Decoherence and the Physics of Open Quantum Systems

Script to Reinhold Bertlmann's Lectures

Tanja Traxler

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1 Density Matrix (Density Operator)

1.1 Description of a quantum state

Introduction

The state vector ψ contains all information about a quantum system. But in many cases detail-information of a system are not known. (In many cases there are interactions between a system and its environment. For example this may lead to spontaneous emission in the atom or to a loss of radiation in a cavity.)

So if we want to describe a quantum system that is not isolated from its environment we have to replace the description by the state vector ψ by a new concept - this will be the *Density Matrix*-notation.

Firstly let us consider the description of a quantum system. If a quantum system is in its energy-eigenstate, it is described by the Hamilton eigenequation

$$H\,|m\rangle = E_m\,|m\rangle \tag{1}$$

Example:

If we take the harmonic oscillator, the energy-eigenstates E_m and the Hamilton-operator H are given by:

$$E_m = \hbar\omega(m + \frac{1}{2}) \tag{2}$$

$$H = \frac{p^2}{2m} + \frac{m\omega^2}{2}x^2 \tag{3}$$

The probability $W(x)$ to find a particle in state $|m\rangle$ with energy E_m at position x is given by:

$$W(x) = |\langle x|m\rangle|^2 = |\varphi_m(x)|^2 \tag{4}$$

Let us now make the assumption that the oscillator is in a superposition of energy-eigenstates. Then for the wave-function we gather:

$$|\psi\rangle = \sum_{m=0}^{\infty} c_m \, |m\rangle \tag{5}$$

$$\Downarrow$$

$$\psi(x) = \langle x \, |\psi\rangle = \sum_{m=0}^{\infty} c_m \varphi_m(x) \tag{6}$$

We calculate the probability $W(x)$ to find the particle at position x:

$$W(x) = |\langle x \, |\psi\rangle \, |^2 = |\psi(x)|^2 = \sum_{m,n} c_m^* \; c_n \; \varphi_m^*(x) \; \varphi_n(x) \tag{7}$$

Splitting the sum we obtain:

$$W(x) = \sum_{m=0}^{\infty} |c_m|^2 |\varphi_m|^2 + \sum_{m \neq n} c_m^* \; c_n \; \varphi_m^*(x) \; \varphi_n(x) \tag{8}$$

where:

$|c_m|^2 = p_m$ is the probability to find the particle in m^{th}-energy-eigenstate
with the features $0 \leq p_m \leq 1$ and $\sum_m p_m = \mathbb{1}$ and
$W_m = |\varphi_m|^2$ is the probability to find the m^{th}-energy-eigenstate at position x.

Resumée

The probability to find a particle prepared in a superposition-state $|\psi\rangle$ at position x is given by the sum of two terms, namly

$$\sum_{m=0}^{\infty} + \sum_{n \neq m}$$

where $\sum_{m=0}^{\infty}$ is the sum of the probabilities of the eigen-states and
$\sum_{n \neq m}$ is the double-sum of the off-diagonal terms. It is this second term that carries the difference of quantum mechanics to classical physics.

Now we will discuss the following situation: We assume that in the given situation, we dont't have all information about the system. The information we have is the probability distribution $\{p_m\}$. The question is: Can we describe a system by the superposition-state ψ? What does the expansion coefficient look like?

For the expansion coefficient $c_m(\alpha_m)$ we make the following ansatz:

$$c_m(\alpha_m) = \sqrt{p_m}\, e^{i\alpha_m} \tag{9}$$

where $c_m(\alpha_m)$ is a complex number and p_m is a real number. α_m is an arbitrary phase, but how can we fix it? As we have no information about the phase α_m we have to average over all possible phases:

$$\langle e^{i\alpha_m} \rangle = \frac{1}{2\pi} \int_0^{2\pi} e^{i\alpha_m} d_{\alpha_m} = 0 \tag{10}$$

Again, we consider the probability $W(x)$:

$$W(x) = \sum_m p_m |\psi_m(x)|^2 + \sum_{n \neq m} \sqrt{p_m}\sqrt{p_n} e^{i(\alpha_n - \alpha_m)} \varphi_m^*(x)\varphi_n(x) \tag{11}$$

We drop the second part to average - then the final result is:

$$\langle W(x) \rangle_{\text{phases}} = \sum_{m=0}^{\infty} p_m W_m(x) \tag{12}$$

This is the correct probability-distribution. The result contains all the information we have. We can associate it with a starting (point) situation.

But: Averaging the state vector gives:

$$|\psi\rangle = \sum_m \sqrt{p_m} e^{i\alpha_m} |m\rangle \longrightarrow 0 \text{ (average)} \tag{13}$$

This of course doesn't make sense! We conclude that we need another concept.

For getting probabilities we will now introduce a different concept for describing the state, therefore we will introduce a new operator: the **density-matrix**.
We start with the probability $W(x)$ to find a particle at position x:

$$W(x) = |\psi(x)|^2 = |\langle x|\psi\rangle|^2 = \langle x| \underbrace{\psi\rangle\langle\psi}\, |x\rangle = \langle x|\rho|x\rangle \tag{14}$$

The decomposition of the density matrix ρ as a superposition of its energy-eigenstates is given by:

$$\rho = \sum_{m,n} \rho_{mn} |m\rangle\langle n| \tag{15}$$

with the coefficients ρ_{mn}:

$$\rho_{mn} = c_m c_n^* \tag{16}$$

Consequently, for the density matrix of all phases we get:

$$\rho = \sum_m p_m |m\rangle\langle m| + \sum_{m \neq n} \sqrt{p_m p_n}\, e^{i(\alpha_m - \alpha_n)} |m\rangle\langle n| \tag{17}$$

Averaging over all phases gives:

$$\langle\rho\rangle_{\text{phases}} = \sum_m p_m |m\rangle\langle m| = \sum_m \rho_{mm} |m\rangle\langle m| \tag{18}$$

We now can see that with the density matrix ρ we obtain all information about a quantum systems. This was the assumption we made in the beginning.

Conclusio

There exists two possibilities for describing a quantum system QS in Hilbert-space HS
i) QS → state vector in HS → pure state - complete info (ideal case) → quantum statistics
ii) QS → state operator density matrix → mixed state - incomplete info (realistic case) → classical statistics, classical averaging in addition.

1.2 Properties of Density Matrices

In the following we will discuss common features of a density matrix as they are very important for quantum statistics. Let the observed quantum system be in state ψ. We consider the observable A in state ψ. Its expectation value is the following:

$$\langle A\rangle = \langle\psi|A|\psi\rangle \tag{19}$$

This structure of the expectation value motivates to define the following operator - the density matrix (for pure states):

$$\rho = |\psi\rangle\langle\psi| \tag{20}$$

Properties of ρ:

- ρ is positive:

$$\rho \geq 0 \tag{21}$$

  By saying: "ρ is positive", we mean, that the eigen-values of ρ are always bigger than or equal to 0. Differently expressed: for all φ it is true that:

$$\langle\varphi|\rho|\varphi\rangle = \langle\varphi|\psi\rangle\langle\psi|\varphi\rangle = |\langle\varphi|\psi\rangle|^2 \geq 0 \tag{22}$$

- ρ is self-adjoint:

$$\rho = \rho^\dagger \tag{23}$$

  Proof:

  Commonly the adjoint $D^\dagger$ of an operator $D = |\varphi\rangle\langle\psi|$ is defined by $D^\dagger = (|\varphi\rangle\langle\psi|)^\dagger = |\psi\rangle\langle\varphi|$, which gives for ρ: $\rho^\dagger = |\psi\rangle\langle\psi|^\dagger = |\psi\rangle\langle\psi| = \rho$.

- Trace of ρ is 1:

$$\mathrm{tr}\rho = 1 \tag{24}$$

The common definition of the trace of an operator D is: $\mathrm{tr}D = \sum_n \langle n|D|n\rangle$ where $\{|n\rangle\}$ is an arbitrary complete orthogonal basis. With this definition we can calculate the trace of ρ:

$$\mathrm{tr}\rho = \sum_n \langle n|\rho|n\rangle = \sum_n \langle n|\psi\rangle\langle\psi|n\rangle = \sum_n \langle\psi|n\rangle\langle n|\psi\rangle = \langle\psi|\psi\rangle = 1$$

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$$\rho^2 = \rho \tag{25}$$

Proof:

$$\rho^2 = |\psi\rangle\langle\psi|\psi\rangle\langle\psi| = |\psi\rangle\langle\psi| = \rho \tag{26}$$

We can now rewrite the expectation value of an observable A like the following:

$$\langle A\rangle = \mathrm{tr}\rho A \tag{27}$$

which coincides with the definition: $\langle A\rangle = \langle\psi|A|\psi\rangle$.

Proof:

$$\mathrm{tr}\rho A = \sum_n \langle n|\psi\rangle\langle\psi|A|n\rangle = \sum_n \langle\psi|A|\underbrace{n\rangle\langle n}|\psi\rangle = \langle\psi|A|\psi\rangle = \langle A\rangle \tag{28}$$

Having found some general features of a density matrix ρ of pure states we will now classify between pure states and mixed states by certain features of the density matrix ρ. In the following we always consider an ensemble of object.

- **Pure States:** All considered objects (systems) are in one and the same state. To proof probability-predictions in the experiment, we have to consider an ensemble of objects with the same preparation.

  Example:

  Let us consider the state $|\psi\rangle = \sum_n c_n|n\rangle$ with the transition-coefficient $c_n = \langle n|\psi\rangle$, where $A|n\rangle = a_n|n\rangle$. Then

$$\langle A\rangle_\psi = \sum_n |c_n|^2 a_n = \sum_n a_n \frac{N_n}{N} \tag{29}$$

  where $|c_n|^2$ is the probability of the transition and N_n the number, how often eigenvalue a_n was measured and N is the ensemble number. Then the density matrix is characterized by:

$$\rho = |\psi\rangle\langle\psi| \tag{30}$$

$$\langle A\rangle = \mathrm{tr}\rho A\ , \quad \rho^\dagger = \rho\ , \quad \rho \geq 0\ , \quad \rho^2 = \rho\ , \quad \mathrm{tr}\rho = 1\ , \quad \mathrm{tr}\rho^2 = 1 \tag{31}$$

- **Mixed States:** This more general case is very important for quantum statistics. In this case not all systems (objects) are in the same state. We consider N objects, let N_i objects of them be in state $|\psi_i\rangle$. The probability p_i that any object of the ensemble is in state $|\psi_i\rangle$ is given by

$$p_i = \frac{N_i}{N} \tag{32}$$

where $\sum_i p_i = 1$. N_i is the number how often the eigenvalue a_n appears and N is the total ensemble number. Then the expectation value of A is given by:

$$\langle A\rangle = \sum_i p_i \langle\psi_i|A|\psi_i\rangle \tag{33}$$

The density matrix is defined by

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i| \tag{34}$$

with the following properties:

$$\langle A\rangle = \mathrm{tr}\rho A \ , \ \rho^\dagger = \rho \ , \ \rho \geq 0 \ , \ \rho^2 \neq \rho \tag{35}$$

$$\mathrm{tr}\rho^2 < 1 \tag{36}$$

Proofs:

$\mathrm{tr}\rho A = \sum_{n,i} p_i \langle n|\psi_i\rangle\langle\psi_i|A|n\rangle = \sum_i p_i \sum_n \langle\psi_i|A|n\rangle\langle n|\psi_i\rangle = \sum_i p_i \langle\psi_i|A|\psi_i\rangle = \langle A\rangle$

$\rho^2 = \sum_i \sum_j p_i p_j |\psi_i\rangle\langle\psi_i|\psi_j\rangle\langle\psi_j| = \sum_i p_i p_i |\psi_i\rangle\langle\psi_i| \neq \rho$

$\mathrm{tr}\rho^2 = \sum_n \langle n| \sum_i \sum_j p_i p_j |\psi_i\rangle\langle\psi_i|\psi_j\rangle\langle\psi_j|n\rangle = \sum_i \sum_j \sum_n p_i p_j \langle\psi_i|\psi_j\rangle\langle\psi_j|n\rangle\langle n|\psi_i\rangle =$
$= \sum_i \sum_j p_i p_j |\langle\psi_i|\psi_j\rangle|^2 < \sum_i p_i \sum_j p_j = 1$

for all $|\varphi\rangle$: $\langle\varphi|\rho|\varphi\rangle = \sum_i p_i \langle\varphi|\psi_i\rangle\langle\psi_i|\varphi\rangle = \sum_i p_i |\langle\varphi|\psi_i\rangle|^2 \geq 0$

As the last property of (36) differs from the case above where we have considered pure states we can associate $\delta = \mathrm{tr}\rho^2$ as a *measure of mixedness*.

1.3 Equation of Motion

The time-evolution of the density matrix is given by the Von Neumann-equation. To derive it we start with the Schrödinger-equation:

$$i\hbar \frac{\partial}{\partial t}|\psi_i\rangle = H|\psi_i\rangle \tag{37}$$

If $H = H^\dagger$ is hermitian, the adjoint equation is given by:

$$-i\hbar \frac{\partial}{\partial t}\langle\psi_i| = \langle\psi_i|H \tag{38}$$

We apply this equations for the density matrix ρ and get:

$$i\hbar\frac{\partial}{\partial t}\rho = i\hbar\sum_i \left(|\dot{\psi}_i\rangle\langle\psi_i| + |\psi_i\rangle\langle\dot{\psi}_i|\right) = H|\psi_i\rangle\langle\psi_i| - |\psi_i\rangle\langle\psi_i|H = H\rho - \rho H \tag{39}$$

Von Neumann-equation:

$$i\hbar\frac{\partial}{\partial t}\rho = [H,\rho] \tag{40}$$

Classical analogy: The von Neumann equation is analogous to the Liouville equation in classical statistical mechanics.

Liouville equation:

$$\frac{\partial}{\partial t}\rho = \{H,\rho\} \tag{41}$$

with the Poisson-bracket: $\{H,\rho\} = \frac{\partial H}{\partial q}\frac{\partial \rho}{\partial p} - \frac{\partial H}{\partial p}\frac{\partial \rho}{\partial q}$. Here ρ is the classical density distribution in two variables p,q: $\rho = \rho(p,q)$.

Dirac rule:

$$\{,\} \to \frac{i}{\hbar}[,] \tag{42}$$

From the Schrödinger equation we also get the unitary *time-shift operator*:

$$U(t,t_0) = e^{-\frac{i}{\hbar}H(t-t_0)} \tag{43}$$

The density-shifts are given by:

$$\rho(t) = U(t,t_0)\rho(t_0)U^\dagger(t,t_0) \tag{44}$$

Proposition 1. *$tr\rho^2$ is time independent!*

This means that pure states remain pure and mixed states remain mixed.

Proof:

tr $\rho^2(t)$ = tr $U\rho(t_0)U^\dagger U\rho(t_0)U^\dagger$ = tr $\rho^2(t_0)UU^\dagger$ = tr $\rho^2(t_0)$

Example from particle physics:

Let us consider the time-evolution of the density matrix ρ of neutral K-mesons. We descibe this decay via the non-hermitian Hamilton-operator

$$H = M - \frac{i}{2}\Gamma \tag{45}$$

where M is the mass and Γ the width of the particle. With this Hamilton-operator we get for the Schrödinger-equation:

$$H|K_S\rangle = \lambda_S|K_S\rangle$$

$$H|K_L\rangle = \lambda_L|K_L\rangle \tag{46}$$

with the complex eigenvalues

$$\lambda_{S,L} = m_{S,L} - \frac{i}{2}\Gamma_{S,L} \tag{47}$$

The time-dependent density matrix $\rho(t)$ is given by:

$$\rho(t) = \sum_{i,j} \rho_{ij}(t)|i\rangle\langle j| \tag{48}$$

where $\rho_{ij} = \langle i|\rho(t)|j\rangle$ and $i, j = S, L$. By applying the von Neumann equation

$$\frac{d\rho(t)}{dt} = -\frac{i}{\hbar}\left(H\rho - \rho H^\dagger\right) \tag{49}$$

we gather for the time-evolution of the density matrix:

$$\dot{\rho}_{SS}(t) = -\frac{i}{\hbar}\left(\lambda_S - \lambda_S^*\right)\ \rho_{SS}(t) \tag{50}$$

$$\dot{\rho}_{LL}(t) = -\frac{i}{\hbar}\left(\lambda_L - \lambda_L^*\right)\ \rho_{LL}(t)$$

With $\lambda_S - \lambda_S^* = -i\Gamma_S$ the differential equation of the diagonal elements is:

$$\dot{\rho}_{SS}(t) = -\frac{1}{\hbar}\Gamma_S\rho_{SS}(t) \tag{51}$$

$$\dot{\rho}_{LL}(t) = -\frac{1}{\hbar}\Gamma_S\rho_{LL}(t)$$

Whereas the differential equation of the off-diagonal elements is:

$$\dot{\rho}_{SL}(t) = -\frac{1}{\hbar}\left(\Gamma + i\Delta m\right)\rho_{SL}(t) \tag{52}$$

where $\lambda_S - \lambda_L^* = m_S - m_L - \frac{i}{2}(\Gamma_S + \Gamma_L) = \Delta m - i\Gamma$ with $\Delta m = m_S - m_L$ and $\Gamma = \frac{\Gamma_S + \Gamma_L}{2}$
As a result for the solution we get the so-called **Wigner-Weisskopf**-approximation:

$$\rho_{SS}(t) = e^{-\frac{1}{\hbar}\Gamma_S t}\rho_{SS}(t) \tag{53}$$

$$\rho_{LL}(t) = e^{-\frac{1}{\hbar}\Gamma_L t}\rho_{LL}(t)$$

$$\rho_{SL}(t) = e^{-\frac{1}{\hbar}\Gamma t}e^{-\frac{i}{\hbar}\Delta m t}\rho_{SL}(t)$$

Example:

As an example let us now consider the time evolution of a spin-$\frac{1}{2}$ particle in an external magnetic field. For this case the Hamilton-operator is given by:

$$H = -\overrightarrow{\mu} \cdot \overrightarrow{B} \tag{54}$$

where $\overrightarrow{B}$ is a constant field parallel to the z-axis and $\overrightarrow{\mu}$ is the magnetic dipole $\overrightarrow{\mu} = g\mu\overrightarrow{s}$ with spin $\overrightarrow{s} = \frac{\hbar}{2}\overrightarrow{\sigma}$, $\overrightarrow{\sigma}$ is the Pauli-sigma-matrix. For electrons the gyromagnetic ratio $g \approx 2$. Bohr's Magneton is given by: $\mu_B = \frac{e\hbar}{2mc}$, we define $\gamma = g \cdot \mu_B$. Therefore for the Hamilton-operator we obtain:

$$H = -\frac{\gamma B}{2} \cdot \sigma_z \tag{55}$$

The solution for the density matrix is given by the von Neumann equation

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[H, \rho] \tag{56}$$

As a solution we get:

$$\begin{aligned} \dot{\rho_{00}} &= \dot{\rho_{11}} = 0 \\ \dot{\rho_{01}} &= \frac{i}{\hbar}\gamma B \rho_{01} \end{aligned} \tag{57}$$

This means that:

$$\rho_{00}(t) = \rho_{00}(0) = const. \tag{58}$$

$$\rho_{11}(t) = \rho_{11}(0) = const.$$

$$\rho_{01}(t) = e^{\frac{i}{\hbar}\gamma B t}\rho_{01}(0) = e^{i\omega t}\rho_{01}(0) \tag{59}$$

$$\rho_{10}(t) = e^{-\frac{i}{\hbar}\gamma B t}\rho_{10}(0) = e^{-i\omega t}\rho_{10}(0)$$

Like Ehrenfest's Theorem tells us, we can see that for the expectation value $\langle\overrightarrow{\sigma}\rangle = \overrightarrow{a}$ we get a classical vector, the so-called **Bloch-vector**.

