi}{2} \end{pmatrix}, \tag{4.62}$$

which is close to the CNOT gate if $\varphi = \pi$. If we apply it to Ψ_2, we find

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

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 φ. The entanglement reaches its maximum of $C = 1$ for $\varphi = \pi$, where CN ≈ 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

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

The subsystem density operators are calculated by tracing over the basis states of the other subsystem, e.g. $\rho_A = Tr_B(\rho)$. The individual elements are then

$$\begin{aligned} \rho_A[1,1] &= \rho[1,1]+\rho[2,2] = \frac{1}{2} \\ \rho_A[2,2] &= \rho[3,3]+\rho[4,4] = \frac{1}{2} \\ \rho_A[1,2] &= \rho[1,3]+\rho[2,4] = \frac{1}{4}(c_-+c_+) = \frac{1}{2}\cos\frac{\varphi}{2} \\ \rho_A[2,1] &= \rho[3,1]+\rho[4,2] = \frac{1}{4}(c_-+c_+) = \frac{1}{2}\cos\frac{\varphi}{2}. \end{aligned}$$

Together

$$\rho_A = Tr_B(\rho) = \frac{1}{2}\begin{pmatrix} 1 & \cos\frac{\varphi}{2} \\ \cos\frac{\varphi}{2} & 1 \end{pmatrix}.$$

For the other subsystem:

$$\begin{aligned} \rho_B[1,1] &= \rho[1,1]+\rho[3,3] = \frac{1}{4}(2-\sin\varphi) \\ \rho_B[2,2] &= \rho[3,3]+\rho[4,4] = \frac{1}{4}(2+\sin\varphi) \\ \rho_B[1,2] &= \rho[1,2]+\rho[3,4] = \frac{1}{4}(1+\cos\frac{\varphi}{4}) \\ &= \frac{1}{2}\cos^2\frac{\varphi}{2} \\ \rho_B[2,1] &= \rho[2,1]+\rho[4,3] = \frac{1}{4}(1+\cos\frac{\varphi}{4}) \\ &= \frac{1}{2}\cos^2\frac{\varphi}{2}. \end{aligned}$$

Together:

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

where we used the trigonometric identity $1 + \cos(\varphi/4) = 2\cos^2(\varphi/2)$. The difference between ρ_A and ρ_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 ρ_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

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

For ρ_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 $\varphi = \pi$:

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

4.6.5 Concurrence : Properties

The two-qubit product state $|\Phi\rangle$ (4.25) has $C = 0$, and in fact any state with $C = 0$ can be written as a product state. Thus $C = 0$ if and only if the state is a product state. The state $|\psi\rangle$ (4.22),

$$|\psi\rangle = a\,|\uparrow\rangle_A \otimes |\uparrow\rangle_B + b\,|\downarrow\rangle_A \otimes |\downarrow\rangle_B$$

has

$$C = 2|ab| = 2|a|\sqrt{1-|a|^2} \leq 1. \qquad (4.63)$$

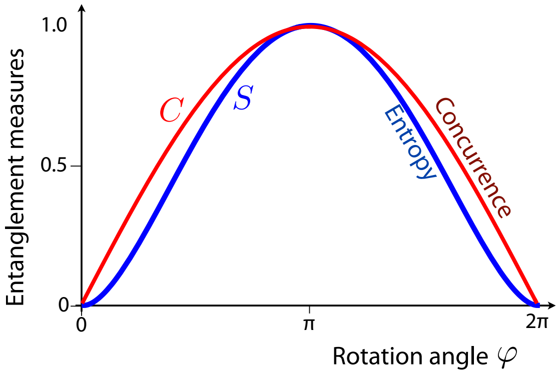


Figure 4.10: Entanglement entropy S and concurrence C of ρ_3 as a function of the rotation angle φ.

Figure 4.10 shows the entanglement entropy $E(\rho_3) = S(\rho_A) = S(\rho_B)$ that is generated by the entangling gate (4.62) as a function of the rotation angle φ. Clearly, the dependence is different from that of the concurrence $C(\Psi_3)$ for the same state, which starts linearly with φ. 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

$$C(\rho) = \max(0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4), \qquad (4.64)$$

where λ_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 λ_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 (4.60).