1.4 Density matrix for spin-1/2 particles

As we know, any 2×2-matrix is a linear combination of the *Pauli-sigma-matrices* σ_x, σ_y, σ_z and the identity matrix 1.

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\ \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},\ \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{60}$$

As $\mathrm{tr}1 = 2$ and $\mathrm{tr}\sigma_i = 0$, generally every density matrix with $\mathrm{tr}\rho = 1$ can be written as:

$$\rho = \frac{1}{2}\left(1 + \overrightarrow{a} \cdot \overrightarrow{\sigma}\right) \tag{61}$$

The vector $\overrightarrow{a}$ represents a sphere, the so-called "Bloch-sphere". All density matrices for spin-$\frac{1}{2}$ particles live on the sphere or inside.
The coefficients of a_i, i=1,2,3 are given by

$$a_i = \mathrm{tr}\rho\ \sigma_i = \langle\sigma_i\rangle \tag{62}$$

We can see, the coefficients tell us something about the polarization of the system, e.g. of an electron- or neutron-beam. In this sense, $a_i = 0$ means, the beam is not polarized, whereas $a_i = 1$ means that the system is completely polarized.
Thus, for the density matrix we gather:

$$\rho = \frac{1}{2}\Big(1 + \langle\overrightarrow{\sigma}\rangle \cdot \overrightarrow{\sigma}\Big) \tag{63}$$

Let $\overrightarrow{a}$ be in z-direction, so that $a_x = a_y = 0$ and $a_z \equiv a$. Thus, we arrive at the following result for the density matrix:

$$\rho = \frac{1}{2}\Big(1 + a\sigma_z\Big) = \frac{1}{2}\begin{pmatrix} 1+a & 0 \\ 0 & 1-a \end{pmatrix} \tag{64}$$

We compare this result to the general decomposition:

$$\rho = \sum_{i,j} \rho_{ij}|i\rangle\langle j| \tag{65}$$

where $\rho_{ij} = \langle i|\rho|j\rangle$. Here $i, j = 1, 2 = \ \uparrow, \downarrow$ and

$$\rho = \rho_{11}|\uparrow\rangle\langle\uparrow| + \rho_{22}|\downarrow\rangle\langle\downarrow| + \rho_{12}|\uparrow\rangle\langle\downarrow| + \rho_{21}|\downarrow\rangle\langle\uparrow| \tag{66}$$

In comparison with eg. (64) we get:

$$\rho_{11} = \frac{1}{2}(1+a)\ ,\ \rho_{22} = \frac{1}{2}(1-a)\ ,\ \rho_{12} = \rho_{21} = 0 \tag{67}$$

Here ρ_{11} and ρ_{22} denote the probabilities to find the particle in the state $\uparrow$ or $\downarrow$. As $\frac{1}{2}(1 \pm a)$ are probabilities, we know that:

$$\begin{aligned} \frac{1}{2}|1 \pm a| &\leq 1 \\ 1 \pm a &\leq 2 \\ |a| &\leq 1 \end{aligned} \tag{68}$$

This means that the state is described by the density matrix ρ, at the same time it is a polarization-operator $\sigma_\uparrow$ or a projection operator $P_\uparrow$. Thus, for $|a| = 1$ we get a totally polarized state. For example, the density matrix for the completely polarized $\uparrow$-state is denoted by:

$$\rho = \frac{1}{2}(1 + \sigma_z) = \sigma_\uparrow \equiv P_\uparrow = |\uparrow\rangle\langle\uparrow| \tag{69}$$

Analogously we have for the density matrix for the completely polarized $\downarrow$-state:

$$\rho = \frac{1}{2}(1 - \sigma_z) = \sigma_\downarrow \equiv P_\downarrow = |\uparrow\rangle\langle\downarrow| \tag{70}$$

The question that remains is: Which ρ characterizes a pure state? For pure states we know that:

$$\rho^2 = \rho \tag{71}$$

So we calculate ρ^2 (recall that $\vec{a}\cdot\vec{\sigma}\ \vec{a}\cdot\vec{\sigma} = \vec{a}^2 = a^2$):

$$\rho^2 = \frac{1}{4}(1 + 2\vec{a}\cdot\vec{\sigma} + \vec{a}\cdot\vec{\sigma}\ \vec{a}\cdot\vec{\sigma})$$

$$\rho^2 = \frac{1}{2}\left(\frac{1+a^2}{2}1 + \vec{a}\cdot\vec{\sigma}\right)$$

If we compare this to $\rho = \frac{1}{2}(1 + \vec{a}\cdot\vec{\sigma})$ with $\rho^2 = \rho$ we get:

$$\frac{1+a^2}{2} = 1$$

$$|\vec{a}| = 1 \tag{72}$$

We see: for *pure states* $|\vec{a}| = 1$, whereas for *mixed states* $|\vec{a}| < 1$.

Finally let us consider an example for a density matrix of a totally mixed state:

$$\rho_{\text{mix}} = \frac{1}{2}(|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|) = \frac{1}{2}1 = \frac{1}{2}(\sigma_\uparrow + \sigma\downarrow) \tag{73}$$

Here the Bloch-vector $\vec{a} = 0$, so the state is totally mixed.

1.5 Density matrix for a pure spin state along an arbitrary direction

Let the observed system be in eigenstate of $\vec{\sigma}\cdot\vec{n}$. Then we write eigenequation of the system:

$$\vec{\sigma}\cdot\vec{n}|\pm\vec{n}\rangle = \pm|\pm\vec{n}\rangle \tag{74}$$

Where:

$$|+\vec{n}\rangle = \cos\frac{\vartheta}{2}\ e^{-i\frac{\varphi}{2}}|\uparrow\rangle + \sin\frac{\vartheta}{2}\ e^{i\frac{\varphi}{2}}|\downarrow\rangle \tag{75}$$

$$|-\vec{n}\rangle = -\sin\frac{\vartheta}{2}\ e^{-i\frac{\varphi}{2}}|\uparrow\rangle + \cos\frac{\vartheta}{2}\ e^{i\frac{\varphi}{2}}|\downarrow\rangle \tag{76}$$

Consequently, the density matrix in $\{|\uparrow\rangle, |\downarrow\rangle\}$-basis is given by:

$$\rho = |+\vec{n}\rangle\langle+\vec{n}| = (\cos\frac{\vartheta}{2}\ e^{-i\frac{\varphi}{2}}|\uparrow\rangle + \sin\frac{\vartheta}{2}\ e^{i\frac{\varphi}{2}}|\downarrow\rangle)\cdot(\cos\frac{\vartheta}{2}\ e^{i\frac{\varphi}{2}}|\uparrow\rangle + \sin\frac{\vartheta}{2}\ e^{-i\frac{\varphi}{2}}|\downarrow\rangle) \tag{77}$$

We remark the sum and the difference of the diagonal elements:

$$\rho_{\uparrow\uparrow} + \rho_{\downarrow\downarrow} = \cos^2\frac{\vartheta}{2} + \sin^2\frac{\vartheta}{2} = 1 \tag{78}$$

$$\rho_{\uparrow\uparrow} - \rho_{\downarrow\downarrow} = \cos^2\frac{\vartheta}{2} - \sin^2\frac{\vartheta}{2} = \cos\vartheta = \langle\sigma_z\rangle$$

We see: the diagonal elements describe the longitudinal polarization. Whereas, for the off-diagonal-elements we get the vertical polarization (projection on x-y-plane):

$$|\rho_{\uparrow\downarrow}| = |\rho_{\downarrow\uparrow}| = \frac{1}{2}\,\sin\vartheta = \frac{1}{2}\,\langle\sigma_v\rangle \tag{79}$$

Spin-measurement along $\overrightarrow{n}$:

In the following we want to show the explicit calculation of the spin-state along an arbitrary direction $\overrightarrow{n}$. Firstly we are interested in the eigenstates and eigenvectors of $\overrightarrow{n}\cdot\overrightarrow{\sigma}$:

$$\overrightarrow{n}\cdot\overrightarrow{\sigma} = n_1\sigma_1 + n_2\sigma_2 + n_3\sigma_3 \tag{80}$$

$$\sigma_1 = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\ ,\ \sigma_2 = \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}\ ,\ \sigma_3 = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} \tag{81}$$

The eigenequations are given by:

$$\overrightarrow{n}\cdot\overrightarrow{\sigma}|\pm\overrightarrow{n}\rangle = \pm|\pm\overrightarrow{n}\rangle \tag{82}$$

Denoting the components of $|+\overrightarrow{n}\rangle$ by (a,b) we gather:

$$a = n_3 a + (n_1 - in_2)b \tag{83}$$

$$a = \frac{n_1 - in_2}{1-n_3}b$$

$$\Rightarrow |a|^2 = \frac{n_1^2 + n_2^2}{(1-n_3)^2}|b|^2$$

The normalization $\langle+\overrightarrow{n}|+\overrightarrow{n}\rangle = 1$ gives:

$$b = \sqrt{\frac{1-n_3}{2}} \tag{84}$$

$$a = \frac{n_1 - in_2}{\sqrt{2(1-n_3)}}$$

Analogously we have for the negative eigenvalue vector components $|-\overrightarrow{n}\rangle$, denoted by (c,d):

$$c = -b^*, d = a^* \tag{85}$$

Re-expressing finally $\overrightarrow{n}$ by polar coordinates and extracting overall phases like $e^{\pm i\frac{\varphi}{2}}$ we obtain equations (75), (76).

density matrix: pure state - mixed state

In the following we are interested in the question: What is the difference between a pure state and a mixed state?

pure state: A pure state is a coherent superposition of states, e.g. $|\uparrow\rangle$, $|\downarrow\rangle$. Off-diagonal-elements do exist, they contain the phase information and are responsible for coherence.

mixed state: A mixed state is an incoherent superposition of states, e.g. $|\uparrow\rangle$, $|\downarrow\rangle$. In this case off-diagonal-elements do not exist, so the phase information is lost, at least partially. It is lost totally for totally mixed state where $|\overrightarrow{a}| = 0$.

Comparison:

The density matrix of the totally mixed state has the following structure:

$$\rho_{\text{mix}} = \frac{1}{2}(|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|) = \frac{1}{2}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} = \frac{1}{2}\mathbb{1} \tag{86}$$

The density matrix of the pure state with $\theta = 90$, $\varphi = 0$ is given by:

$$\rho_{\text{pure}} = \begin{pmatrix}\cos^2\frac{\theta}{2} & \frac{1}{2}\sin\theta e^{-i\varphi}\\ \frac{1}{2}\sin\theta e^{i\varphi} & \sin^2\frac{\theta}{2}\end{pmatrix} = \frac{1}{2}\begin{pmatrix}1 & 1\\ 1 & 1\end{pmatrix} \tag{87}$$

Now we will consider the expectation value of an operator, so to say the measurement outcome. If we consider the spin along the z-axis, we can see, that we can find no difference between the mixed and the pure state:

$$\langle\sigma_z\rangle_{\text{mix}} = \text{tr}\rho_{\text{mix}}\sigma_z = \text{tr}\frac{1}{2}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} = 0 \tag{88}$$

$$\langle\sigma_z\rangle_{\text{pure}} = \text{tr}\rho_{\text{pure}}\sigma_z = \text{tr}\frac{1}{2}\begin{pmatrix}1 & 1\\ 1 & 1\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} = 0 \tag{89}$$

In both cases 50% of the spins are orientated along $\uparrow$ and 50% along $\downarrow$. Now we choose projections on a definite spin, therefore we define the following projection operators:

$$P_\uparrow = |\uparrow\rangle\langle\uparrow| = \begin{pmatrix}1 & 0\\ 0 & 0\end{pmatrix} \tag{90}$$

$$P_\downarrow = |\downarrow\rangle\langle\downarrow| = \begin{pmatrix}0 & 0\\ 0 & 1\end{pmatrix}$$

$$P_+ \equiv \rho(\theta = 90, \varphi = 0) = \frac{1}{2}\begin{pmatrix}1 & 1\\ 1 & 1\end{pmatrix} \tag{91}$$

$$P_- \equiv \rho(\theta = 90, \varphi = 180) = \frac{1}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$$

Consequently, for the expectation values we obtain:

$$\langle P_\uparrow \rangle_{\text{mix}} = \text{tr } \rho_{\text{mix}} \text{P}_\uparrow = \text{tr} \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \frac{1}{2} \tag{92}$$

$$\langle P_\uparrow \rangle_{\text{pure}} = \text{tr } \rho_{\text{pure}} \text{P}_\uparrow = \text{tr} \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = \frac{1}{2}$$

$$\langle P_\downarrow \rangle_{\text{mix}} = \text{tr} \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = \frac{1}{2} \tag{93}$$

$$\langle P_\downarrow \rangle_{\text{pure}} = \text{tr} \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = \frac{1}{2}$$

We see: There is no difference up to now between the mixed and the pure states. But if we choose the spin measurement along the x-axis we get:

$$\langle P_+ \rangle_{\text{mix}} = \text{tr } \rho_{\text{mix}} \text{P}_+ = \text{tr} \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} = \frac{1}{4}\text{tr}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} = \frac{1}{2} \tag{94}$$

$$\langle P_- \rangle_{\text{mix}} = \text{tr } \rho_{\text{mix}} \text{P}_- = \text{tr} \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\frac{1}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} = \frac{1}{4}\text{tr}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} = \frac{1}{2}$$

Whereas:

$$\langle P_+ \rangle_{\text{pure}} = \text{tr } \rho_{\text{pure}} \text{P}_+ = \text{tr} \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}\frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} = \frac{1}{2}\text{tr}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} = 1 \tag{95}$$

$$\langle P_- \rangle_{\text{pure}} = \text{tr } \rho_{\text{pure}} \text{P}_- = \text{tr} \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}\frac{1}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} = \frac{1}{4}\text{tr}\begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} = 0$$

Resumée

For **pure states** it is characteristic that there exists a maximal test such that the outcome accurs with 100%. But for **mixed states** such a test is not possible.

1.6 Density matrix for mixed states

In the following we will discuss the example of an silver-atom. The atom is emitted by an oven and runs through a Stern-Gerlach-experiment, which acts like a polarizer. The silver-atom carries a spin, which looks into all directions. Each spin-direction has the same probability. Thus there is a statistical mixture of $|+\overrightarrow{n}\rangle$ -states with equal probabilities.

The density matrix is defined by:

$$\rho_{\text{pure}} = |\psi_i\rangle\langle\psi_i| =: \rho_i \tag{96}$$

$$\rho_{\text{mix}} = \sum_i p_i \rho_i \tag{97}$$

with the probabilities p_i with $\sum_i = 1$. We now exchange the sum by an integral:

$$\sum_i \;\rightarrow\; \frac{1}{4\pi}\int d\Omega \tag{98}$$

So we integrate the average space-angle over all directions with the normalization constant 4π. Thus, for the density matrix we get:

$$\rho_{\text{mix}} = \frac{1}{4\pi}\int d\Omega \rho(\Omega) \tag{99}$$

We recall the density matrix for the pure spin state $|+\overrightarrow{n}\rangle$:

$$\rho = \begin{pmatrix} \cos^2\frac{\theta}{2} & \frac{1}{2}\sin\theta\; e^{-i\varphi} \\ \frac{1}{2}\sin\theta\; e^{i\varphi} & \sin^2\frac{\theta}{2} \end{pmatrix} \tag{100}$$

Thus for the integration over all spin-states we have:

$$\rho_{\text{mix}} = \frac{1}{4\pi}\int_0^{2\pi} d\varphi \int_0^{\pi} \sin\theta d\theta \rho(\theta,\varphi) = \frac{1}{4\pi} 2\pi \int_{-1}^{1} d\xi \rho(\xi,\varphi) \tag{101}$$

where $\xi = \cos\theta$. Consequently, the as a result for the integration for the mixed density matrix we gather:

$$\rho_{\text{mix}} = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \frac{1}{2}\mathbb{1} \tag{102}$$

We can now easily calculate ρ^2_{mix}:

$$\rho^2_{\text{mix}} = \frac{1}{4}\mathbb{1} = \frac{1}{2}\rho_{\text{mix}} \tag{103}$$

We see: $\rho^2_{\text{mix}} \neq \rho_{\text{mix}}$. So indeed the state we consider is a mixed state.

Remark No 1: The expectation value of the spin in the mixed state is given by:

$$\langle\sigma_i\rangle_{\text{mix}} = \text{tr}\rho_{\text{mix}}\sigma_i = \frac{1}{2}\;\text{tr}\sigma_i = 0 \tag{104}$$

The spin is not polarized, all directions are equal, therefore the expectation value (average value) is zero.

Remark No 2: The off-diagonal-elements of the density matrix are given by:

$$\rho^{\text{mix}}_{\uparrow\downarrow} = \rho^{\text{mix}}_{\downarrow\uparrow} = 0 \tag{105}$$

$$\Downarrow$$

$$\langle \overrightarrow{\sigma_\perp} \rangle = 0 \tag{106}$$

We see: The expectation value of the transverse spin disappears.

Remark No 3: ρ_{mix} represents a statistical mixture of the different states $|+\overrightarrow{n}\rangle$, which have the same probability for all directions.

Important Note: There are different mixtures that lead to the same density matrix! Differently said: One and the same density matrix can be produced differently!

Example:

- Mixture of states $|\uparrow\rangle$ and $|\downarrow\rangle$ with equal weights:

$$\rho_{mix} = \frac{1}{2}(|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|) = \frac{1}{2}\mathbb{1} \tag{107}$$

  In the following we will see: We can get the same density matrix with a different mixture:

- Mixture of 3 states $|+\overrightarrow{n}\rangle$ with equal weights so that the angle between two states is always 120. Generally the state is given by:

$$|+\overrightarrow{n}\rangle = \cos\frac{\theta}{2}\, e^{-i\varphi}|\uparrow\rangle + \sin\frac{\theta}{2}\, e^{i\varphi}|\downarrow\rangle \tag{108}$$

  So we choose the following mixture of three states:

  $\frac{1}{\sqrt{3}}|\uparrow\rangle = |1\rangle$
  $\frac{1}{\sqrt{3}}(\cos\frac{120}{2}|\uparrow\rangle + \sin\frac{120}{2}|\downarrow\rangle) = |2\rangle$
  $\frac{1}{\sqrt{3}}(\cos\frac{120}{2}|\uparrow\rangle - \sin\frac{120}{2}|\downarrow\rangle) = |3\rangle$

  Thus, for the mixed density matrix we gather:

$$\rho_{\text{mix}} = \sum_{i=1}^{3} |i\rangle\langle i| = \frac{1}{3}|\uparrow\rangle\langle\uparrow| +$$

$$+\frac{1}{3}[\cos^2 60|\uparrow\rangle\langle\uparrow| + \sin^2 60|\downarrow\rangle\langle\downarrow| + \sin 60\, \cos 60(|\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|)] +$$

$$+\frac{1}{3}[\cos^2 60|\uparrow\rangle\langle\uparrow| + \sin^2 60|\downarrow\rangle\langle\downarrow| - \sin 60\, \cos 60(|\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|)] =$$

$$= \left(\frac{1}{3} + \frac{2}{3}\frac{1}{4}\right) |\uparrow\rangle\langle\uparrow| + \frac{2}{3}\frac{3}{4}|\downarrow\rangle\langle\downarrow| =$$

$$= \frac{2+1}{6}\begin{pmatrix}1 & 0\\ 0 & 0\end{pmatrix} + \frac{1}{2}\begin{pmatrix}0 & 0\\ 0 & 1\end{pmatrix} = \frac{1}{2}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} = \frac{1}{2}\mathbb{1} \tag{109}$$

The physical prediction depends only on the density matrix. This means that we cannot distinguish between the different types of statistical mixtures, which lead to the same density matrix. We can understand the different types like different aspects of one and the same incomplete information, which we have about a system. This leads to the *entropy*-notation for a quantum system: The *entropy* is a measure for the degree of uncertainty of a quantum system.

Theorem 1. *Thirring: In a mixed system we have only partial information about a quantum system. The entropy measures how much is missing from the maximal information.*

1.7 Density matrix in thermal equilibrium

In the following we will discuss the important example: the quantum system as a harmonic oscillator. In thermal equilibrium the n-th energy eigenstate is occupied with the probability:

$$p_n = Ne^{-n\beta} \tag{110}$$

where $\beta = \frac{\hbar\omega}{kT}$ and N is the normalization constant. Thus, the density matrix is given by:

$$\rho = \sum_{n=0}^{\infty} p_n |n\rangle\langle n| = N\sum_{n=0}^{\infty} e^{-n\beta}|n\rangle\langle n| \tag{111}$$

We calculate the normalization constant from the condition that $\mathrm{tr}\rho = 1$:

$$1 = \mathrm{tr}\rho = \sum_n \langle n|\rho|n\rangle = N\sum_{n=0}^{\infty} e^{-n\beta} = N\frac{1}{(1-e^{-\beta})} \tag{112}$$

$$\Downarrow$$

$$N = \left(1 - e^{-\beta}\right) \tag{113}$$

Consequently, we get for the density matrix:

$$\rho = \left(1 - e^{-\beta}\right)\sum_{n=0}^{\infty} e^{-n\beta}|n\rangle\langle n| \tag{114}$$

We will now consider the relation between the average energy $\langle H\rangle$ and the temperature T:

$$\langle H\rangle = \mathrm{tr}\rho H = \sum_n \langle n|\rho H|n\rangle = \sum_n \langle n|\rho|n\rangle\hbar\omega\left(n + \frac{1}{2}\right) =$$

$$= \hbar\omega \left[\left(1 - e^{-\frac{\hbar\omega}{kT}}\right) \sum_{n=0}^{\infty} n e^{-n\frac{\hbar\omega}{kT}} + \frac{1}{2} \right] \tag{115}$$

The probability for the n-th state is:

$$\langle n|\rho|n\rangle = p_n = (1 - e^{-\beta})e^{-n\beta} \tag{116}$$

In the following we will consider the relation between the average energy $\langle H \rangle$ and the average number of photons $\overline{n}$:

$$\langle H \rangle = \sum_n \langle n|\rho|n\rangle \hbar\omega \left(n + \frac{1}{2}\right) = \sum_n p_n \hbar\omega \left(n + \frac{1}{2}\right) \tag{117}$$

The average number of thermal quanta is given by:

$$\overline{n} = \sum_{n=0}^{\infty} p_n n = \sum_n \left(1 - e^{-\beta}\right) n e^{-n\beta} = -\left(1 - e^{-\beta}\right) \frac{\partial}{\partial\beta} \sum_n e^{-n\beta} = \frac{e^{-\beta}}{1 - e^{-\beta}} = \frac{1}{e^{\beta} - 1} \tag{118}$$

This means that the mean number of thermal quanta is determined by the temperature T. Consequently, for the mean energy we get:

$$\langle H \rangle = \sum_n p_n \hbar\omega \left(n + \frac{1}{2}\right) = \hbar\omega \left(\overline{n} + \frac{1}{2}\right) \tag{119}$$

We now express the density matrix in terms of the mean number of thermal quanta:

$$\rho = \left(1 - e^{-\beta}\right) \sum_n e^{-n\beta} |n\rangle\langle n| = \frac{1}{\overline{n} + 1} \sum_{n=0}^{\infty} \left(\frac{\overline{n}}{\overline{n} + 1}\right)^n |n\rangle\langle n| \tag{120}$$

Remark: "black body" radiation

The atom emits and absorbs photons with an energy of $E = \hbar\omega$. For the relation of the number of atoms in ground N_g and in excited state N_e in thermal equilibrium we have:

$$\frac{N_e}{N_g} = e^{-\frac{E}{kT}} \tag{121}$$

In thermal equilibrium the absorption and emission rates must be equal:

$$N_g \overline{n} = N_e(\overline{n} + 1) \tag{122}$$

Note

"+1" stands for spontaneous emission of an additional photon in the exited state. From this relation we can calculate the average number of photons $\overline{n}$:

$$\frac{\overline{n}}{\overline{n}+1} = \frac{N_e}{N_g} = e^{-\frac{\hbar\omega}{kT}} \tag{123}$$

$$\Downarrow$$

$$\overline{n} = \frac{1}{e^{\beta}-1} \tag{124}$$

Thus, for the energy for the mean photon number we gather:

$$\overline{n}\hbar\omega = \frac{\hbar\omega}{e^{\beta}-1} \tag{125}$$

In 1 dimension the energy density of the photons is:

$$dN = \frac{L}{2\pi}dk \tag{126}$$

In 3 dimensions it is:

$$dN = \frac{V}{(2\pi)^3}d^3K \cdot 2 \tag{127}$$

The factor "2" stands for the two independent degrees of freedom of the polarization. With $d^3k = 4\pi k^2 dk$ we get:

$$dN = \frac{V\omega^2}{\pi^2 c^3}d\omega \tag{128}$$

Classically for the energy density of photons we have:

$$dE = kTdN \tag{129}$$

Thus, we get the classical radiation equation (Rayleigh-Jeans):

$$u(\omega) = \frac{1}{V}\frac{dE}{d\omega} = \frac{kT}{\pi^2 c^3}\omega^2 \tag{130}$$

Quantum mechanically the energy density of photons is given by:

$$dE = \overline{n}\hbar\omega dN \tag{131}$$

So we arrive at the quantum mechanical radiation equation (Planck):

$$u(\omega) = \frac{1}{V}\frac{dE}{d\omega} = \frac{\hbar}{\pi^2 c^3}\frac{\omega^3}{e^{\frac{\hbar\omega}{kT}}-1} \tag{132}$$

1.8 Composite quantum systems

The composite quantum system consists of subsystems, for instance Alice and Bob (in quantum information theory) or 2 atoms, or 2 particles, or 2 degrees of freedom of the same object, for example the spin-path of a neutron, etc. For a combined system

$$AB = A + B \tag{133}$$

described in the Hilbert-space-notation we get a tensor product of the subspaces:

$$\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B \tag{134}$$

If the state vectors in the subsystems are $\{|\varphi_i\rangle^A \ \epsilon \ \mathcal{H}_A\}$ and $\{|\varphi_j\rangle^A \ \epsilon \ \mathcal{H}_B\}$ then the space vector for the combined (composite) system is given by:

$$|\psi\rangle = \sum_{i,j} c_{ij} |\varphi_i\rangle^A \otimes |\varphi_j\rangle^B \tag{135}$$

Note:

$|\varphi_i\rangle^A \otimes |\varphi_j\rangle^B$ forms a basis in the tensorspace with the dimension:

$$\dim\mathcal{H}_{AB} = \dim\mathcal{H}_A \cdot \mathcal{H}_B \tag{136}$$

We will now consider two operators that are acting in Hilbert-space, namely operator A action in $\mathcal{H}_A$ and operator B acting in $\mathcal{H}_B$. We introduce the norm of an operator:

$$\|A\|_2^2 = \mathrm{tr}A^\dagger A < \infty \tag{137}$$

and the scalar product:

$$(A_1, A_2) = \mathrm{tr}A_1^\dagger A_2 \tag{138}$$

The Hilbert-Schmidt operators form a Hilbert space, the so-called Hilbert-Schmidt-space. The tensor product of an operator can be defined via the action on vectors:

$$(A \otimes B)(|\varphi_i\rangle^A \otimes |\varphi_j\rangle^B) \equiv A|\varphi_i\rangle^A \otimes B|\varphi_j\rangle^B \tag{139}$$

Any operator acting on $\mathcal{H}_{AB}$ is expressible by a linear combination of tensor products:

$$O = \sum_i a_i A_i \otimes B_i \tag{140}$$

In particular, observables of the subsystems A and B can be written:

$$A \otimes \mathbb{1}_B \tag{141}$$

$$\mathbb{1}_A \otimes B$$

where 1_A and 1_B are the identities in the subsystems. We now will consider the density matrix of the composite system, which is an operator action on $\mathcal{H}_{AB}$. If the subsystems

are uncorrelated the density matrix of the composite system is given by the density operators of the subsystems:

$$\rho^{AB} \equiv \rho = \rho^A \otimes \rho^B \tag{142}$$

where ρ^A is action on $\mathcal{H}_A$ and ρ^B is action on $\mathcal{H}_B$. The expectation value of the tensor product of operators factorizes:

$$\langle A \otimes B \rangle = \mathrm{tr} A \otimes B\rho = \mathrm{tr}(A \otimes B)(\rho^A \otimes \rho^B) = \mathrm{tr}[A\rho^A \otimes B\rho^B] =$$

$$= \mathrm{tr}_A A\rho^A \cdot \mathrm{tr}_B B\rho^B = \langle A \rangle \cdot \langle B \rangle \tag{143}$$

where tr_A and tr_B denote the partial traces over the subsystems. If an operator on the total space $\mathcal{H}_{AB}$ is given by:

$$O = |a_1\rangle\langle a_2| \otimes |b_1\rangle\langle b_2| \tag{144}$$

with the vectors $|a_i\rangle \, \epsilon \, \mathcal{H}_A$ and $|b_i\rangle \, \epsilon \, \mathcal{H}_B$, then the partial trace over the subsystem B is defined by:

$$\mathrm{tr}_B O = |a_1\rangle\langle a_2|\mathrm{tr}|\mathrm{b}_1\rangle\langle \mathrm{b}_2| = \langle \mathrm{b}_2|\mathrm{b}_1\rangle|\mathrm{a}_1\rangle\langle \mathrm{a}_2| \; \epsilon \; \mathcal{H}_\mathrm{A} \tag{145}$$

Thus, the reduced density matrices are defined by:

$$\rho^A = \mathrm{tr}_B \rho \; \epsilon \; \mathcal{H}_A \text{ (describes state on system A)} \tag{146}$$

$$\rho^B = \mathrm{tr}_A \rho \; \epsilon \; \mathcal{H}_B \text{ (describes state on system B)}$$

This definition will be intuitively clear when we consider the product state

$$\rho = \sigma \otimes \tau \tag{147}$$

where $\sigma \, \epsilon \, \mathcal{H}_A$ and $\tau \, \epsilon \, \mathcal{H}_B$. Then we gather:

$$\mathrm{tr}\rho^A = \mathrm{tr}_B \sigma \otimes \tau = \sigma \tag{148}$$

$$\mathrm{tr}\rho^B = \mathrm{tr}_A \sigma \otimes \tau = \tau$$

The reduced density matrix ρ^A completely describes the statistical properties of all observables of the subsystem A:

$$\langle A \rangle_\rho = \mathrm{tr} A\rho = \mathrm{tr}(A \otimes \mathbb{1}_B)\rho = \mathrm{tr}_A A\rho^A = \langle A \rangle_{\rho A} \tag{149}$$

Example:

As an example let us consider qubits. The states of the subsystems are given by:

$$|\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \; , |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{150}$$

Thus for the composite system we get:

$$|\uparrow\rangle \otimes |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \tag{151}$$

Let's consider the operators:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \ , \ \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \tag{152}$$

For the composite system we obtain:

$$\sigma_x \otimes \sigma_y = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix} \tag{153}$$

Schmidt decomposition theorem (only for pure states)

For any state vector $|\psi\rangle \ \epsilon \ \mathcal{H}_A \otimes \mathcal{H}_B$ there exist orthonormal bases - the *Schmidt*-bases

$$\{|\chi_i\rangle^A \epsilon \mathcal{H}_A\} \text{ and } \{|\chi_i\rangle^B \epsilon \mathcal{H}_B\} \tag{154}$$

such that

$$|\psi\rangle = \sum_i c_i |\chi_i\rangle^A \otimes |\chi_i\rangle^B \tag{155}$$

with the Schmidt coefficients c_i. From the normalization $\langle\psi|\psi\rangle = 1$ we get:

$$\sum_i |c_i|^2 = 1 \tag{156}$$

Proof of the *Schmidt decomposition theorem*:

Without loss of generality we can suppose that $\dim\mathcal{H}_A = \dim\mathcal{H}_B$. Then the coefficient matrix in general decomposition is given by:

$$C = (c_{ij}) \text{ is square matrix} \tag{157}$$

$$\Downarrow$$

$$|\psi\rangle = \sum_{i,j} c_{ij} |\varphi_i\rangle^A \otimes |\varphi_j\rangle^B \tag{158}$$

We now use the *singular value decomposition theorem* of matrices:

$$C = U C^{\text{diag}} V \tag{159}$$

where U and V are unitary matrices and C^{diag} is a diagonal matrix with non-negative eigen-values. In components we can write:

$$c_{ij} = u_{ik} c_{kk}^{\text{diag}} v_{kj} \tag{160}$$

Then for the state vector $|\psi\rangle$ we get:

$$|\psi\rangle = \sum_{i,j} c_{ij} |\varphi_i\rangle^A \otimes |\varphi_j\rangle^B = \sum_{ijk} u_{ik} c_k v_{kj} |\varphi_i\rangle^A \otimes |\varphi_j\rangle^B = \sum_k c_k |\chi_k\rangle^A \otimes |\chi_k\rangle^B \text{ q.u.e.d.} \tag{161}$$

Remark:

Note that the Schmidt basis can always be chosen such that the Schmidt-coefficients $c_i \geq 0$ are real and non-negative.

Definition

The *Schmidt number* N_S is defined by the number of Schmidt coefficients $c_i > 0$. N_S is invariant under unitary transformations U^A and U^B on the subspaces $\mathcal{H}_A$ and $\mathcal{H}_B$. N_S is uniquely defined for a space-vector $|\psi\rangle$ (it does not depend on a particular Schmidt basis).

A state $|\psi\rangle$ is called *product state* if it can be written as a tensor product

$$|\psi\rangle = |\varphi\rangle^A \otimes |\varphi\rangle^B \tag{162}$$

A state $|\psi\rangle \; \epsilon \; \mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$ is called *entangled* if it cannot be written as a tensor product. From the Schmidt decomposition theorem follows:

$$|\psi\rangle \text{ is entangled if } N_S > 1 \tag{163}$$

$$|\psi\rangle \text{ is a product state if } N_S = 1$$

$$|\psi\rangle \text{ is maximal entangled if all Schmidt coefficients are equal } |c_i| = |c| \tag{164}$$

We will now consider the density matrix of a composite quantum system in a pure state.

Lemma 1. *If a system is in a pure state $\rho = |\psi\rangle\langle\psi|$ then the reduced density matrices $\rho^A = \text{tr}_B \rho$ and $\rho^B = \text{tr}_A \rho$ have same eigenvalues.*

Proof:

$$\rho^A = \text{tr}_B |\psi\rangle\langle\psi| = \text{tr}_B [\sum_i c_i |\chi_i\rangle^A \otimes |\chi_i\rangle^B (\sum_j c_j^* \; {}^A\langle\chi_j| \otimes^B \langle\chi_j|)] =$$

$$= \text{tr}_B [\sum_{ij} c_j c_j^* |\chi_j\rangle\langle\chi_j|^A \otimes |\chi_i\rangle\langle\chi_j|^B] = \text{tr} |c_i|^2 |\chi_i\rangle\langle\chi_i|^A \tag{165}$$

Analogously:

$$\rho^B = \mathrm{tr}_A|\psi\rangle\langle\psi| = \sum_i |c_i|^2 |\chi_i\rangle\langle\chi_i|^B \text{ q.u.e.d.} \tag{166}$$

Remark:

Generally subsystems are in mixed states when the composite system is in a pure state. If a composite state ρ is maximal entangled, then the reduced densities ρ^A and $\rho^B \sim 1$ are maximal mixed. A composite state ρ is a product state if ρ^A and ρ^B are in pure states.

1.9 Purification of a quantum state

Motivation:

The purification of a quantum state is a frequently used technique in quantum communication and quantum information.

We can associate pure states with mixed states. For example let us consider a given quantum state ρ^A of the system Alice. Then we introduce another system R as a reference system. (Note: There is not necessarily a direct physical significance.) We now define the **pure state** $|AR\rangle$ of the joint system AR

$$\rho = |AR\rangle\langle AR| \; \epsilon \; \mathcal{H}_{AR} = \mathcal{H}_A \otimes \mathcal{H}_R \tag{167}$$

such that the reduced density matrix is given by:

$$\rho^A = \mathrm{tr_R}|\mathrm{AR}\rangle\langle\mathrm{AR}| \tag{168}$$

Thus the pure state ρ reduces to ρ^A when we look only at A. Purification can be done for any state. Let us suppose a mixed state. Then the purification can be constructed:

$$\rho^A = \sum_i p_i |\varphi_i\rangle\langle\varphi_i|^A \tag{169}$$

with the complete orthogonal basis $\{|\varphi_i\rangle^A \; \epsilon \; \mathcal{H}_A\}$. To purify ρ^A we introduce the system R with the same state space as A: $\{|\varphi_i\rangle^R \; \epsilon \; \mathcal{H}_R\}$. We now define the pure state for the joint system AR - according to the *Schmidt decomposition* - as:

$$|AR\rangle = \sum_i \sqrt{p_i} |\varphi_i\rangle^A \otimes |\varphi_i\rangle^R \tag{170}$$

Then the reduced density matrix for A is given by:

$$\mathrm{tr}_R\rho = \mathrm{tr}_R|AR\rangle\langle AR| = \sum_{i,j} \sqrt{p_i p_j} |\varphi_i\rangle\langle\varphi_j|^A \mathrm{tr}|\varphi_i\rangle\langle\varphi_j|^R = \sum_i p_i |\varphi_i\rangle\langle\varphi_i|^A = \rho^A \tag{171}$$

Thus $\rho = |AR\rangle\langle AR|$ is a purification of ρ^A.