4.6.6 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 system. Any two qubits of this system can be pairwise entangled and their entanglement can be measured, e.g., by the concurrence C_{ik}, which measures the pairwise entanglement between qubits i and k. Each of these is determined by tracing over the third qubit and then using eq. (4.64) to calculate the concurrence for the resulting 2-qubit state, which may be pure or mixed.

For the 3-qubit system, we can define the average two-tangle

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

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

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

where ρ_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, ρ_i is pure and therefore $\rho_i = \rho_i^2$ and $Tr(\rho_i^2) = 1$ and $C_{i(jk)} = 0$. For an entangled state, $Tr(\rho_i^2) < 1$ 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 τ_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:

$$\tau_3 = C^2_{i(jk)} - (C^2_{ij} + C^2_{ik}). \tag{4.65}$$

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

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

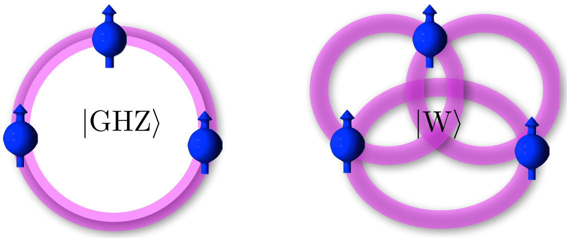


Figure 4.11: Different types of entanglement in 3-partite states.

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. [57]), $\tau_2^{(k)}$ the two-way entanglement of qubit k with the other qubits, and τ_3 the ‘essential three-way entanglement’ defined by eq. (4.65).

4.6.7 Positive Partial Transpose (PPT)

The Positive Partial Transpose (PPT) was introduced by Peres [58] and by the Horodeckis [59] as a necessary condition, for the joint density matrix ρ 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

$$\rho = \sum_{ijkl} p_{ijkl}\, |i\rangle\langle j| \otimes |k\rangle\langle l|. \tag{4.66}$$

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 (4.66) 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 ρ^{T_B} has a negative eigenvalue, then ρ is entangled. A positive partial transpose is thus a necessary condition for a density operator to be separable. In the 2 × 2 and 2 × 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.

4.6.8 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

$$\begin{aligned} \rho_2 &= \frac{1}{2}\left(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle\right)\left(\langle\uparrow\uparrow| + \langle\downarrow\downarrow|\right) \\ &= \frac{1}{2}\left(|\uparrow\uparrow\rangle\langle\uparrow\uparrow| + |\uparrow\uparrow\rangle\langle\downarrow\downarrow| \right. \\ &\quad \left. +|\downarrow\downarrow\rangle\langle\uparrow\uparrow| + |\downarrow\downarrow\rangle\langle\downarrow\downarrow|\right) \\ &= \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}. \end{aligned} \tag{4.67}$$

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

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

To obtain the eigenvalues of this state, we have to diagonalize the central 2×2 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 ρ_2 is entangled, as we expect for a Bell state.

4.6.9 Decay of entanglement

Superposition states like ρ_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 ρ_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 ρ_2 of eq. (4.67).

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

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

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 λ_1, λ_2, and λ_4 are always positive, λ_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 the other eigenvalues, and the resulting state fulfills the PPT criterion.

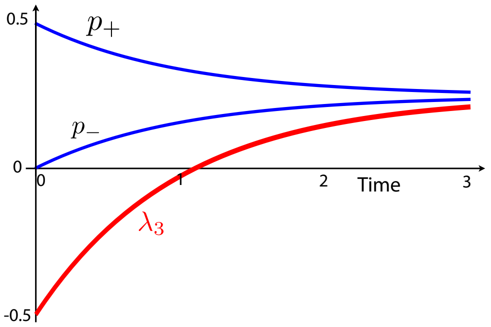


Figure 4.12: Time dependence of the populations and the eigenvalue λ_3 of ρ_2 for $T_1 = T_2 = 1$.

Fig. 4.12 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 ≈ 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.