Procedure of purification:

A mixed state ρ^A can be purified by defining a pure state $|AR\rangle$ with such a Schmidt basis for A in which the mixed state ρ^A is diagonal. The Schmidt coefficients are $\sqrt{p_i}$ where p_i are the eigenvalues of ρ^A. We see: With the Schmidt decomposition purification can be obtained.

1.10 Examples of composite states

1. Bell states

Let us now consider the maximal entangled *Bell states*:

$$|\psi^{\mp}\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle \otimes |\downarrow\rangle \mp |\downarrow\rangle \otimes |\uparrow\rangle) \tag{172}$$

$$|\phi^{\mp}\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle \otimes |\uparrow\rangle \mp |\downarrow\rangle \otimes |\downarrow\rangle)$$

The Bell density matrices are denoted by $\rho^{\mp}$ and $\omega^{\mp}$:

$$\rho^{\mp} = |\psi^{\mp}\rangle\langle\psi^{\mp}| \tag{173}$$

$$\omega^{\mp} = |\phi^{\mp}\rangle\langle\phi^{\mp}|$$

Explicitly we get for ρ^{-}:

$$|\uparrow\rangle \otimes |\downarrow\rangle = \begin{pmatrix}1\\0\end{pmatrix}\begin{pmatrix}0 & 1\end{pmatrix} = \begin{pmatrix}0 & 1\\0 & 0\end{pmatrix} \ , |\downarrow\rangle \otimes |\uparrow\rangle = \begin{pmatrix}0\\1\end{pmatrix}\begin{pmatrix}1 & 0\end{pmatrix} = \begin{pmatrix}0 & 0\\1 & 0\end{pmatrix}$$

$$\begin{pmatrix}1 & 0\\0 & 0\end{pmatrix} \otimes \begin{pmatrix}0 & 0\\0 & 1\end{pmatrix} = \begin{pmatrix}0 & 0 & 0 & 0\\0 & 1 & 0 & 0\\0 & 0 & 0 & 0\\0 & 0 & 0 & 0\end{pmatrix}$$

$$\Downarrow$$

$$\rho^{-} = \frac{1}{2}(|\uparrow\rangle\langle\uparrow| \otimes |\downarrow\rangle\langle\downarrow| - |\uparrow\rangle\langle\downarrow| \otimes |\downarrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow| \otimes |\uparrow\rangle\langle\uparrow| - |\downarrow\rangle\langle\uparrow| \otimes |\uparrow\rangle\langle\downarrow|) =$$

$$= \frac{1}{2}\begin{pmatrix}0 & 0 & 0 & 0\\0 & 1 & -1 & 0\\0 & -1 & 1 & 0\\0 & 0 & 0 & 0\end{pmatrix} \tag{174}$$

In terms of the *Pauli matrices* the Bell states can be expressed like the following:

$$\rho^{\mp} = \frac{1}{4}(\mathbb{1} \mp \sigma_x^A \otimes \sigma_x^B \mp \sigma_y^A \otimes \sigma_y^B - \sigma_z^A \otimes \sigma_z^B) \tag{175}$$

$$\omega^{\mp} = \frac{1}{4}(\mathbb{1} \mp \sigma_x^A \otimes \sigma_x^B \pm \sigma_y^A \otimes \sigma_y^B + \sigma_z^A \otimes \sigma_z^B)$$

with the Pauli matrices $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.

2. Werner state - mixed entangled

$$\rho_W = p\rho^- + (1-p)\frac{1}{4}\mathbb{1} \tag{176}$$

where $0 \leq p \leq 1$. One can find that for $0 \leq p \leq \frac{1}{3}$ the *Werner state* is separable, for $\frac{1}{3} < p \leq \frac{1}{2}$ it behaves classically and for $\frac{1}{2} < p \leq 1$ it can be used for teleportation. For $\frac{1}{3} \leq p \leq \frac{1}{\sqrt{2}}$ the Bell Inequality is not violated but still the state is entangled.

The density matrix for Alice and Bob is given by:

$$\rho_\alpha = \frac{1}{4}(\mathbb{1} - \alpha \overrightarrow{\sigma}^A \otimes \overrightarrow{\sigma}^B) \tag{177}$$

For $-\frac{1}{3} \leq \alpha \leq 1$ the density matrix is well-defined, this means that it is a positive operator. For $-\frac{1}{3} \leq \alpha \leq \frac{1}{3}$ the state is separable and for $\frac{1}{3} < \alpha < 1$ it is mixed entangled. Just for $\alpha = 1$ we get a pure state namly the anti-symmetric *Bell-Singlet state*, which is maximal entangled.

Separable states

We now define the set of separable states:

$$S = \{\rho = \sum_i p_i \rho_i^A \otimes \rho_i^B \mid 0 \leq p_i \leq 1, \sum_i p_i = \mathbb{1}\} \tag{178}$$

A state ω is entangled when it is not separable so $\omega \, \epsilon \, S^c$ where S^c is the complement to S. One can show that S is convex and that S and S^c combine to the Hilbert-space:

$$S \cup S^c = \mathcal{H} \tag{179}$$

Reduced density matrix of entangled states

The reduced density matrix for an entangled state is given by:

$$\rho^- = \frac{1}{2}\left(|\uparrow\rangle\langle\uparrow| \otimes |\downarrow\rangle\langle\downarrow| - |\uparrow\rangle\langle\downarrow| \otimes |\downarrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow| \otimes |\uparrow\rangle\langle\uparrow| - |\downarrow\rangle\langle\uparrow| \otimes |\uparrow\rangle\langle\downarrow|\right) \tag{180}$$

We trace over Bob:

$$\mathrm{Tr}|\downarrow\rangle\langle\downarrow| = \sum_{i=\uparrow,\downarrow} = \langle i|\downarrow\rangle\langle\downarrow|i\rangle = \langle\downarrow|\downarrow\rangle\langle\downarrow|\downarrow\rangle = 1 \tag{181}$$

$$\mathrm{Tr}|\uparrow\rangle\langle\uparrow| = \sum_{i=\uparrow,\downarrow} = \langle i|\uparrow\rangle\langle\uparrow|i\rangle = \langle\uparrow|\uparrow\rangle\langle\uparrow|\uparrow\rangle = 1$$

$$\mathrm{Tr}|\uparrow\rangle\langle\downarrow| = \langle\uparrow|\uparrow\rangle\langle\downarrow|\uparrow\rangle + \langle\downarrow|\uparrow\rangle\langle\downarrow|\downarrow\rangle = 0$$
$$\mathrm{Tr}|\downarrow\rangle\langle\uparrow| = 0$$

Thus for the reduced density matrix for Alice we get:

$$\rho^A = \mathrm{Tr}_B\rho^- = \frac{1}{2}(|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|) = \frac{1}{2}\mathbb{1} \tag{182}$$

Note: The state ρ^A is maximally mixed with the measure:

$$\delta = \mathrm{Tr}(\rho^A)^2 = \frac{1}{4}\mathrm{Tr}\mathbb{1} = \frac{1}{2} < 1 = \mathrm{Tr}\rho^A \tag{183}$$

Remark:

The joint state of Alice and Bob consists of 2 qubits. If we want to know Alice' state we have to trace over Bob. Then the state of Alice is maximally mixed. Thus we don't have the maximal information about state A. We can express this maximal uncertainty with the *von Neumann entropy* S - which will be defined in the following chapter - of the reduced density matrix ρ^A:

$$S(\rho^A) = -\frac{1}{2}\log_2\frac{1}{2}\cdot 2 = -\frac{1}{2}(-1)2 = 1 \tag{184}$$

Whereas for a pure and maximally entangled state there is no uncertainty and the *von Neumann entropy* vanishes:

$$S(\rho^-) = -\mathrm{tr}\rho^-\log_2\rho^- \to 0 \tag{185}$$

2 Quantum entropies

2.1 Von Neumann Entropy - definition

Let be a given state ρ. Then the **von Neumann entropy** is defined by

$$S(\rho) = -\mathrm{tr}\ \rho\ \log\rho \tag{186}$$

Note:

Here log = ln, whereas for qubits it's better to use $\log_2 x = \frac{\ln x}{\ln 2}$.
The trace of the operator (density matrix) is defined via its eigenvalues. Thus for the entropy we get:

$$S(\rho) = -\sum_i \lambda_i\ \log\lambda_i \tag{187}$$

For a totally mixed state we have:

$$\rho_{\mathrm{mix}} = \frac{1}{d}\mathbb{1}_{\mathrm{d}} \tag{188}$$

$$S(\rho_{\text{mix}}) = -\text{tr}\ \rho_{\text{mix}}\ \log\rho_{\text{mix}} = -\text{tr}\frac{1}{d}\mathbb{1}\ \log\frac{1}{d}\mathbb{1} = -\sum_i \frac{1}{d}\lambda_i\ \log\frac{\lambda_i}{d} = \log\ d \tag{189}$$

The entropy can be normalized:

$$0 \leq S(\rho) \leq 1 \tag{190}$$

Examples:

- **pure state**: $|\alpha\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + e^{i\alpha}|\downarrow\rangle$
  Here the density matrix is given by:

$$\rho_\alpha = \frac{1}{2}\begin{pmatrix} 1 & e^{-i\alpha} \\ e^{i\alpha} & 1 \end{pmatrix} \tag{191}$$

  We calculate the eigenvalues:

$$\begin{vmatrix} 1-\lambda & e^{-i\alpha} \\ e^{i\alpha} & 1-\lambda \end{vmatrix} = 0\ \Rightarrow\ (1-\lambda)^2 ==\Rightarrow \lambda_1 = 2, \lambda_2 = 0 \tag{192}$$

$$\Downarrow$$

$$\rho_\alpha^{\text{diag}} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \tag{193}$$

  Thus for the von Neumann entropy we get:

$$S(\rho_\alpha) = -\text{tr}\rho_\alpha^{\text{diag}}\ \log\rho_\alpha^{\text{diag}} = -1\ \log\ 1 - 0\ \log\ 0 = 0 \tag{194}$$

  So we can distinguish between the following cases:
  i) $0 < S(\rho) \leq 1$ mixed state
  ii) $S(\rho) = 1$ maximal mixed
  iii) $S(\rho) = 0$ pure state

- **mixed state**: The density matrix is given in the spectral decomposition:

$$\rho = \sum_i p_i |\varphi_i\rangle\langle\varphi_i| \tag{195}$$

  where $p_i \geq 0$ and $\sum_i p_i = 1$. Then the entropy becomes:

$$S(\rho) = -\text{tr}\rho\ \log\rho = -\text{tr}\sum_i p_i|\varphi_i\rangle\langle\varphi_i|\ \log\sum_j p_j|\varphi_j\rangle\langle\varphi_j| = \tag{196}$$

$$= -\text{tr}\sum_i p_i \sum_j \sum_k c_k (p_j)^k |\varphi_i\rangle\langle\varphi_i|\varphi_j\rangle\langle\varphi_j|... = -\sum_i p_i\ \log p_i \equiv H(\{p_i\})$$

  where $H(\{p_i\})$ denotes the *Shannon Information Entropy* of a classical probability distribution $\{p_i\}$ for random numbers i.

Resumée:

A statistical mixture is achieved by mixing pure states with weights p_i. Then the von Neumann entropy expresses the uncertainty - the lack of knowledge (partial information) - about the realization of a particular state in the mixture.

Remark:

When mixing 2 or more random variables we can define the *binary entropy*. The entropy of a binary outcome of 2 random variables is given by:

$$H_{\text{bin}}(p) = -p \log p - (1-p) \log(1-p) \tag{197}$$

where $0 \leq p \leq 1$.

2.2 Properties of Von Neumann Entropy

As we already know the von Neumann entropy is given by:

$$S(\rho) = -\text{tr}\rho \log\rho \tag{198}$$

where ρ denotes a quantum state.

The von Neumann entropy has the following properties:

- $$S(\rho) \geq 0 \tag{199}$$

  If $S(\rho) = 0 \Rightarrow \rho$ is a pure state.

- $$S(\rho) \leq \log\, d \tag{200}$$

  If $S(\rho) = \log\, d \Rightarrow \rho$ is a totally mixed state: $\rho = \frac{1}{d}\mathbb{1}_{\text{d}}$.

- $$S(U\rho U^\dagger) = S(\rho) \tag{201}$$

  This means that $S(\rho)$ is invariant under unitary transformations U,
  where $U^\dagger U = 1$.

- $S(\rho)$ is a concave functional. This a very important property! For the map of ρ in Hilbert space this means: map $\rho \rightarrow S(\rho)$. So for any set $\{p_i\}$ we know:

  $$S\left(\sum_i p_i\rho_i\right) \geq \sum_i p_i S(\rho_i) \tag{202}$$

  where $0 \leq p_i \leq 1$ and $\sum_i p_i = 1$. Remark: If $\rho_i \equiv \rho$ for all indices i $\Rightarrow S(\sum_i p_i\rho_i) = \sum_i p_i S(\rho_i)$.

Physically this property tells us that the uncertainty about a state $\sum_i p_i\rho_i$ is greater (or equal) than the uncertainties of states ρ_i in mixture. Proof: see end of this section

- Suppose that p_i is a probability with the properties $p_i \geq 0$, $0 \leq p_i \leq 1$ and $\sum_i p_i = 1$. Let ρ_i be quantum states with support on orthogonal subspaces. Then there holds the following **entropy theorem**:

  Theorem 2.
  $$S(\sum_i p_i\rho_i) = H(\{p_i\}) + \sum_i p_i S(\rho_i) \tag{203}$$

  where $H(\{p_i\}) = -\sum_i p_i \log p_i$ denotes the *Shannon entropy* of the probability distribution $\{p_i\}$.

  Proof:

  Let be λ_i^j eigenvalues and $|e_i^j\rangle$ eigenvectors of ρ_i. Since the subspaces are orthogonal we can suppose that $p_i\lambda_i^j$ are eigenvalues and $|e_i^j\rangle$ are eigenvectors of $\sum_i p_i\rho_i$. Then:
  $$S(\rho) = S\left(\sum_i p_i\rho_i\right) = -\sum_j \overline{\lambda}^j \log\overline{\lambda}^j \tag{204}$$

  where $\overline{\lambda}^j$ are eigenvalues of ρ. With $\log p_i\lambda_i^j = \log p_i + \log\lambda_i^j$ we can write:

  $$S(\rho) = -\sum_{i,j} p_i\lambda_i^j \log p_i\lambda_i^j = -\sum_i p_i \log p_i \sum_j \lambda_i^j - \sum_i p_i \sum_j \lambda_i^j \log\lambda_i^j =$$

  $$= H(\{p_i\}) + \sum_j p_i S(\rho_i) \tag{205}$$

- **Joint entropy theorem for composite systems**

  Suppose that p_i is the probability with the properties $p_i \geq 0$ and $\sum_i p_i = 1$. Let ρ_i be any density matrix on subsystem A. Let $|i\rangle$ be an orthogonal basis on subsystem B corresponding to index i of ρ_i. Finally let be *joint state*
  $$\rho^{AB} = \sum p_i\rho_i \otimes |i\rangle\langle i| \tag{206}$$

  Then we have the **joint entropy theorem**:

  Theorem 3.
  $$S(\rho^{AB}) = H(\{p_i\}) + \sum_i p_i S(\rho_i) \tag{207}$$

Proof:

Let us consider states with support on orthogonal subspaces: $\rho_i' = \rho_i \otimes |i\rangle\langle i|$. From the entropy theorem for ρ_i' follows:

$$S(\rho^{AB}) = S\left(\sum_i p_i \rho_i'\right) = H(\{p_i\}) + \sum_i p_i S(\rho_i')$$

And we can show that:

$$S(\rho_i') = -\mathrm{tr}\rho_i' \log \rho_i' = -\mathrm{tr}\rho_i \otimes |i\rangle\langle i| \log \rho_i \otimes |i\rangle\langle i| = -\mathrm{tr}_A \rho_i \log \rho_i = S(\rho_i)$$

which completes the proof.

- **entropy of composite system**: Let us consider a density matrix ρ on Hilbert-space $\mathcal{H}_A \otimes \mathcal{H}_B = \mathcal{H}_{AB}$. The density matrices on the subsystems are given by:

$$\rho^A = \mathrm{tr}_B \rho \; \epsilon \; \mathcal{H}_A \; , \; \rho^B = \mathrm{tr}_A \rho \; \epsilon \; \mathcal{H}_B \tag{208}$$

The entropy of the composite system satisfies the *subadditivity property*

$$S(\rho) \leq S(\rho^A) + S(\rho^B) \;\; \text{upper bound} \tag{209}$$

For $\rho = \rho^A \otimes \rho^B$ we get: $S(\rho) = S(\rho^A) + S(\rho^B)$. Physically this means that the uncertainty of the product state (Alice and Bob uncorrelated) is larger than the uncertainty about the composite system. This means that by tracing over subsystem A, B we lose information about correlations between A and B, thus, increasing the entropy. The Proof for the subadditivity follows quickly from the relative entropy, see Section 2.3., Eq. (234).

Generally we can say if ρ is a pure state $\rho = |\psi\rangle\langle\psi| \Rightarrow S(\rho) = 0$.

From the Schmidt decomposition theorem follows that the subsystems have the same eigenvalues $|c_i|$ with the Schmidt coefficients c_i.

$$S(\rho^A) = S(\rho^B) = -\sum_i |c_i|^2 \log |c_i|^2 \geq 0 \tag{210}$$

with the strict positivity > 0 if ρ is entangled.

We also want to mention the **Araki-Lieb inequality**

$$\text{lower bound} \;\; |S(\rho^A) - S(\rho^B)| \leq S(\rho) \tag{211}$$

Proof of the concavity of the von Neumann entropy:

With the properties we have discussed before we are in position to prove the concavity of the von Neumann entropy:

$$S\left(\sum_i p_i\rho_i\right) \geq \sum_i p_i S(\rho_i) \tag{212}$$

Proof: Let be ρ_i states of the system A. We introduce an auxiliary system B whose state space has the orthogonal basis $|i\rangle$ corresponding to the index i of ρ_i. The *joint state* is defined by:

$$\rho^{AB} = \sum_i p_i\rho_i \otimes |i\rangle\langle i| \tag{213}$$

To prove the concavity we use the subadditivity of the entropy, we have:

$$\rho^A = \mathrm{tr}_B\rho^{AB} = \sum_i p_i\rho_i \tag{214}$$

$$\rho^B = \mathrm{tr}_A\rho^{AB} = \sum_i p_i|i\rangle\langle i|$$

$$S(\rho^A) = S\left(\sum_i p_i\rho_i\right) \tag{215}$$

$$S(\rho^B) = S\left(\sum_i p_i|i\rangle\langle i|\right) = -\mathrm{tr}\left[\sum_i p_i|i\rangle\langle i|\log\sum_i p_i|i\rangle\langle i|\right] = -\sum_i p_i\log p_i =$$
$$= H(\{p_i\}) \tag{216}$$

where $H(\{p_i\})$ denotes the *Shannon information entropy*. Quite generally holds the *joint entropy theorem*:

$$S(\rho^{AB}) = H(\{p_i\}) + \sum_i p_i S(\rho_i) \tag{217}$$

We apply the subadditivity property:

$$S(\rho^{AB}) \leq S(\rho^A) + S(\rho^B) \tag{218}$$

Thus, we gather:

$$H(\{p_i\}) + \sum_i p_i S(\rho_i) \leq S(\sum_i p_i\rho_i) + H(\{p_i\}) \tag{219}$$

$$\Downarrow$$

$$\sum_i p_i S(\rho_i) \leq S(\sum_i p_i\rho_i) \tag{220}$$

2.3 Quantum relative entropy

In the following we will consider *quantum relative entropy* in analogy to *classical relative entropy*. Let be $p(x)$ and $q(x)$ two probability distributions. Now we define an entropy measure $H(p(x)||q(x))$ for the "closeness" of the two distributions $p(x)$ and $q(x)$:

$$H(p(x)||q(x)) := \sum_x p(x)\ \log\frac{p(x)}{q(x)} = -H(p(x)) - \sum_x p(x)\ \log\ q(x) \tag{221}$$

Theorem 4. *Non-negativity of relative entropy:*

$$H\left(p(x)||q(x)\right) \geq 0 \tag{222}$$

If $p(x) = q(x) \Rightarrow H(p(x)||q(x)) = 0$.

Proof:

For "log" we chose "$\log_2$". Then there exists a number x such that:

$$\log_2 x \ln 2 = \ln x \leq x - 1 \tag{223}$$

$$\Downarrow$$

$$-\log_2 x \geq \frac{1-x}{\ln 2} \tag{224}$$

Consequently, we have:

$$H(p(x)||q(x)) = -\sum_x p(x)\log_2\frac{q(x)}{p(x)} \geq \frac{1}{\ln 2}\sum_x p(x)(1-\frac{q(x)}{p(x)}) = \tag{225}$$

$$= \frac{1}{\ln 2}\sum_x (p(x)-q(x)) = \frac{1}{\ln 2}(1-1) = 0 \quad \text{q.e.d.}$$

To consider the quantum case let be ρ, σ two density matrices. We define the *relative entropy* $S(\rho||\sigma)$ of ρ to σ:

$$S(\rho||\sigma) := \mathrm{tr}\rho\ \log\ \rho - \mathrm{tr}\rho\ \log\ \sigma \tag{226}$$

This is an entropy-like measure for the "closeness" of two density matrices.
We define the *kernel* of an operator:

$$\text{kern}\ \sigma = \{v\ \epsilon H|\sigma v = 0\},\ \lambda = 0 \tag{227}$$

where v is an eigenvector, and λ is its eigenvalue. The *support* of an operator is defined by:

$$\text{supp}\ \rho = \{w\ \epsilon H|\rho w = \lambda w\},\ \lambda \neq 0 \tag{228}$$

If we now consider entropy we get the following results:

- $$S \to \infty \quad \text{if kern } \sigma \cap \text{supp } \rho \neq \emptyset \text{ nontrivial} \tag{229}$$

- $$S < \infty \quad \text{if kern } \sigma \cap \text{supp } \rho = \emptyset \text{ trivial} \tag{230}$$

Let us consider a composite system $\rho \, \epsilon \, H_{AB}$ and an uncorrelated system $\rho^A \otimes \rho^B$. Then we have the following lemma:

Lemma 2.

$$S(\rho||\rho^A \otimes \rho^B) = S(\rho^A \otimes \rho^B) - S(\rho) = S(\rho^A) + S(\rho^B) - S(\rho) \tag{231}$$

Proof:

$$S(\rho||\rho^A \otimes \rho^B) = \text{tr}\rho \, \log\rho - \text{tr}\rho \, \log\rho^A \otimes \rho^B = -S(\rho) - \text{tr}\rho \left(\log\rho^A + \log\rho^B\right) =$$

$$= -S(\rho) - \text{tr}_A \, \rho^A \log\rho^A - \text{tr}_B \, \rho^B \log\rho^B = S(\rho^A) + S(\rho^B) - S(\rho) \tag{232}$$

The entropy of the composite system ρ relative to the uncorrelated system $\rho^A \otimes \rho^B$ corresponds to the change of the *von Neumann entropies* of ρ to $\rho^A \otimes \rho^B$, i.e. the information-loss when we trace over the subsystems.

Properties of relative quantum entropy

- non-negativity-theorem - *Klein-inequality*

$$S(\rho||\sigma) \geq 0 \quad \text{"="} \text{ if } \quad \rho = \sigma \tag{233}$$

From this property follows the subadditivity of the *von Neumann entropy*:

$$0 \leq S(\rho||\rho^A \otimes \rho^B) = S(\rho^A) + S(\rho^B) - S(\rho)$$

$$\Downarrow$$

$$S(\rho) \leq S(\rho^A) + S(\rho^B) \tag{234}$$

- The *relative quantum entropy* invariant with respect to unitary transformations:

$$S(U\rho U^\dagger||U\sigma U^\dagger) = S(\rho||\sigma) \tag{235}$$

where $UU^\dagger = \mathbb{1}$

- The *relative quantum entropy* is jointly convex:

$$S(\rho||\sigma) = \lambda S(\rho_1||\sigma_2) + (1-\lambda) S(\rho_2||\sigma_2) \tag{236}$$

for $0 \leq \lambda \leq 1$, $\rho = \lambda\rho_1 + (1-\lambda)\rho_2$ and $\sigma = \lambda\sigma_1 + (1-\lambda)\sigma_2$.

- Tracing over both subsystems reduces the relative entropy:

$$S(\rho^A||\sigma^A) \leq S(\rho||\sigma) \tag{237}$$

where $\rho^A = \mathrm{tr}_B\rho$ and $\sigma^A = \mathrm{tr}_B\sigma$. In particular if $\rho = \rho^A \otimes \rho^B$:

$$S(\rho^A||\sigma^A) = S(\rho^A \otimes \rho^B||\sigma^A \otimes \rho^B) \tag{238}$$

Proof:

$$\begin{gathered} S(\rho^A \otimes \rho^B||\sigma^A \otimes \rho^B) = \\ = \mathrm{tr}\ \rho^A \otimes \rho^B\ \log\ (\rho^A \otimes \rho^B) - \mathrm{tr}\ \rho^A \otimes \rho^B\ \log\ (\sigma^A \otimes \rho^B) = \\ = \mathrm{tr}\ \rho^A \otimes \rho^B\ \log\ \rho^A - \mathrm{tr}\ \rho^A \otimes \rho^B\ \log\ \sigma^A = \\ = \mathrm{tr}_A\ \rho^A\ \log\ \rho^A - \mathrm{tr}_A\ \rho^A\ \log\ \sigma^A = S(\rho^A||\sigma^A) \end{gathered}$$

2.4 Quantum linear entropy

The *quantum linear entropy* is a measure for the mixedness of a state. It is defined by:

$$S_{\mathrm{lin}}(\rho) = \mathrm{tr}(\rho - \rho^2) = 1 - \mathrm{tr}\rho^2 \tag{239}$$

with the property $0 \leq S_{\mathrm{lin}} \leq 1$ and $S_{\mathrm{lin}} \leq 0$ for pure states. For d dimensions we get:

$$S_{\mathrm{lin}}(\rho) = 1 - \frac{1}{d} \tag{240}$$

2.5 Measurement and entropy

We are now interested in the behaviour of a quantum system under a measurement. In the following we will consider *projective measurements*.

Let us consider an observable A. It is a hermitian operator onto a state space. There exists a spectral decomposition:

$$A = \sum_i a_i P_i \tag{241}$$

where P_i are projectors onto eigenstates of A with the properties:

$$P_i = |i\rangle\langle i|\ ,\ P_i^2 = P_i\ ,\ P_i^\dagger = P_i\ ,\ \sum_i P_i = 1 \tag{242}$$

The eigenequation of the eigenstates of A with eigenvalues a_i is given by:

$$A|i\rangle = a_i|i\rangle \tag{243}$$

For the probability of measuring an eigenvalue a_i in a general state $|\psi\rangle$ we gather:

$$p_i = \langle\psi|P_i|\psi\rangle = \langle\psi|i\rangle\langle i|\psi\rangle = |\langle i|\psi\rangle|^2 \tag{244}$$

We are now interested in the outcome of a_i after the measurement. Before the measurement the system is in state $|\psi\rangle$. After the measurement it is in the following state:

$$\frac{1}{\sqrt{p_i}} P_i|\psi\rangle = \frac{|i\rangle\langle i|\psi\rangle}{|\langle i|\psi\rangle|} = c_i|i\rangle \tag{245}$$

where $c_i \, \epsilon \, \mathbb{C}$ is the phase and $|i\rangle$ is eigen-state. The expectation value of the observable A is given by:

$$\langle A\rangle = \langle\psi|A|\psi\rangle = \sum_i a_i\langle\psi|P_i|\psi\rangle = \sum_i p_i a_i \tag{246}$$

Within the density matrix formalism, the initially state $\rho = |\psi\rangle\langle\psi|$ is after measurement the following state:

$$\frac{1}{p_i} P_i|\psi\rangle\langle\psi|P_i = \frac{1}{p_i} P_i\rho P_i = |i\rangle\langle i| = \rho_i \tag{247}$$

The state after the measurement process ρ' is defined by:

$$\rho' = \sum_i p_i|i\rangle\langle i| = \sum_i p_i \frac{1}{p_i} P_i\rho P_i = \sum_i P_i\rho P_i \tag{248}$$

Question:

How does the entropy behave under measurement?

Answer:

It depends on the kind of measurement - the entropy may increase or decrease.

Theorem 5. *Projective measurements increase entropy!*

To be more precise: Let be $\{P_i\}$ projection operators of a complete orthogonal system and ρ a density matrix of the state of the system. Then the density matrix of the state after the measurement is given by:

$$\rho' = \sum_i P_i\rho P_i \tag{249}$$

The entropy fulfills the following inequality:

$$S(\rho') \geq S(\rho) \quad \text{"="} \text{ if } \quad \rho' = \rho \tag{250}$$

Proof:

To prove this inequality we apply the *Klein inequality*:

$$0 \leq S(\rho||\rho') = \text{tr } \rho \log \rho - \text{tr } \rho \log \rho' = -S(\rho) - \text{tr } \rho \log \rho' \tag{251}$$

So we only have to prove that $-\text{tr } \rho \log \rho' = S(\rho')$:

$$-\text{tr } \rho \log \rho' = -\text{tr } \sum_i P_i \rho \log \rho' = -\text{tr } \sum_i P_i P_i \rho \log \rho' =$$

$$= -\text{tr } \sum_i P_i \rho \log \rho' P_i = -\text{tr } \sum_i P_i \rho P_i \log \rho' = -\text{tr } \rho' \log \rho' = S(\rho')$$

Remark:

However, generalized measurements can decrease entropy! For example let us consider a qubit in state ρ that is measured by two operators M_1 and M_2 which are defined like following:

$$M_1 = |0\rangle\langle 0| \ , \ M_2 = |0\rangle\langle 1| \tag{252}$$

The result of the measurement is unknown; the state after measurement is given by:

$$\rho' = M_1 \rho M_1^\dagger + M_2 \rho M_2^\dagger \tag{253}$$

Here the entropy can decrease. F.i. chose the totally mixed state:

$$\rho = \frac{1}{2}\mathbb{1} \tag{254}$$

$\Rightarrow$ the entropy before the measurement $S(\rho) = 1$. After the measurement the density matrix is given by:

$$\rho' = \frac{1}{2}|0\rangle\langle 0|\mathbb{1}|0\rangle\langle 0| + \frac{1}{2}|0\rangle\langle 1|\mathbb{1}|1\rangle\langle 0| = |0\rangle\langle 0| \tag{255}$$

Thus, for the entropy after the measurement we gather:

$$S(\rho') = S(|0\rangle\langle 0|) = 0 \tag{256}$$

3 Open quantum systems

3.1 Classical analogy

The time evolution of a quantum system described by a state ρ is given by the *von Neumann*-equation:

$$\frac{\partial}{\partial t}\rho(t) = -\frac{i}{\hbar}[H, \rho] \tag{257}$$

The classical analogy to this equation is the *Liouville*-equation for the probability of the density $\rho(q, p, t)$ in a phase space (q, p) of a statistical system:

$$\frac{\partial}{\partial t}\rho = \{H, \rho\} \tag{258}$$

with the *Poisson brackets*:

$$\{ \ , \ \} = \frac{\partial}{\partial q}\frac{\partial}{\partial p} - \frac{\partial}{\partial p}\frac{\partial}{\partial q} \tag{259}$$

The general equation of motion in statistical mechanics is described by the *Liouville*-equation:

$$\frac{\partial}{\partial t}\rho(t) = \mathcal{L}\rho(t) \tag{260}$$

where $\mathcal{L}$ is the so-called *Liouville*-operator. It has the formal solution:

$$\rho(t) = Te^{[\int_{t_0}^{t} \mathcal{L}(t')dt']}\rho(t_0) \tag{261}$$

3.2 Open quantum system - dynamics

In reality a quantum system S is always coupled to environment E via interactions - there is no isolated system. In the physical description we consider the environment E as a reservoir with infinite degrees of freedom, for example like a heat bath (in case of thermal equilibrium).

To study the dynamics of a quantum system in interaction with its environment (that is what we call "*open quantum system*") we have to consider the total system $S + E$, because the dynamis of subsystem S is determined by the dynamics of the total system. The total Hilbertspace is constructed by the tensor product:

$$\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_E \tag{262}$$

The total Hamilton-operator has the following form:

$$H(t) = H_S \otimes \mathbb{1}_E + \mathbb{1}_S \otimes H_E + H_I(t) \tag{263}$$

where H_S is the Hamiltonian of the open system, H_E is the Hamiltionian of the environment and $H_I(t)$ denotes the interaction between system and environment.

All observables refer to a subsystem S of the form:

$$A \otimes \mathbb{1}_E \quad \text{with} \quad A \,\epsilon\, \mathcal{H}_S \tag{264}$$

The density matrix of the system ρ^S - which is of central interest for us - we obtain by tracing over the environment E:

$$\rho^S = \mathrm{tr}_E \rho \tag{265}$$

The expectation value of A is represented by:

$$\langle A \rangle = \mathrm{tr}_S \rho^S A \tag{266}$$

The total system $S+E$ is closed and therefore follows a unitary t-evolution. The unitary time-evolution is determined by the operator:

$$U(t, t_0) = Te^{-i\int_{t_0}^{t} H(t)dt} \tag{267}$$

Thus, we can write the evolution of the density matrix of the reduced system in the following way:

$$\rho^S(t) = \mathrm{tr}_E U(t, t_0)\rho(t_0)U^t(t, t_0) \tag{268}$$

For a closed system we know that: $\frac{\partial}{\partial t}\rho(t) = -i[H(t), \rho(t)]$, ($\hbar = 1$). Thus, with tracing over the environment we get the equation of motion for the density matrix of the system:

$$\frac{\partial}{\partial t}\rho^S(t) = -i\mathrm{tr}_E[H(t), \rho(t)] \tag{269}$$

An example for the open quantum system description is an atom (system) in an external electromagnetical field (environment).

3.3 Dynamical map, Operator sum representation, quantum dynamical semigroups

Let us suppose that at $t = 0$ the system and the environment are uncorrelated. Therefore, the density operator can be described by a tensor product of ρ^S and ρ^E:

$$\rho(0) = \rho^S(0) \otimes \rho^E \tag{270}$$

From the chapter above we already know the time-evolution of the reduced system:

$$\rho^S(0) \;\rightarrow\; \rho^S(t) = V(t)\rho^S(0) \equiv \mathrm{tr}_E U(t,0)\rho^S(0) \otimes \rho^E U^t(t,0) \tag{271}$$

where $V(t)$: $\mathcal{H}_S \rightarrow \mathcal{H}_E$ is called *dynamical map*. In the following we will show that a dynamical map $V(t)$ can be completely characterized by operators action on $\mathcal{H}_S$. Therefore let us consider the spectral decomposition of the density matrix of the environment ρ^E:

$$\rho^E = \sum_k p_k |\phi_k\rangle\langle\phi_k| \tag{272}$$

where $0 \leq p_k \leq 1$ and $\sum p_k = 1$.

We can visualize the evolution in the following diagram:

$$\begin{array}{ccc} \rho(0) = \rho^S(0) \otimes \rho^E & \rightarrow^{U(t,0)}_{\text{unitary time-evolution}} & \rho(t) = U(t,0)\rho^S(0) \otimes \rho^E U^\dagger(t,0) \\ & \downarrow \ \mathrm{tr}_E & \\ \rho^S(0) & \rightarrow^{V(t)}_{\text{dynamical map}} & \rho^S(t) = V(t)\rho^S(0) \end{array} \tag{273}$$

For the overall density matrix ρ of $S + E$ we can choose that

- at beginning $t = 0$ the density matrix is given as a pure product state:

$$\rho(0) = \rho^S(0) \otimes \rho^E \tag{274}$$

- at $t = 0$ the environment represents a pure state - this is experimentally achievable and simplifies our discussions:

$$\rho^E = |\phi_0\rangle\langle\phi_0| \tag{275}$$

Then we consider the unitary time-evolution of the total system $S + E$ and study its effects on the system by tracing over E.

$$\rho_{\text{tot}} \;\rightarrow\; U\rho^S(0) \otimes \rho^E U^\dagger$$

$$\Downarrow$$

$$\rho^S = \text{tr}_E \rho \;\rightarrow\; \sum_k \rangle \phi_k | U \rho^S(0) \otimes |\phi_0\rangle\langle\phi_0| U^\dagger |\phi_k\rangle$$

where $\{|\phi_k\rangle\}$ denote the complete states of the environment.

We introduce operators on $\mathcal{H}_S$ - the so-called *Kraus-operators*:

$$W_k =: \langle\phi_k|U|\phi_0\rangle \tag{276}$$

$$W_k^\dagger =: \langle\phi_0|U^\dagger|\phi_k\rangle$$

with the property

$$\sum_k W_k^\dagger W_k = \sum_k \langle\phi_0|U^\dagger|\phi_k\rangle\langle\phi_k|U|\phi_0\rangle = \langle\phi_0|U^\dagger U|\phi_0\rangle = \langle\phi_0|\mathbb{1}_{S+E}|\phi_0\rangle = \mathbb{1}_S \tag{277}$$

Then we find for the dynamical map - the time evolution of the density matrix of the system - a representation in terms of a sum of *Kraus-operators*:

$$\rho^S(0) \;\rightarrow\; \sum_k W_k \rho^S(0) W_k^\dagger = V[\rho^S(0)] = \rho^S(t) \tag{278}$$

Properties of the dynamical map $V(t)$:

- The dynamical map $V(t)$ is trace conserving.

$$tr_S \rho^S(t) = tr_S V[\rho^S] = tr_S \sum_k W_k \rho^S(0) W_k^\dagger = tr_S \rho^S(0) \tag{279}$$

- $V(t)$ is a convex linear map.

$$V(t) \sum_i p_i \rho_i = \sum_i p_i V(t) \rho_i \;,\; \sum_i p_i = 1 \;\rightarrow\; \text{convex sum} \tag{280}$$

- The dynamical map $V(t)$ is completely positive.

$$V(t) \otimes 1_n \geq 0 \;\; \text{on } \mathcal{H}_S \otimes \mathbb{C}^n \tag{281}$$

Remark:

Let be a map $V(t)[\rho] \geq 0$ for all $\rho \geq 0$ and for all $t \geq 0$ on a finite dimensional complex Hilbert space. Then the map V is *completely positive* if the extention

$$V_n(t) = V(t) \otimes \mathbb{1}_n \tag{282}$$

defined on $\mathcal{H} \otimes \mathbb{C}^n$ for all n is positive

$$V_n(t)[\rho \otimes \omega] = V(t)[\rho] \otimes \omega \geq 0 \tag{283}$$

for all $\rho \in \mathcal{H}$ and for all $\omega \in \mathbb{C}^n$.