4.6.10 Quantum discord

Another measure of nonclassical correlations between two subsystems is the quantum discord. The concept was introduced in 2001 by Ollivier and Zurek [60] and by Henderson and Vedral [61]. 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.

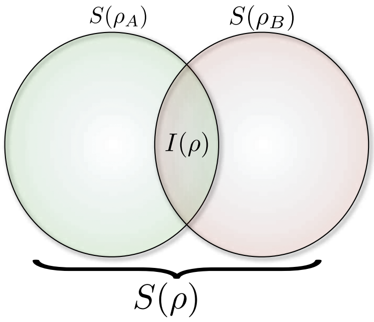


Figure 4.13: Schematic representation of the mutual information $I(\rho)$ between subsystems A and B.

We first remember the von Neumann or information entropy $S(\rho) = -Tr(\rho \log_2 \rho)$ defined in section 4.6.2. 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 ρ_A and ρ_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

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

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

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

where $\left\{\Pi_j^A\right\}$ is the set of projective operators on subsystem A and $\rho_{B|\Pi_j^A}$ are the resulting states.

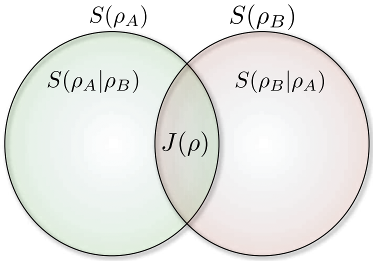


Figure 4.14: Schematic representation of $J(\rho)$ for the classical case or for a specific set of observables.

The quantum conditional entropy is also an entanglement measure: if it is negative, the state is entangled.

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

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

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 ρ 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.

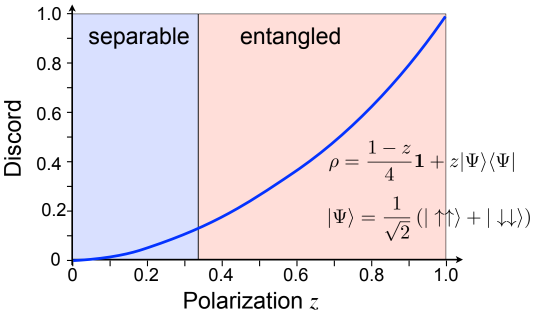


Figure 4.15: Discord as a function of the polarization for a partially mixed Bell state.

Figure 4.15 shows, as an example, the quantum discord for a partially mixed Bell state

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

where

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

is one of the Bell states. For all nonzero values of the polarization z, the discord is positive, while the entanglement only starts at a finite value.

The quantum discord was quite popular for some time. 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.

4.6.11 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 theses 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 ρ_A and ρ_B in the set is also inside.

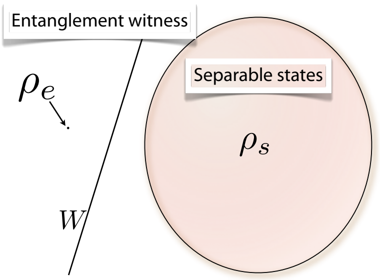


Figure 4.16: Schematic representation of an entanglement witness W, separating the entangled state ρ_e from the convex set of all separable states ρ_s.

This is compared to an entangled state ρ_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

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

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 [62] is a concise and clear masterpiece. Cohen-Tannoudji *et al.* [63] is a detailed student-friendly textbook. Ballentine [64] has interesting modern applications, whereas Peres [65] 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 (4.19) 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 state (4.20) 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 $|\theta, \phi\rangle$ (4.21) 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:
   a) $ac|\uparrow\uparrow\rangle + ad|\uparrow\downarrow\rangle + bc|\downarrow\uparrow\rangle + bd|\downarrow\downarrow\rangle$
   b) $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$
5. Calculate the expectation values $\langle(\mathbf{S}_\alpha\rangle$ and the variances $\langle(\mathbf{S}_\alpha - \langle \mathbf{S}_\alpha\rangle)^2\rangle$ $(\alpha = x, y, z)$ for the pure state

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

   and the mixed state

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

   Calculate the purity η (4.35) 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 $|\Psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle)$.