Theorem 6. *$V(t)$ is completely positive $\Leftrightarrow$ $V(t) \otimes V(t) \geq 0$ is positive.*

This theorem is important for entangled systems, a counter example to complete positivity is the partial transposition.

Let us now assume that the characteristic time scale of the environment is much smaller than the characteristic time scale of the system $\tau_E \ll \tau_S$, so to say, that the memory effects of the system about the environment are negligible (classical "Markov process"). The characteristic time scales are determined by some correlation functions proportional to $e^{-\frac{t}{\tau_E}}$ in case of the environment and $e^{-\frac{t}{\tau_S}}$ in case of the system.

Then the dynamical map V forms a semigroup:

$$V(t_1)V(t_2) = V(t_1 + t_2) \text{ where } t_1, t_2 \geq 0 \tag{284}$$

We construct a generator of the semigroup:

$$V(t) = e^{\mathcal{L}t} \tag{285}$$

$$\Downarrow$$

$$\rho^S(t) = V(t)\rho^S(0) = e^{\mathcal{L}t}\rho^S(0) \tag{286}$$

and find a so-called *master equation*:

$$\frac{\partial}{\partial t}\rho^S(t) = \mathcal{L}\rho^S(t) \tag{287}$$

in analogy to the classical *Liouville*-equation discussed in the beginning.

3.4 Measurement process - dynamical map

Resumée:

For the dynamical map of the density matrix there exists an operator decomposition. In the open quantum system formulation we consider a quantum system S in interaction with its environment E. We can assume that at the beginning $t = 0$:

- The density matrix of $S + E$ is represented by a product state:

$$\rho(0) = \rho^S(0) \otimes \rho^E \tag{288}$$

- The density matrix of the environment is a pure state:

$$\rho^E = |\phi_0\rangle\langle\phi_0| \tag{289}$$

  where $\{|\phi_k\rangle\}$ form a completely orthogonal system.

Visualized in a diagram:

$$\rho(0) \;\rightarrow\; U\rho^S(0)\otimes\rho^E U^\dagger \tag{290}$$

$$\downarrow tr_E$$

$$\rho^S(0) \;\rightarrow\; \sum_k \langle\phi_k|U(t)\rho^S(0)\otimes|\phi_0\rangle\langle\phi_0|U(t)^\dagger|\phi_k\rangle \tag{291}$$

With the *Kraus-operator* W_k

$$W_k =: \langle\phi_k|U(t)|\phi_0\rangle \tag{292}$$

the master-equation can finally be written as:

$$\rho^S(t) = \sum_k W_k(t)\rho^S(0)W_k^\dagger(t) = V(t)[\rho^S(0)] \tag{293}$$

The master-equation fulfills the following properties:

- trace conserving
- convex linear
- completely positive map

von Neumann measurement, projective measurement

Let us consider the observable $A = \sum_n a_n P_n$ with the eigen-values a_n and the projection-operator $P_n = |n\rangle\langle n|$, $P_n^2 = P_n$, $\sum_n P_n = 1$ with the eigen-equation: $A|n\rangle = a_n|n\rangle$. The expectation value of A is given by:

$$\langle A\rangle = \mathrm{tr}\rho^S A = \sum p_n a_n \tag{294}$$

where $p_n = tr\rho^S P_n$ is the probability for an eigen-value a_n.

The *von Neumann-measurement* or *projective measurement* looks like the following:

$$\rho^S \;\rightarrow\; \sum_n p_n|n\rangle\langle n| = \sum_n P_n\rho^S P_n^\dagger \tag{295}$$

For measurement of this type the *Kraus-operator* is identical to the projection operator.

$$W_k \equiv P_n \tag{296}$$

Positive Operator Value Measurements POVM

We again consider the total system $S + E$ with some interaction $S \leftrightarrow E$. We define an unitary operator U such that at the same time:

- apply operator M_n on system S: $|\psi\rangle \rightarrow M_n|\psi\rangle$ with $|\psi\rangle$, $M_n|\psi\rangle \; \epsilon \; \mathcal{H}_S$
- state of environment changes $|e_0\rangle \rightarrow |e_n\rangle$, where $\{|e_n\rangle\} \; \epsilon \; \mathcal{H}_E$:

So the operation can be written as:

$$U(|\psi\rangle \otimes |e_0\rangle) = \sum_n M_n|\psi\rangle \otimes |e_n\rangle \tag{297}$$

where M_n has to fulfill the following property (normalization):

$$1 = \langle e_0|\langle\psi|U^\dagger U|\psi\rangle|e_o\rangle = \sum_{m,m'} \langle e_{m'}|\langle\psi|M^\dagger_{m'}M_m|\psi\rangle|e_m\rangle = \sum_m \langle\psi|M^\dagger_m M_m|\psi\rangle \tag{298}$$

$$\Downarrow$$

$$\sum_m M^\dagger_m M_m = 1 \tag{299}$$

In the method of the *Positive Operator Valued Measurements POVM* we measure the state of the environment by an operator B:

$$B = \mathbb{1}_S \otimes \sum_n b_n|e_n\rangle\langle e_n| = \sum_n b_n P^E_n \tag{300}$$

The expectation value of B is given by:

$$\langle B\rangle = \mathrm{tr}\rho_{SE}B = \mathrm{tr}U|\psi\rangle|e_0\rangle\langle e_0|\langle\psi|U^\dagger \mathbb{1}_S \otimes \sum_n b_n|e_n\rangle\langle e_n| =$$

$$[\mathrm{tr}|\psi\rangle\langle\varphi| = \langle\varphi|\psi\rangle]$$

$$= \langle e_0|\langle\psi|U^\dagger \mathbb{1}_S \otimes \sum_n b_n|e_n\langle e_n|U|\psi\rangle|e_0\rangle = \sum_n p_n b_n \tag{301}$$

where p_n denotes the probability to get the measurement-result b_n.

$$p_n = \langle e_0|\langle\psi|U^\dagger \mathbb{1}_S \otimes |e_n\rangle\langle|U|\psi|e_0\rangle =$$

$$= \sum_{m,m'} \langle e_{m'}|\langle\psi|M^\dagger_{m'} \mathbb{1}_S \otimes |e_n\rangle\langle e_n|M_m|\psi_\rangle|e_m\rangle = \langle\psi|M^\dagger_n M_n|\psi\rangle \tag{302}$$

The effect of the measurement process is the following:

$$\rho^{SE}_0 \;\; \rightarrow \;\; \sum_n p_n|\psi^{SE}_n\rangle\langle\psi^{SE}_n| \tag{303}$$

$$\downarrow \mathrm{tr}_E$$

$$\rho^S = |\psi\rangle\langle\psi| \;\; \rightarrow \;\; \mathrm{tr}_E \sum_n M_n|\psi\rangle|e_n\rangle\langle e_n|\langle\psi|M^\dagger_m = \sum_n M_n\rho^S M^\dagger_m \tag{304}$$

For this type of measurement the *Kraus-operator* is identical to M_n:

$$W_n \equiv M_n \tag{305}$$

3.5 Quantum channels - dynamical maps

Let us now consider a quantum operation with a spin- $\frac{1}{2}$ particle. Alice transmits such a particle to Bob:

$$\text{Alice} \rightsquigarrow \text{Bob} \tag{306}$$

There exists a noise caused by the interaction of the particle with the environment. In the following we will discuss different processes of this intereaction, the so-called *quantum channels* and the corresponding dynamical maps.

Depolarising channel

The first quantum channel we consider is the *depolarising channel*. This is a process with contributions from a total mixture:

$$\rho \;\rightarrow\; p\frac{1}{2}\mathbb{1} + (1-p)\rho \tag{307}$$

where p is the probability for an error and $(1-p)$ is the probability that the initial qubit remains O.K.

The dynamical map of this channel is given by:

$$V[\rho] = \frac{p}{2}\mathbb{1} + (1-p)\rho \tag{308}$$

To find out how the *Kraus-operators* look like we use the following lemma:

Lemma 3.

$$\frac{1}{2}(\mathbb{1}\rho\mathbb{1} + \overrightarrow{\sigma}\rho\overrightarrow{\sigma}) = \mathbb{1} \tag{309}$$

In general we can decompose the density matrix for qubits as:

$$\rho = \frac{1}{2}(1 + \overrightarrow{a}\cdot\overrightarrow{\sigma}) \tag{310}$$

where $\overrightarrow{a}$ is the Bloch-vector. Inserting Lemma 2 we get for the dynamical map:

$$V[\rho] = \frac{p}{2}\frac{1}{2}(\mathbb{1}\rho\mathbb{1} + \overrightarrow{\sigma}\rho\overrightarrow{\sigma}) + (1-p)\mathbb{1}\rho\mathbb{1} = \tag{311}$$

$$= \frac{p}{4}\overrightarrow{\sigma}\rho\overrightarrow{\sigma} + (\mathbb{1} - \frac{3p}{4})\mathbb{1}\rho\mathbb{1} = \frac{p'}{3}\overrightarrow{\sigma}\rho\overrightarrow{\sigma} + (1-p')\mathbb{1}\rho\mathbb{1}$$

where $p' = \frac{3p}{4}$. Thus the *Kraus-Operators* are given by:

$$W_0 = \sqrt{1-p'}\mathbb{1} \tag{312}$$

$$W_i = \sqrt{\frac{p'}{4}}\sigma_i$$

The Bloch-sphere shrinks by the factor $(1-p)$.

Bit-flip channel

The *Bit-flip channel* describes the process where spins are flipped:

$$\begin{aligned} |\uparrow\rangle &\rightarrow |\downarrow\rangle \text{ analogous: } |0\rangle \rightarrow |1\rangle \\ |\downarrow\rangle &\rightarrow |\uparrow\rangle \text{ analogous: } |1\rangle \rightarrow |0\rangle \end{aligned} \tag{313}$$

Thus we have for the dynamical map of this process:

$$V[\rho] = p\ \sigma_x \rho \sigma_x + (1-p)\rho \tag{314}$$

The *Kraus-operators* are given by:

$$\begin{aligned} W_0 &= \sqrt{p}1 \\ W_1 &= \sqrt{p}\sigma_x \end{aligned} \tag{315}$$

For this case the Bloch-sphere is invariant in x. In y, z it is shrinking by the factor $(1-2p)$.

Phase-flip channel

The *Phase-flip channel* describes the process where the spin obtains phases:

$$\begin{aligned} |\uparrow\rangle &\rightarrow |\uparrow\rangle \\ |\downarrow\rangle &\rightarrow -|\downarrow\rangle \end{aligned} \tag{316}$$

Then the dynamical map for this process can be expressed by:

$$V[\rho] = p\ \sigma_z \rho\ \sigma_z + (1-p)\rho \tag{317}$$

with the *Kraus-operators*:

$$\begin{aligned} W_0 &= \sqrt{1-p}\mathbb{1} \\ W_1 &= \sqrt{p}\ \sigma_z \end{aligned} \tag{318}$$

For this case the Bloch-sphere is invariant in z. In x, y it is shrinking by the factor $(1-2p)$.

Bit-flip-phase channel

The *Phase-flip channel* describes the process where the spin obtains phases:

$$\begin{aligned} |\uparrow\rangle &\rightarrow i|\downarrow\rangle \\ |\downarrow\rangle &\rightarrow -i|\uparrow\rangle \end{aligned} \tag{319}$$

The dynamical map for this process is given by:

$$V[\rho] = p\ \sigma_y \rho\ \sigma_y + (1-p)\rho \tag{320}$$

with the *Kraus-operators*:

$$W_0 = \sqrt{1-p}\mathbb{1} \tag{321}$$
$$W_1 = \sqrt{p}\ \sigma_y$$

For this case the Bloch-sphere is invariant in y. In z, x it is shrinking by the factor $(1-2p)$.

Amplitude damping channel

The *amplitude damping channel* describes the process where the spin decays $|\downarrow\rangle \rightarrow |\uparrow\rangle$ via emission of a photon:

$$\rho_\downarrow = |\downarrow\rangle\langle\downarrow| \ \rightarrow\ |\uparrow\rangle\langle\uparrow| = \rho_\uparrow \tag{322}$$

Explicitly:

$$\sigma_+\ \rho_\downarrow\ \sigma_- = |\uparrow\rangle\langle\downarrow|\downarrow\rangle\langle\downarrow|\downarrow\rangle\langle\uparrow| = |\uparrow\rangle\langle\uparrow| = \rho_\uparrow \tag{323}$$

with $\sigma_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$ and $\sigma_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$. Thus, one *Kraus-Operator* will be:

$$W_1 = \sqrt{p}\ \sigma_+ \tag{324}$$

From the normalization follows the other *Kraus-operator*:

$$\sum_i W_i^\dagger W_i = 1 \tag{325}$$

$$p\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$
$$\Downarrow$$
$$a = 1\ ,\ b = 1-p$$
$$\Downarrow$$
$$W_0 = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{1-p} \end{pmatrix} \tag{326}$$

For the dynamical map we finally have:

$$V[\rho_\downarrow] = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{1-p} \end{pmatrix}\rho_\downarrow\begin{pmatrix} 1 & 0 \\ 0 & \sqrt{1-p} \end{pmatrix} + p\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}\rho_\downarrow\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} =$$
$$= p\rho_\uparrow + (1-p)\rho_\downarrow \tag{327}$$

3.6 Master Equation

In the following we'll construct the most general form of the Liouville equation for a finite dimensional complex Hilbert-space $\mathcal{H}_S$ with $dim\mathcal{H}_S = N^2$. We will construct out of *Kraus-operators* an equation which contains the Hamilton-operator (plus remaining operators). This method goes back to Lindblad 1976 and to Gorini-Kossakoneski-Sudarshan.

The master equation a la Lindblad is given by:

$$\frac{d}{dt}\rho^S(t) = -\frac{i}{\hbar}[H, \rho^S(t)] - D[\rho^S(t)] \tag{328}$$

where ρ^S is the density matrix of the system and $D[\rho^S]$ is the so-called *dissipator*:

$$D[\rho^S] = \frac{1}{2}\sum_{k=1}^{N^2-1} \lambda_k \left(A_k^\dagger A_k \rho^S + \rho^S A_k^\dagger A_k - 2A_k \rho^S A_k^\dagger\right) \tag{329}$$

The dissipator can be rewritten:

$$D[\rho^S] = \frac{1}{2}\sum_k \lambda_k([A_k^\dagger, A_k\rho^S] + [\rho^S A_k^\dagger, A_k]) \tag{330}$$

with the Lindblad-operators A_k and the (positive) decoherence constants $\lambda_k \geq 0$ which are a quantitative measure for decoherence.

Remark:
Here we assume a weak coupling limit between the system and the environment:

$$H \equiv H_{S+E} = H_S + H_E + H_{int} \tag{331}$$

For H_E, $H_{int} \to 0 \Rightarrow H = H_S$.

Proof of the Lindblad-master-equation:

We consider the dynamical map for the time-evolution of the density matrix of the system:

$$\rho^S \;\to\; V[\rho^S] = \sum_k W_k \rho^S W_k^\dagger \tag{332}$$

with the Kraus-operator:

$$W_k = \langle\phi_k|U|\phi_0\rangle \tag{333}$$

with the unitary operator $U = e^{-\frac{i}{\hbar}Ht}$ and the property $\sum_k W_k^\dagger W_k = 1$. As we know, the dynamical map fulfills the following properties:

- trace conserving
- convex linear

- completely positive

About the time evolution we make the following assumptions:

- The characteristic time scale of the system δt is much smaller than the lifetime of the system τ_S:
$$\delta t \ll \tau_S \tag{334}$$
- The characteristic time scale of the environment τ_E should "forget" about the system, this is a so-called *Markov process*:
$$\tau_E \ll \delta t \tag{335}$$

For the proof we start from the dynamical map under the assumptions made above:

$$\rho^S(\delta t) = V[\rho^S(0)] = \sum_k W_k \rho^S(0) W_k^\dagger = \rho^S(0) + \mathcal{O}(\delta t) \tag{336}$$

We see: First Kraus-operator $\sim 1_S + \mathcal{O}(\delta t)$, all further Kraus-operators $\sim \mathcal{O}(\delta t)$. Under these conditions we construct:

$$W_0 = \mathbb{1}_S + \left(K - \frac{i}{\hbar} H\right) \delta t \tag{337}$$

$$W_k = A_k \sqrt{\delta t}$$

where K and H are hermitian operators and A_k is the Lindblad operator. From the normalization we get:

$$\sum_k W_k^\dagger W_k = \mathbb{1}_S + \left(2K + \sum_k A_k^\dagger A_k\right) \delta t + \mathcal{O}(\delta t^2) \tag{338}$$

$$\Downarrow$$

$$K = -\frac{1}{2} \sum A_k^\dagger A_k \tag{339}$$

Thus, we find for the time evolution of the system S:

$$\rho^S(\delta t) = W_0 \rho^S W_0^\dagger + \sum W_k \rho^S(0) W_k^\dagger =$$

$$= \left(\mathbb{1}_S + \left(K - \frac{i}{\hbar} H\right) \delta t\right) \rho^S(0) \left(\mathbb{1}_S + \left(K + \frac{i}{\hbar} H\right) \delta t\right) + \delta t \sum_k A_k \rho^S(0) A_k^\dagger =$$

$$= \rho^S(0) + \delta t \{-\frac{i}{\hbar} \left[H, \rho^S(0)\right] - \frac{1}{2} \left(\sum A_k^\dagger A_k \rho^S(0) + \rho^S(0) A_k^\dagger A_k - 2 A_k \rho^S(0) A_k^\dagger\right)\} \tag{340}$$

$$\Downarrow$$

$$\lim_{\delta t \to 0} \frac{\rho^S(\delta t) - \rho^S(0)}{\delta t} = \frac{d}{dt} \rho^S(t)|_{t=0} = -\frac{i}{\hbar} [H, \rho^S(t)]|_{t=0} - D[\rho^S(t)]|_{t=0} \tag{341}$$

Note:
Here we have derived Eq. (341) at $t = 0$ but it holds for any time and we have rescaled $A_k \to \sqrt{\lambda_k} A_k$.

Remarks:

- $\exists$ 1 Kraus-operator $\Leftrightarrow \nexists$ Lindblad operator. $\Rightarrow$ For $\lambda_k = 0$ there is no interaction. For this case H is the Hamiltonian of the system: $H = H_S$ and in the limit of weak coupling we also have $H \to H_S$ since $H_{int} \to 0$.
- The Hamiltonian is not unique, the master equation is invariant under the operation:

$$A_k \to A_k + a_k \mathbb{1}_S$$
$$H \to H + \frac{1}{2i} \sum_k (a_k^* A_k - a_k A_k^\dagger) + b \mathbb{1}_S$$

  Furthermore, the dissipator is invariant under unitary transformations

$$A_k \to U A_k$$

  where $UU^\dagger = \mathbb{1}$.

- The right hand side of the equation is linear functional in ρ^S:

$$\frac{d}{dt} \rho^S(t) = \mathcal{L}[\rho^S] \tag{342}$$

  formally:

$$\rho^S(t) = T e^{\int_0^t \mathcal{L}(t) dt} \rho^S(0) = e^{\mathcal{L}t} \rho^S(0) \text{ where } \mathcal{L} \text{ is constant} \tag{343}$$
$$\rho^S(t) = V(t) \rho^S(0) \to V(t) = e^{\mathcal{L}t}$$

3.7 Example: Spontaneous emission

Let us consider an atom with two energy levels. The Hamilton operator is given by:

$$H = -\frac{\hbar\omega}{2} \sigma_z \tag{344}$$

Then we have for the ground state $|0\rangle$ and for the excited state $|1\rangle$ the following energy-eigenequations:

$$H|1\rangle = \frac{\hbar\omega}{2} |1\rangle \tag{345}$$
$$H|0\rangle = -\frac{\hbar\omega}{2} |0\rangle$$

The energy difference between the excited state and the ground state is equal to the energy of the spontaneously emitted photon:

$$E_1 - E_0 = \hbar\omega \tag{346}$$

The transition operator (emission operator) which causes the transition from $|1\rangle$ to $|0\rangle$ is given by:

$$\sigma_+ = |0\rangle\langle 1| \tag{347}$$

$$\Downarrow$$

$$\sigma_+|1\rangle = |0\rangle\langle 1|1\rangle = |0\rangle \tag{348}$$

Thus we chose as Lindblad operator:

$$A_1 = \sqrt{\Gamma}\sigma_+ \tag{349}$$

$$A_1^\dagger = \sqrt{\Gamma}\sigma_-$$

where Γ is the rate for the emission of a photon. It is inverse to the lifetime.

We consider a 2-dimensional Hilbert space:

$$|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \ , \ |0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{350}$$

$$\sigma_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \ , \ \sigma_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \tag{351}$$

Therefore we finally obtain the following *master equation* describing the spontaneous emission:

$$\frac{d}{dt}\rho(t) = -\frac{i}{\hbar}[H,\rho] - \frac{1}{2}\Gamma(\sigma_-\sigma_+\rho + \rho\sigma_-\sigma_+ - 2\sigma_+\rho\sigma_-) \tag{352}$$

To find the solutions of the master equation, firstly we calculate the components of the terms of the dissipator:

$$\sigma_-\sigma_+\rho = \begin{pmatrix} 0 & 0 \\ \rho_{10} & \rho_{11} \end{pmatrix} \ , \ \sigma_+\rho\ \sigma_- = \begin{pmatrix} \rho_{11} & 0 \\ 0 & 0 \end{pmatrix} \ , \ \rho\ \sigma_-\sigma_+ = \begin{pmatrix} 0 & \rho_{01} \\ 0 & \rho_{11} \end{pmatrix} \tag{353}$$

Thus, for the master equation in components we gather:

$$\frac{d}{dt}\begin{pmatrix} \rho_{00} & \rho_{01} \\ \rho_{10} & \rho_{11} \end{pmatrix} = i\omega \begin{pmatrix} 0 & \rho_{01} \\ -\rho_{10} & 0 \end{pmatrix} + \Gamma \begin{pmatrix} \rho_{11} & -\frac{1}{2}\rho_{01} \\ -\frac{1}{2}\rho_{10} & -\rho_{11} \end{pmatrix} \tag{354}$$

With $\dot{\rho_{00}} = \Gamma\rho_{11}$ and $\dot{\rho_{11}} = -\Gamma\rho_{11}$ we get the solutions for the diagonal-elements of the density matrix:

$$\rho_{11}(t) = \rho_{11}(0)e^{-\Gamma t} \tag{355}$$

$$\Downarrow$$

$$\dot{\rho_{00}}(t) = \Gamma\rho_{11}(0)e^{-\Gamma t} \tag{356}$$

$$\Downarrow$$

$$\rho_{00}(t) = \rho_{00}(0) + \rho_{11}(0)(1 - e^{-\Gamma t}) \tag{357}$$

For the off-diagonal elements we get the following solutions:

$$\rho_{01}(t) = \rho_{01}(0)e^{+i\omega t - \frac{\Gamma}{2}t} \tag{358}$$

$$\rho_{10}(t) = \rho_{10}(0)e^{-i\omega t - \frac{\Gamma}{2}t}$$

Remark:
The mean decay time is $T_1 = \frac{1}{\Gamma}$. The excited state decays with the probability $e^{-\Gamma t}$ and the probability for the ground state increases with $(1 - e^{-\Gamma t})$. The lifetime of coherence is $T_2 = \frac{2}{\Gamma}$, twice as large as the mean decay time: $T_2 = 2T_1$

The emission process corresponds to the amplitude damping channel.

3.8 Master Equation for decoherence via scattering process

Let us assume that the dynamics of the system is separable from the environment, so to say that H_I is small, i.e. the typical time of scattering $\tau_E \ll \tau_S$.

We make the following ansatz:

$$i\frac{\partial \rho}{\partial t} = [H_S, \rho] + i\frac{\partial \rho}{\partial t}|_{\text{scatt}} \tag{359}$$

Question:

Why are macroscopic objects localized in space? $\Rightarrow$ The coherence of macroscopic objects at different positions is destroyed by scattering.

Description of scattering:

Let our object be in state $|a\rangle$. It is localized at x in eigen-state $|x\rangle$. We describe the process of scattering as follows:

$$|x\rangle|a\rangle \rightarrow_t |x\rangle S_x|a\rangle \tag{360}$$

where S_x denotes the scattering matrix. If we have initially a wave-packet, it evolves as:

$$\int d^3x\varphi(x)|x\rangle|a\rangle \rightarrow_t \int d^3x\varphi(x)|x\rangle S_x|a\rangle \tag{361}$$

The reduced density matrix in x-space can be written as:

$$\rho = \int dxdx'\rho(x, x', t)|x\rangle\langle x'| \tag{362}$$

Analogeously to discrete space:

$$\rho = \sum_{m,n} \rho_{mn}|m\rangle\langle n| \text{ with } \rho_{mn} = \langle m|\rho|n\rangle \tag{363}$$

The matrix element after scattering is given by:

$$\rho(x,x',t) = \langle x|\rho|x'\rangle =$$

$$= \mathrm{tr}\langle x| \int dydy'\varphi(y)|y\rangle S_y|a\rangle\langle a|S_y^\dagger\langle y'|\varphi*(y')|x'\rangle = \varphi(x)\varphi*(x')\langle a|S_{x'}^\dagger S_x|a\rangle \tag{364}$$

where we take the trace over the scattered states $S_y|a\rangle$. For the single scattering process we get: $x' \to x \Rightarrow \rho(x,x',t) \to 1$. So there is no scattering. If there are many scatterings they add up to an exponential damping of the non-diagonal elements of $\rho(x,x',t)$:

$$\dot\rho(x,x',t)|_{\mathrm{scatt}} = -\Lambda\rho(x,x',t)|_{\mathrm{scatt}} = -\Lambda(x-x')^2\rho(x,x',t)|_{\mathrm{scatt}} \tag{365}$$

where we extracted a factor $(x-x')^2$ since $\dot\rho \to 0$ for $x' \to x$ (no scattering).

$$\Downarrow$$

$$\rho(x,x',t)|_{\mathrm{scatt}} = \rho(x,x',0)|_{\mathrm{scatt}} e^{-\Lambda t(x-x')^2} \tag{366}$$

where the *localization rate* Λ is given by:

$$\Lambda = k^2\frac{Nv}{V}\sigma_{eff} \tag{367}$$

k denotes to the wave number, v the velocity, $\frac{Nv}{V}$ the incoming flux, while σ_{eff} is the total cross section.

Example:

For example, a dust particle in air scattered by sunlight with a size of 10^{-3} cm $\Rightarrow$ $\Lambda = 10^{21}$.

Finally we arrive at the follwing master equation for scattering - decoherence:

$$i\frac{\partial}{\partial t}\rho(x,x',t) = \left[\frac{1}{2m}\left(\frac{\partial^2}{\partial x'^2} - \frac{\partial^2}{\partial x^2}\right) + \frac{m\omega^2}{2}(x^2-x'^2) - i\Lambda(x-x')^2\right]\rho(x,x',t) \tag{368}$$

The first term stands for the kinetic part of the system, the second for the potential part, an harmonic ascillator, and the third term represents the scattering part. Recall the oscillator Hamiltonian:

$$H = -\frac{1}{2m}\frac{d^2}{dx^2} + \frac{m\omega^2}{2}x^2 \tag{369}$$

In operator version we get:

$$\frac{d}{dt}\rho = -i[H,\rho] - \Lambda[x,[x,\rho]] \tag{370}$$

We now extend our master equation (368), (370) to the *Caldeira-Leggett*-model: We consider a system weakly coupled to a heat-bath of oscillators in a high temperature limit. We distinguish between decoherence and dissipation (loss of energy, loss of momentum):

$$\frac{\partial}{\partial t}\rho = -i[H,\rho] - i\frac{\gamma}{2}[x,\{p,q\}] - \Lambda[x,[x,\rho]] \tag{371}$$

$$i\frac{\partial}{\partial t}\rho(x,x',t) = \left[\frac{1}{2m}\left(\frac{\partial^2}{\partial x'^2} - \frac{\partial^2}{\partial x^2}\right) + i\gamma(x-x')\left(\frac{\partial}{\partial x'} - \frac{\partial}{\partial x}\right) - i\Lambda(x-x')\right]\rho(x,x',t) \tag{372}$$

where γ is the damping constant which is proportional to inverse of the relaxation time τ_R^{-1}. The localization rate Λ is given by: $\Lambda = 2\gamma m k_B t/\hbar^2$. The proportion of the decoherence time τ_D to the relaxation time τ_R for a particle with mass m and temperature T is given by:

$$\frac{\tau_D}{\tau_R} = \frac{\gamma}{\Lambda}\frac{1}{\delta x^2} = \frac{\hbar^2}{2mk_Bt}\frac{1}{\delta x^2} \tag{373}$$

Example: $m = 1g$, $T = 300K$, $\delta x = 1cm \Rightarrow \frac{\tau_D}{\tau_R} \approx 10^{-40} \rightarrow$ we see: dust is classical. Decoherence is more important ($\approx \Lambda$) than dissipation ($\approx \gamma$).

Example: Schrödinger cats - Gaussion like wave-packets

At $t = 0$ let be 2 Gaussion wave packets, socalled Schrödinger cat states. Then the density matrix $\rho(x, x', t = 0)$ is also Gaussian-like. There exists 4 peaks: 2 peaks main diagonal (Schrödinger cat states) and 2 peaks off-diagonal. The off-diagonal-peaks are responsible for coherence. See figure (1).

For $t > 0$: We gather $\rho(x, x', t) > 0$ as a solution of the master equation. If there exists decoherence the off-diagonal elements vanish with the exponential damping $\rho = \rho_0 e^{-\Lambda t(x-x')^2}$. The main diagonal terms remain rather constant. See figure (2).

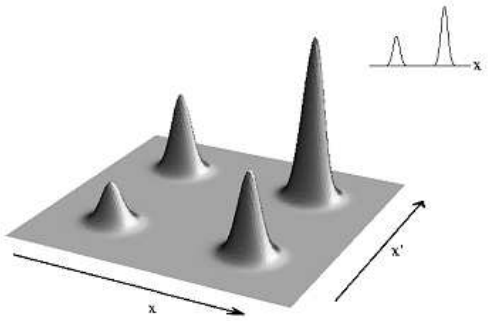


Figure 1: **Density matrix of a superposition of two Gaussian wave packets**, the wave function is shown in the inset. Coherence between the two parts of the wave function is represented by the two off-diagonal peaks. Source: Claus Kiefer, Erich Joos: "Decoherence: Concepts and Examples", quant-ph/9803052

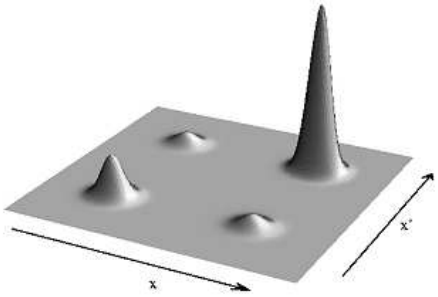


Figure 2: **Density matrix of a superposition of two Gaussian wave packets**, the density matrix after interference is partially destroyed by decoherence. The position distribution, along the diagonal, is not changed appreciably. Source: Claus Kiefer, Erich Joos: "Decoherence: Concepts and Examples", quant-ph/9803052

Illustration with Wigner function:

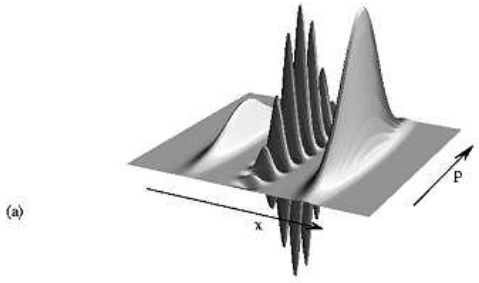
The *Wigner function* is given by:

$$W(x,p) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dy e^{ipy}\rho\left(x-\frac{y}{2}, x+\frac{y}{2}\right) \tag{374}$$

The Fourier-transform of the shifted density matrix is a kind of "probability" function in phase space (x,p), not anymore positive definite! Typical features are:

- There exist oscillations for non-classical states.
- There don't exist oscillation for classical states.

The *Wigner functions* for the above described Schrödinger cat states which shows decoherence are illustrated in Figure (3).



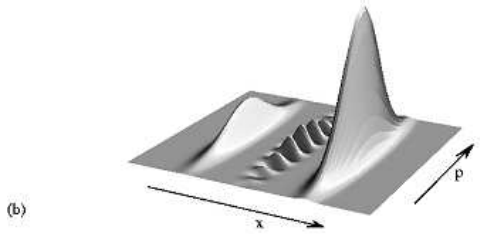


Figure 3: **The Wigner function equivalent to the density matrices shown in Fig. (1), (2)**. (a) represents the superposition of two Gaussian wave packets. Strong oscillations together with negative values indicate coherence between the two wave packets. (b) oscillations are partially damped by decoherence. Source: Claus Kiefer, Erich Joos: "Decoherence: Concepts and Examples", quant-ph/9803052

3.9 Wigner Function

The *Wigner function* is a convenient tool, frequently used, to demonstrate the coherence features of quantum states. It is defined by:

$$W(x,p) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dy e^{ipy}\psi^*\left(x+\frac{y}{2}\right)\psi\left(x-\frac{y}{2}\right) \tag{375}$$

i.e. the Fourier-transformation of shifted wave-packets, like a kind of "probability" distribution - not positive definite anymore! We consider the density matrix representation:

$$\rho = |\psi\rangle\langle\psi| \tag{376}$$

$$\psi(x) = \langle x|\psi\rangle \ , \ \psi^*(x) = \langle\psi|x\rangle$$

$$\Downarrow$$

$$\psi^*(x')\psi(x) = \langle\psi|x'\rangle\langle x|\psi\rangle = \langle x|\psi\rangle\langle\psi|x'\rangle = \langle x|\rho|x'\rangle = \rho(x,x')$$

Thus, for the *Wigner function* we get:

$$W(x,p) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dy e^{ipy}\langle x-\frac{y}{2}|\rho|x+\frac{y}{2}\rangle = \frac{1}{2\pi}\int_{-\infty}^{\infty} dy e^{ipy}\rho\left(x-\frac{y}{2},x+\frac{y}{2}\right) \tag{377}$$

We now shift $\frac{y}{2} \to y$:

$$W(x,p) = \frac{1}{\pi}\int_{-\infty}^{\infty} dy e^{2ipy}\rho(x-y,x+y) \tag{378}$$

The *Wigner function* has the following properties:

- For the integral over p we get the probability density in x-space:

$$\int_{-\infty}^{\infty} dpW(x,p) = \int_{-\infty}^{\infty} dy \frac{1}{2\pi} \int_{-\infty}^{\infty} dp e^{ipy} \langle x - \frac{y}{2}|\rho|x + \frac{y}{2}\rangle =$$

$$= \langle x|\rho|x\rangle = W(x) = \langle x|\psi\rangle\langle\psi|x\rangle = \psi(x)\psi^*(x) = |\psi(x)|^2 \tag{379}$$

- For the integral over x we get the probability density in p-space:

$$\int_{-\infty}^{\infty} dxW(x,p) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy e^{ipy} \langle x - \frac{y}{2}|\rho|x + \frac{y}{2}\rangle =$$

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} dx' \int_{-\infty}^{\infty} dx'' e^{-ip(x'-x'')} \langle x'|\rho|x''\rangle = \int_{-\infty}^{\infty} dx' \int_{-\infty}^{\infty} dx'' \langle p|x'\rangle\langle x'|\rho|x''\rangle\langle x''|p\rangle =$$

$$= \langle p|\rho|p\rangle = W(p) = \psi(p)\psi^*(p) \tag{380}$$

- Normalization

$$\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dpW(x,p) = 1 \tag{381}$$

- The trace of the density matrix corresponds to an overlap of Wigner functions in phase space.

  Lemma 4.

$$\mathrm{tr}\rho_1\rho_2 = 2\pi \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dpW_{\rho_1}(x,p)W_{\rho_2}(x,p) \tag{382}$$

  Proof:

$$2\pi \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dpW_{\rho_1}(x,p)W_{\rho_2}(x,p) =$$

$$= \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dy' \frac{1}{2\pi} \int_{-\infty}^{\infty} dp e^{ip(y+y')} \langle x - \frac{y}{2}|\rho_1|x + \frac{y}{2}\rangle\langle x - \frac{y'}{2}|\rho_2|x + \frac{y'}{2}\rangle =$$

$$= \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dy' \delta(y+y') \langle x - \frac{y}{2}|\rho_1|x + \frac{y}{2}\rangle\langle x - \frac{y'}{2}|\rho_2|x + \frac{y'}{2}\rangle =$$

$$= \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \langle x - \frac{y}{2}|\rho_1|x + \frac{y}{2}\rangle\langle x + \frac{y}{2}|\rho_2|x - \frac{y}{2}\rangle =$$

$$= \int_{-\infty}^{\infty} dx' \int_{-\infty}^{\infty} dx'' \langle x'|\rho_1|x''\rangle\langle x''|\rho_2|x'\rangle =$$

$$= \int_{-\infty}^{\infty} dx' \langle x'|\rho_1\rho_2|x'\rangle = tr\rho_1\rho_2$$

- The Wigner function has negative values.

  Proof:

  Let be given 2 density matrices ρ_1 and ρ_2 so that $\mathrm{tr}\rho_1\rho_2 = 0 \Rightarrow$ according to Lemma (4):

  $$\int dxdpW_{\rho_1}(x,p)W_{\rho_2}(x,p) = 0 \tag{383}$$

  $\Rightarrow W_{\rho_1}(x,p)$ or/and $W_{\rho_2}(x,p)$ must be negative for special values.

4 Kaonic Qubits

4.1 K-mesons

Neutral K-mesons (Kaons) are fundamental particles that consist of two quarks, namly of a down-quark d and a strange-quark s. In the following we will write K^0 for a Kaon with quarkcontent $(d\bar{s})$ and the anti-particle we denote by $\overline{K^0}$ with $(\bar{d}s)$. The mass of a Kaon is about $M_K = 497MeV$. The behaviour of Kaons is ruled by the following quantum principles:

- superposition
- oscillation
- decay
- quasi spin
- regeneration

4.2 Quantum states of K-mesons

Quantum-mechanically we can describe Kaons in the following way, we characterize them by quantum numbers. The eigen-equations of the strangeness-quantum-number are given by:

$$S|K^0\rangle = +|K^0\rangle \ , \ S|\overline{K^0}\rangle = -|\overline{K^0}\rangle \tag{384}$$

with strangeness operator S and strangeness eigen-values $+$ and $-$.

Parity:

$$P|K^0\rangle = -|K^0\rangle \tag{385}$$

Charge conjugation:

$$C|K^0\rangle = |\overline{K^0}\rangle \tag{386}$$

Charge conjugation - Parity:

$$CP|K^0\rangle = -|\overline{K^0}\rangle \ , \ CP|\overline{K^0}\rangle = -|K^0\rangle \tag{387}$$

We now construct eigen-states to the CP-operator:

$$|K_1^0\rangle = \frac{1}{\sqrt{2}}\left(|K^0\rangle - |\overline{K^0}\rangle\right) \ , \ |K_2^0\rangle = \frac{1}{\sqrt{2}}\left(|K^0\rangle + |\overline{K^0}\rangle\right) \tag{388}$$

with the eigen-equations

$$CP|K_1^0\rangle = +|K_1^0\rangle \ , \ CP|K_2^0\rangle = -|K_2^0\rangle \tag{389}$$

From experiments we know, that Kaons decay with different decay times and the physical states we call K_S (short-lived-state) and K_L (long-lived-state). K_S decays into two pions with a decay-time of $\Gamma_S^{-1} = \tau_S = 10^{-10}s$. K_L decays into three pions with a decay-time of $\Gamma_L^{-1} = \tau_L = 5{\cdot}10^{-8}s$. These states differ slightly in mass $\Delta m = m_L - m_S = 3,49{\cdot}10^{-6}eV$. We also know that CP is violated due to weak-interactions with a probability of $|\varepsilon| \approx 10^{-3}$. Thus, we can write the states $|K_S\rangle$ and $|K_L\rangle$ as superposition of $|K_1^0\rangle$ and $|K_2^0\rangle$:

$$|K_S\rangle = \frac{1}{\sqrt{2}}\left(|K_1^0\rangle + \varepsilon|K_2^0\rangle\right) \ , \ |K_L\rangle = \frac{1}{\sqrt{2}}\left(\varepsilon|K_1^0\rangle + |K_2^0\rangle\right) \tag{390}$$

$$|K_S\rangle = \frac{1}{N}\left(p|K^0\rangle - p|\overline{K^0}\rangle\right) \ , \ |K_L\rangle = \frac{1}{N}\left(p|K^0\rangle + p|\overline{K^0}\rangle\right) \tag{391}$$

where $p = 1 + \varepsilon$ and $q = 1 - \varepsilon$ and $N = \sqrt{|p|^2 + |q|^2}$. The complex quantity ε is called *CP violating parameter*.

4.3 Strangeness oscillation

The decay is given by the non-hermitian effective Hamiltonian H:

$$H = M - \frac{i}{2}\Gamma \tag{392}$$

where M and Γ are hermitian operators. M corresponds to the mass and Γ is the decay-matrix.

The eigenequations of the effective Hamiltonian are satisfied by the states $|K_S\rangle$ and $|K_L\rangle$:

$$H|K_{S,L}\rangle = \lambda_{S,L}|K_{S,L}\rangle \tag{393}$$

with the energyeigen-values $\lambda_{S,L} = m_{S,L} - \frac{i}{2}\Gamma_{S,L}$ where $\Gamma_{S,L}$ is the width of the states.

From the Schrödinger equation we get the *Wigner-Weisskopf*-approximation:

$$|K_S(t)\rangle = e^{-i\lambda_S t}|K_S\rangle = e^{-\frac{\Gamma_S}{2}t}e^{-im_S t}|K_S\rangle \tag{394}$$

$$|K_L(t)\rangle = e^{-i\lambda_L t}|K_L\rangle = e^{-\frac{\Gamma_L}{2}t}e^{-im_L t}|K_L\rangle$$

Since $|K^0\rangle = \frac{N}{2p}(|K_S\rangle + |K_L\rangle)$ and $|\overline{K^0}\rangle = \frac{N}{2q}(-|K_S\rangle + |K_L\rangle)$ we have for the time-evolution of the strangeness-states:

$$|K^0(t)\rangle = g_+(t)|K^0\rangle + \frac{q}{p}g_-(t)|\overline{K^0}\rangle \tag{395}$$

$$|\overline{K^0}(t)\rangle = \frac{p}{q} g_-(t)|K^0\rangle + g_+(t)|\overline{K^0}\rangle$$

with $g_{+,-}(t) = \frac{1}{2}[\pm e^{-i\lambda_S t} + e^{-i\lambda_L t}]$. Suppose that a K^0-beam is produced at $t = 0$ then there occur transitions from $|K^0\rangle$ to $|\overline{K^0}\rangle$ with the following transitions-probabilities:

$$|\langle K^0|K^0(t)\rangle|^2 = g_+(t)g_+^*(t) = \frac{1}{4}[e^{-\Gamma_S t} + e^{-\Gamma_L t} - 2e^{-\Gamma t}\cos(\Delta m t)] \tag{396}$$

$$|\langle \overline{K^0}|\overline{K^0(t)}\rangle|^2 = g_+(t)g_+^*(t) \tag{397}$$

$$|\langle K^0|\overline{K^0(t)}\rangle|^2 = \frac{|p|^2}{|q|^2} g_-(t)g_-^*(t) = \frac{1}{4}\frac{|p|^2}{|q|^2}[e^{-\Gamma_S t} + e^{-\Gamma_L t} + 2e^{-\Gamma t}\cos(\Delta m t)] \tag{398}$$

$$|\langle \overline{K^0}|K^0(t)\rangle|^2 = \frac{|q|^2}{|p|^2} g_-(t)g_-^*(t) \tag{399}$$

where $\Delta m = m_L - m_S$ and $\Gamma = \frac{1}{2}(\Gamma_L + \Gamma_S)$.

4.4 Quasi-Spin of Kaon - Photon analogy

We can introduce the quasi-spin (strangeness) of a Kaon in analogy to the spin of a particle or to the polarization of a photon:

$$|K^0\rangle \quad \leftrightarrow \quad |\uparrow\rangle \quad \leftrightarrow \quad |V\rangle \tag{400}$$

$$|\overline{K^0}\rangle \quad \leftrightarrow \quad |\downarrow\rangle \quad \leftrightarrow \quad |H\rangle$$

$$|K_S\rangle \quad \leftrightarrow \quad |\rightarrow\rangle \quad \leftrightarrow \quad |L\rangle \tag{401}$$

$$|K_L\rangle \quad \leftrightarrow \quad |\leftarrow\rangle \quad \leftrightarrow \quad |R\rangle$$

Attention:

$$\langle K_S|K_L\rangle = \frac{2Re\varepsilon}{1 + |\varepsilon|^2} = 2Re\varepsilon \tag{402}$$

Whereas:

$$\langle L|R\rangle = 0 \tag{403}$$

where $|L\rangle = \frac{1}{\sqrt{2}}(|V\rangle - i|H\rangle)$ and $|R\rangle = \frac{1}{\sqrt{2}}(|V\rangle + i|H\rangle)$. Then we can describe the Kaon-features with the Pauli-matrices and we can decompose the Hamilton-operator in the following way:

$$H = a\mathbb{1} + \overrightarrow{b}\,\overrightarrow{\sigma} \tag{404}$$

In comparison with the effective Hamilton operator $H = M - \frac{i}{2}\Gamma$ we get:

$$b_1 = b\,\cos\alpha\ ,\ b_2 = b\,\sin\alpha \tag{405}$$

$$b_3 = 0 \quad \text{because of CPT-invariance}$$

$$a = (\lambda_L + \lambda_S)\frac{1}{2}\ ,\ b = (\lambda_L - \lambda_S)\frac{1}{2} \tag{406}$$

Because of the CP-violation the angle α corresponds to the parameter ε from chapter 4.2. via the following relation:

$$e^{i\alpha} = \frac{1-\varepsilon}{1+\varepsilon} \tag{407}$$

If we insert these relations we obtain for the Hamiltonian:

$$H = a\mathbb{1} + b\sigma_1 + 2i\varepsilon b\sigma_2 \tag{408}$$

4.5 Decoherence of entangled Kaons

Now let us describe and measure possible decoherence of entangled Kaons. Decoherence provides us some information on the quality of the entangled state.

Experimentally a Bell-state is produced:

$$|\psi^-\rangle = \frac{1}{\sqrt{2}}\left(|e_1\rangle - |e_2\rangle\right) \tag{409}$$

with the following notation:

$$|e_1\rangle = |K_S\rangle_l \otimes |K_L\rangle_r \ , \ |e_2\rangle = |K_L\rangle_l \otimes |K_S\rangle_r \tag{410}$$

where the indices l and r denote the left-moving and the right-moving particle and we have chosen the eigenstates of the Hamiltonian. Thus, the density matrix is described by:

$$\rho^- = |\psi^-\rangle\langle\psi^-| = \frac{1}{2}\left(|e_1\rangle\langle e_1| + |e_2\rangle\langle e_2| - |e_1\rangle\langle e_2| - |e_2\rangle\langle e_1|\right) \tag{411}$$

Possible decoherence arises from the interaction of the quantum system with its environment. To study decoherence we therefore consider the master equation

$$\frac{d}{dt}\rho = -iH\rho + i\rho H^\dagger - D[\rho] \tag{412}$$

In our model the *Lindblad-operators* A_j act like projectors:

$$A_j = \sqrt{\lambda}P_j \tag{413}$$

with $j = 1, 2$ and the projectors $P_j = |e_j\rangle\langle e_j|$. The operators P_j project onto the eigenstates of the 2-particle Hamiltonian $H = H_l \otimes \mathbb{1}_r + \mathbb{1}_l \otimes H_r$. The solution of the master equation provides the time dependence of the density matrix:

$$\rho(t) = \frac{1}{2}e^{-\Gamma t}\left(|e_1\rangle\langle e_1| + |e_2\rangle\langle e_2| - e^{-\lambda t}\left(|e_1\rangle\langle e_2| + |e_2\rangle\langle e_1|\right)\right) \tag{414}$$

where λ is the decoherence parameter. Decoherence arises through the factor $e^{-\lambda t}$ in the off-diagonal elements. It means that for $t > 0$ the density matrix $\rho(t)$ is not pure any more but mixed.

Experimentally kaons are produced in particle colliders, e.g. at e^+e^--collider DAΦNE,

Frascati or at $p\overline{p}$-collider LEAR, CERN. The Kaons produced in such an experiment are entangled and detected with respect to their strangeness.

For the actual experiment let us consider the case:

$$K^0 \text{ will be measured at the left hand side at time } t_l$$

$$\overline{K^0} \text{ will be measured at the right hand side at time } t_r$$

and $t_l \geq t_r$. Then the probability of such a measurement is calculated by

$$P(K^0, t_l; \overline{K^0}, t_r) = \mathrm{tr}_l\{|K^0\rangle\langle K^0|_l \mathrm{tr}_r[\mathbb{1}_l \otimes |\overline{K^0}\rangle\langle\overline{K^0}|_r \rho(t_r)]\} \tag{415}$$

Analogously can be calculated the case K^0 left and K^0 right. The result for the probabilities is:

$$P_\lambda(K^0, t_l; \overline{K^0}, t_r) = P_\lambda(\overline{K^0}, t_l; K^0, t_r) = \tag{416}$$

$$= \frac{1}{8}\left(e^{-\Gamma_S t_l - \Gamma_L t_r} + e^{-\Gamma_L t_l - \Gamma_S t_r} + e^{-\lambda t_r} 2\cos(\Delta m \Delta t) \cdot e^{-\Gamma(t_l + t_r)}\right)$$

$$P_\lambda(K^0, t_l; K^0, t_r) = P_\lambda(\overline{K^0}, t_l; \overline{K^0}, t_r) = \tag{417}$$

$$= \frac{1}{8}\left(e^{-\Gamma_S t_l - \Gamma_L t_r} + e^{-\Gamma_L t_l - \Gamma_S t_r} - e^{-\lambda t_r} 2\cos(\Delta m \Delta t) \cdot e^{-\Gamma(t_l + t_r)}\right)$$

with $\Delta t = t_l - t_r$. Note that at equal times $t_l = t_r = t$ the like-strangeness probabilities

$$P_\lambda(K^0, t; K^0, t) = P_\lambda(\overline{K^0}, t; \overline{K^0}, t) = \frac{1}{4} e^{-2\Gamma t}(1 - e^{-\lambda t}) \tag{418}$$

do not vanish, in contrast to the pure quantum mechanical EPR-correlations. The interesting quantity is the *asymmetry of probabilities*; it is directly sensitive to the interference term and can be measured experimentally. For pure quantum mechanics we have

$$A^{QM}(\Delta t) =$$

$$= \frac{P(K^0, t_l; \overline{K^0}, t_r) + P(\overline{K^0}, t_l; K^0, t_r) - P(K^0, t_l; K^0, t_r) - P(\overline{K^0}, t_l; \overline{K^0}, t_r)}{P(K^0, t_l; \overline{K^0}, t_r) + P(\overline{K^0}, t_l; K^0, t_r) + P(K^0, t_l; K^0, t_r) + P(\overline{K^0}, t_l; \overline{K^0}, t_r)} =$$

$$= \frac{\cos(\Delta m \Delta t)}{\cosh(\frac{1}{2}\Delta\Gamma\Delta t)} \tag{419}$$

with $\Delta\Gamma = \Gamma_L - \Gamma_S$, and for our decoherence model we find, by inserting the probabilities (416), (417),

$$A^\lambda(t_l, t_r) = \frac{\cos\Delta m \Delta t}{\cosh(\frac{1}{2}\Delta\Gamma\Delta t)} e^{-\lambda \min\{t_l, t_r\}} = A^{QM}(\Delta t) e^{-\lambda \min\{t_l, t_r\}} \tag{420}$$

Thus, the decoherence effect, simply given by the factor $e^{-\lambda \min\{t_l, t_r\}}$, depends only on the time of the first measured kaon, in our case: $\min\{t_l, t_r\} = t_r$.

Experiment

Now we compare our model with the results of the CPLEAR experiment at CERN where $K^0\overline{K^0}$ pairs are produced in the $p\overline{p}$-collider: $p\overline{p} \to K^0\overline{K^0}$. These pairs are prodominantly in an antisymmetric state with quantum numbers $J^{PC} = 1^-$ and the strangeness of the kaons is detected via strong interactions in surrounding absorbers (made of copper and carbon). The experimental set-up has two configurations. In configuration $C(0)$ both

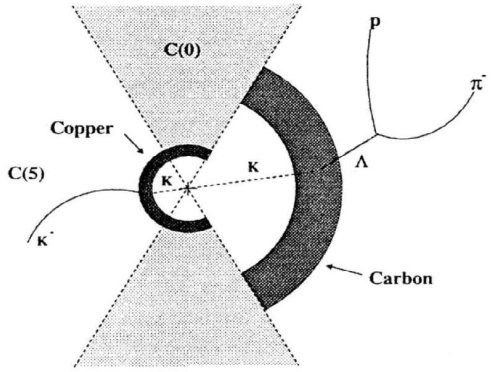


Figure 4: **Set-up of the CPLEAR-Experiment** Source: R. A. Bertlmann: "Entanglement, Bell Inequalities and Decoherence in Particle Physics", quant-ph/041028

kaons propagate 2 cm, they have nearly equal proper times ($t_r \approx t_l$) when they are measured by the absorbers. This fulfills the condition for an EPR-type experiment. In configuration $C(5)$ one kaon propagates 2 cm and the other kaon 7 cm, thus, the flight-path difference is 5 cm on average, corresponding to a proper time difference $|t_r - t_l| \approx 1.2\tau_S$.

Fitting the decoherence parameter λ by comparing the asymmetry with the experimental data we find, when averaging over both configurations, the following bounds on λ:

$$\overline{\lambda} = (1.84^{+2.50}_{-2.17}) \cdot 10^{-12}\text{MeV} \quad \text{and} \quad \overline{\Lambda} = \frac{\overline{\lambda}}{\Gamma_S} = 0.25^{+0.34}_{-0.32} \tag{421}$$

The results are certainly compatible with quantum mechanics ($\lambda = 0$), nevertheless, the experimental data allow an upper pound $\overline{\lambda}_{\text{up}} = 4.34 \cot 10^{-12}$ MeV for possible decoherence in the entangled $K^0\overline{K^0}$ system. But this decoherence is small $\Lambda = 0.25 + 0.34 < 1$.

Summary:

From the data we see the Kaons are still entangled although they extended over a macroscopic distance of about 7 cm. They form a quantum system of massive particles with a mass of about 1 GeV.

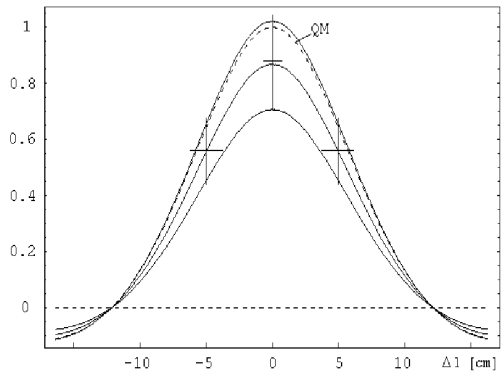


Figure 5: **Data from the CPLEAR-Experiment**, The asymmetry as a function of the distance of the kaons. Source: R. A. Bertlmann: "Entanglement, Bell Inequalities and Decoherence in Particle Physics", quant-ph/041028

References

[1] Heinz-Peter Breuer, Francesco Petruccione: "The Theory of Open Quantum Systems", Oxford University Press, 2002

[2] Domenico Giulini, Erich Joos, Claus Kiefer, Joachim Kupsch: "Decoherence and the Appearance of a Classical World in Quantum Theory", Springer Verlag, 1996